Dakota, A Multilevel Parallel Object-Oriented Framework for
Design Optimization, Parameter Estimation, Uncertainty
Quantification, and Sensitivity Analysis:

Brian M. Adams, Mohamed S. Ebeida, Michael S. Eldred, Gianluca Geraci,
John D. Jakeman, Kathryn A. Maupin, Jason A. Monschke, Laura P. Swiler,
J. Adam Stephens, Dena M. Vigil, Timothy M. Wildey
Optimization and Uncertainty Quantification Department

William J. Bohnhoff
Radiation Transport Department

Keith R. Dalbey
Mission Analysis and Simulation Department

John P. Eddy
System Readiness and Sustainment Technologies Department

Joseph R. Frye, Russell W. Hooper
Multiphysics Applications Department

Kenneth T. Hu
Validation and Uncertainty Quantification Department

Patricia D. Hough, Mohammad Khalil
Quantitative Modeling and Analysis Department

Elliott M. Ridgway
Data-driven and Neural Computing
Sandia National Laboratories
P.O. Box 5800
Albuquerque, New Mexico 87185

Ahmad Rushdi
Electrical and Computer Engineering
University of California
One Shields Avenue
Davis, CA 95616-5294
Abstract

The Dakota toolkit provides a flexible and extensible interface between simulation codes and iterative analysis methods. Dakota contains algorithms for optimization with gradient and nongradient-based methods; uncertainty quantification with sampling, reliability, and stochastic expansion methods; parameter estimation with nonlinear least squares methods; and sensitivity/variance analysis with design of experiments and parameter study methods. These capabilities may be used on their own or as components within advanced strategies such as surrogate-based optimization, mixed integer nonlinear programming, or optimization under uncertainty. By employing object-oriented design to implement abstractions of the key components required for iterative systems analyses, the Dakota toolkit provides a flexible and extensible problem-solving environment for design and performance analysis of computational models on high performance computers.

This report serves as a reference manual for the commands specification for the Dakota software, providing input overviews, option descriptions, and example specifications.
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Chapter 1

Main Page

The Dakota software (http://dakota.sandia.gov/) delivers advanced parametric analysis techniques enabling quantification of margins and uncertainty, risk analysis, model calibration, and design exploration with computational models. Its methods include optimization, uncertainty quantification, parameter estimation, and sensitivity analysis, which may be used individually or as components within surrogate-based and other advanced strategies.

Author

The Reference Manual documents all the input keywords that can appear in a Dakota input file to configure a Dakota study. Its organization closely mirrors the structure of dakota.input.summary. For more information see Dakota Input Specification. For information on software structure, refer to the Developers Manual [3], and for a tour of Dakota features and capabilities, including a tutorial, refer to the User’s Manual[4].

1.1 How to Use this Manual

- To learn how to run Dakota from the command line, see Running Dakota
- To learn to how to restart Dakota studies, see Restarting Dakota Studies
- To learn about the Dakota restart utility, see The Dakota Restart Utility

To find more information about a specific keyword

1. Use the search box at the top right (currently only finds keyword names)
2. Browse the Keywords tree on the left navigation pane
3. Look at the Dakota Input Specification
4. Navigate through the keyword pages, starting from the Keywords Area

To find more information about a Dakota related topic

1. Browse the Topics Area on the left navigation pane
2. Navigate through the topics pages, starting from the **Topics Area**

A small number of examples are included (see **Sample Input Files**) along with a description of the test problems (see **Test Problems**).

A bibliography for the Reference Manual is provided in **Bibliographic References**
Chapter 2

Running Dakota

The Dakota executable file is named dakota (dakota.exe on Windows) and is most commonly run from a terminal or command prompt.

2.1 Usage

If the dakota command is entered at the command prompt without any arguments, a usage message similar to the following appears:

usage: dakota [options and <args>]
   -help (Print this summary)
   -version (Print Dakota version number)
   -input <$val> (REQUIRED Dakota input file $val)
   -output <$val> (Redirect Dakota standard output to file $val)
   -error <$val> (Redirect Dakota standard error to file $val)
   -parser <$val> (Parsing technology: nidr[strict][:dumpfile])
   -no_input_echo (Do not echo Dakota input file)
   -check (Perform input checks)
   -pre_run [$val] (Perform pre-run (variables generation) phase)
   -run [$val] (Perform run (model evaluation) phase)
   -post_run [$val] (Perform post-run (final results) phase)
   -read_restart [$val] (Read an existing Dakota restart file $val)
   -stop_restart <$val> (Stop restart file processing at evaluation $val)
   -write_restart [$val] (Write a new Dakota restart file $val)

Of these command line options, only input is required, and the -input switch can be omitted if the input file name is the final item appearing on the command line (see Examples); all other command-line inputs are optional.

- help prints the usage message above.
- version prints version information for the executable.
- check invokes a dry-run mode in which the input file is processed and checked for errors, but the study is not performed.
- input provides the name of the Dakota input file.
- output and error options provide file names for redirection of the Dakota standard output (stdout) and standard error (stderr), respectively.
• The parser option is for debugging and will not be further described here.

• By default, Dakota will echo the input file to the output stream, but no_input_echo can override this behavior.

• read_restart and write_restart commands provide the names of restart databases to read from and write to, respectively.

• stop_restart command limits the number of function evaluations read from the restart database (the default is all the evaluations) for those cases in which some evaluations were erroneous or corrupted. Restart management is an important technique for retaining data from expensive engineering applications.

• \texttt{-pre\_run}, \texttt{-run}, and \texttt{-post\_run} instruct Dakota to run one or more execution phases, excluding others. The commands must be followed by filenames as described in \textit{Execution Phases}.

Command line switches can be abbreviated so long as the abbreviation is unique, so the following are valid, unambiguous specifications: \texttt{-h}, \texttt{-v}, \texttt{-c}, \texttt{-i}, \texttt{-o}, \texttt{-e}, \texttt{-s}, \texttt{-w}, \texttt{-re}, \texttt{-pr}, \texttt{-ru}, and \texttt{-po} and can be used in place of the longer forms of the command line options.

For information on restarting Dakota, see \textit{Restarting Dakota Studies} and \textit{The Dakota Restart Utility}.

### 2.2 Examples

To run Dakota with a particular input file, the following syntax can be used:

\texttt{dakota -i dakota.in}

or more simply

\texttt{dakota dakota.in}

This will echo the standard output (stdout) and standard error (stderr) messages to the terminal. To redirect stdout and stderr to separate files, the \texttt{-o} and \texttt{-e} command line options may be used:

\texttt{dakota -i dakota.in -o dakota.out -e dakota.err}

or

\texttt{dakota -o dakota.out -e dakota.err dakota.in}

Alternatively, any of a variety of Unix redirection variants can be used. Refer to[?] for more information on Unix redirection. The simplest of these redirects stdout to another file:

\texttt{dakota dakota.in > dakota.out}

### 2.3 Execution Phases

Dakota has three execution phases: \texttt{pre\_run}, \texttt{run}, and \texttt{post\_run}.

• \texttt{pre\_run} can be used to generate variable sets

• \texttt{run} (core run) invokes the simulation to evaluate variables, producing responses

• \texttt{post\_run} accepts variable/response sets and analyzes the results (for example, calculate correlations from a set of samples). Currently only two modes are supported and only for sampling, parameter study, and DACE methods:

(1) \texttt{pre\_run} only with optional tabular output of variables:

\texttt{dakota -i dakota.in -pre\_run :::myvariables.dat}

(2) \texttt{post\_run} only with required tabular input of variables/responses:

\texttt{dakota -i dakota.in -post\_run myvarsresponses.dat::}
2.4 Restarting Dakota Studies

Dakota is often used to solve problems that require repeatedly running computationally expensive simulation codes. In some cases you may want to repeat an optimization study, but with a tighter final convergence tolerance. This would be costly if the entire optimization analysis had to be repeated. Interruptions imposed by computer usage policies, power outages, and system failures could also result in costly delays. However, Dakota automatically records the variable and response data from all function evaluations so that new executions of Dakota can pick up where previous executions left off. The Dakota restart file (dakota.rst by default) archives the tabulated interface evaluations in a binary format. The primary restart commands at the command line are -read_restart, -write_restart, and -stop_restart.

2.4.1 Writing Restart Files

To write a restart file using a particular name, the -write_restart command line input (may be abbreviated as -w) is used:

```
dakota -i dakota.in -write_restart my_restart_file
```

If no -write_restart specification is used, then Dakota will still write a restart file, but using the default name dakota.rst instead of a user-specified name.

To turn restart recording off, the user may use the restart_file keyword, in the interface block. This can increase execution speed and reduce disk storage requirements, but at the expense of a loss in the ability to recover and continue a run that terminates prematurely. This option is not recommended when function evaluations are costly or prone to failure. Please note that using the deactivate restart_file specification will result in a zero length restart file with the default name dakota.rst, which can overwrite an exiting file.

2.4.2 Using Restart Files

To restart Dakota from a restart file, the -read_restart command line input (may be abbreviated as -r) is used:

```
dakota -i dakota.in -read_restart my_restart_file
```

If no -read_restart specification is used, then Dakota will not read restart information from any file (i.e., the default is no restart processing).

To read in only a portion of a restart file, the -stop_restart control (may be abbreviated as -s) is used to specify the number of entries to be read from the database. Note that this integer value corresponds to the restart record processing counter (as can be seen when using the print utility (see The Dakota Restart Utility) which may differ from the evaluation numbers used in the previous run if, for example, any duplicates were detected (since these duplicates are not recorded in the restart file). In the case of a -stop_restart specification, it is usually desirable to specify a new restart file using -write_restart so as to remove the records of erroneous or corrupted function evaluations. For example, to read in the first 50 evaluations from dakota.rst:

```
dakota -i dakota.in -r dakota.rst -s 50 -w dakota_new.rst
```

The dakota_new.rst file will contain the 50 processed evaluations from dakota.rst as well as any new evaluations. All evaluations following the 50th in dakota.rst have been removed from the latest restart record.

2.4.3 Appending to a Restart File

If the -write_restart and -read_restart specifications identify the same file (including the case where -write_restart is not specified and -read_restart identifies dakota.rst), then new evaluations will be appended to the existing restart file.
2.4.4 Working with multiple Restart Files

If the -write_restart and -read_restart specifications identify different files, then the evaluations read from the file identified by -read_restart are first written to the -write_restart file. Any new evaluations are then appended to the -write_restart file. In this way, restart operations can be chained together indefinitely with the assurance that all of the relevant evaluations are present in the latest restart file.

2.4.5 How it Works

Dakota’s restart algorithm relies on its duplicate detection capabilities. Processing a restart file populates the list of function evaluations that have been performed. Then, when the study is restarted, it is started from the beginning (not a warm start) and many of the function evaluations requested by the iterator are intercepted by the duplicate detection code. This approach has the primary advantage of restoring the complete state of the iteration (including the ability to correctly detect subsequent duplicates) for all methods/iterators without the need for iterator-specific restart code. However, the possibility exists for numerical round-off error to cause a divergence between the evaluations performed in the previous and restarted studies. This has been rare in practice.

2.5 The Dakota Restart Utility

The Dakota restart utility program provides a variety of facilities for managing restart files from Dakota executions. The executable program name is dakota_restart_util and it has the following options, as shown by the usage message returned when executing the utility without any options:

Usage:
dakota_restart_util command <arg1> [<arg2> <arg3> ...] --options
dakota_restart_util print <restart_file>
dakota_restart_util to_neutral <restart_file> <neutral_file>
dakota_restart_util from_neutral <neutral_file> <restart_file>
dakota_restart_util to_tabular <restart_file> <text_file>
    [--custom_annotated [header] [eval_id] [interface_id]]
    [--output_precision <int>]
dakota_restart_util remove <double> <old_restart_file> <new_restart_file>
dakota_restart_util remove_ids <int_1> ... <int_n> <old_restart_file> <new_restart_file>
dakota_restart_util cat <restart_file_1> ... <restart_file_n> <new_restart_file>

options:
--help show dakota_restart_util help message
--custom_annotated arg tabular file options: header, eval_id, interface_id
--freeform tabular file: freeform format
--output_precision arg (=10) set tabular output precision

Several of these functions involve format conversions. In particular, the binary format used for restart files can be converted to ASCII text and printed to the screen, converted to and from a neutral file format, or converted to a tabular format for importing into 3rd-party graphics programs. In addition, a restart file with corrupted data can be repaired by value or id, and multiple restart files can be combined to create a master database.

2.5.1 Print Command

The print option is useful to show contents of a restart file, since the binary format is not convenient for direct inspection. The restart data is printed in full precision, so that exact matching of points is possible for restarted runs or corrupted data removals. For example, the following command

dakota_restart_util print
dakota.rst

results in output similar to the following:
2.5. THE DAKOTA RESTART UTILITY

------------------------------------------
Restart record 1 (evaluation id 1):
Parameters:
  1.8000000000000000e+00 intake_dia
  1.0000000000000000e+00 flatness

Active response data:
Active set vector = { 3 3 3 3 }
-2.4355973813420619e+00 obj_fn
-4.7428486677140930e-01 nln_ineq_con_1
-4.5000000000000001e-01 nln_ineq_con_2
  1.3971343170299741e-01 nln_ineq_con_3
[ -4.3644298963447897e-01 1.4999999999999999e-01 ] obj_fn gradient
[ 1.3855136437818300e-01 0.0000000000000000e+00 ] nln_ineq_con_1 gradient
[ 0.0000000000000000e+00 1.4999999999999999e-01 ] nln_ineq_con_2 gradient
[ 0.0000000000000000e+00 -1.9485571585149869e-01 ] nln_ineq_con_3 gradient
------------------------------------------

Restart record 2 (evaluation id 2):
Parameters:
  2.1640000000000001e+00 intake_dia
  1.7169994018008317e+00 flatness

Active response data:
Active set vector = { 3 3 3 3 }
-2.4869127192988878e+00 obj_fn
6.925695879998943e-01 nln_ineq_con_1
-3.4245008972987528e-01 nln_ineq_con_2
  8.7142207937157910e-03 nln_ineq_con_3
[ -4.3644298963447897e-01 1.4999999999999999e-01 ] obj_fn gradient
[ 2.9814239699997572e+01 0.0000000000000000e+00 ] nln_ineq_con_1 gradient
[ 0.0000000000000000e+00 1.4999999999999999e-01 ] nln_ineq_con_2 gradient
[ 0.0000000000000000e+00 -1.6998301774282701e-01 ] nln_ineq_con_3 gradient
...

Restart file processing completed: 11 evaluations retrieved.

# 2.5.2 Neutral File Format

A Dakota restart file can be converted to a neutral file format using a command like the following:
```
dakota_restart_util to_neutral dakota.rst dakota.neu
```
which results in a report similar to the following:

```
Writing neutral file dakota.neu
Restart file processing completed: 11 evaluations retrieved.
```

Similarly, a neutral file can be returned to binary format using a command like the following:
```
dakota_restart_util from_neutral dakota.neu dakota.rst
```
which results in a report similar to the following:

```
Reading neutral file dakota.neu
Writing new restart file dakota.rst
Neutral file processing completed: 11 evaluations retrieved.
```

The contents of the generated neutral file are similar to the following (from the first two records for the Cylinder example in[4]).
CHAPTER 2. RUNNING DAKOTA

This format is not intended for direct viewing (print should be used for this purpose). Rather, the neutral file capability has been used in the past for managing portability of restart data across platforms (recent use of more portable binary formats has largely eliminated this need) or for advanced repair of restart records (in cases where the remove command was insufficient).

2.5.3 Tabular Format

Conversion of a binary restart file to a tabular format enables convenient import of this data into 3rd-party post-processing tools such as Matlab, TECplot, Excel, etc. This facility is nearly identical to the output activated by the tabular_data keyword in the Dakota input file specification, but with two important differences:

1. No function evaluations are suppressed as they are with tabular_data (i.e., any internal finite difference evaluations are included).

2. The conversion can be performed later, i.e., for Dakota runs executed previously.

An example command for converting a restart file to tabular format is:

dakota_restart_util to_tabular dakota.rst dakota.m

which results in a report similar to the following:

Writing tabular text file dakota.m
Restart file processing completed: 10 evaluations tabulated.

The contents of the generated tabular file are similar to the following (from the example in the Restart section of[4]). Note that while evaluations resulting from numerical derivative offsets would be reported (as described above), derivatives returned as part of the evaluations are not reported (since they do not readily fit within a compact tabular format):

```
%eval_id interface x1  x2  obj_fn  nln_ineq_con_1  nln_ineq_con_2
1 NO_ID 0.9 0.1 1.0002 0.26 0.76
2 NO_ID 0.90009 1.1 0.001996404857 0.2601620081 0.759955
3 NO_ID 0.89991 1.1 0.0002003604863 0.2598380081 0.760045
4 NO_ID 0.9 1.10011 0.0002004407265 0.259945 0.7602420121
5 NO_ID 0.9 1.09989 0.0001995607255 0.260055 0.7597580121
6 NO_ID 0.58256179 0.4772224441 0.1050555937 0.1007670171 -0.0635963386
7 NO_ID 0.5826200462 0.4772224441 0.1050386469 0.1008348962 -0.0635687195
8 NO_ID 0.5825035339 0.4772224441 0.1050725476 0.1006991449 -0.0635105077
9 NO_ID 0.58256179 0.4772701663 0.1050283245 0.100743156 -0.0634908333
10 NO_ID 0.58256179 0.4771747219 0.1050827044 0.1007908783 -0.06356517983
...  
```

Controlling tabular format: The command-line options --freeform and --custom_annotated give control of headers in the resulting tabular file. Freeform will generate a tabular file with no leading row nor columns (variable and response values only). Custom annotated format accepts any or all of the options:

- header: include %-commented header row with labels
2.5. THE DAKOTA RESTART UTILITY

- eval_id: include leading column with evaluation ID
- interface_id: include leading column with interface ID

For example, to recover Dakota 6.0 tabular format, which contained a header row, leading column with evaluation ID, but no interface ID:

dakota_restart_util to_tabular dakota.rst dakota.m --custom_annotated header eval_id

Resulting in

```
$eval_id x1 x2 obj_fn nln_ineq_con_1 nln_ineq_con_2
1 0.9 1.1 0.0002 0.26 0.76
2 0.90009 1.1 0.0001996404857 0.2601620081 0.759955
3 0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...```

Finally, `--output_precision integer` will generate tabular output with the specified integer digits of precision.

2.5.4 Concatenation of Multiple Restart Files

In some instances, it is useful to combine restart files into a single master function evaluation database. For example, when constructing a data fit surrogate model, data from previous studies can be pulled in and reused to create a combined data set for the surrogate fit. An example command for concatenating multiple restart files is:

dakota_restart_util cat dakota.rst.1 dakota.rst.2 dakota.rst.3 dakota.rst.all

which results in a report similar to the following:

```
Writing new restart file dakota.rst.all
dakota.rst.1 processing completed: 10 evaluations retrieved.
dakota.rst.2 processing completed: 110 evaluations retrieved.
dakota.rst.3 processing completed: 65 evaluations retrieved.
```

The `dakota.rst.all` database now contains 185 evaluations and can be read in for use in a subsequent Dakota study using the `-read_restart` option to the `dakota` executable.

2.5.5 Removal of Corrupted Data

On occasion, a simulation or computer system failure may cause a corruption of the Dakota restart file. For example, a simulation crash may result in failure of a post-processor to retrieve meaningful data. If 0’s (or other erroneous data) are returned from the user’s analysis driver, then this bad data will get recorded in the restart file. If there is a clear demarcation of where corruption initiated (typical in a process with feedback, such as gradient-based optimization), then use of the `-stop_restart` option for the `dakota` executable can be effective in continuing the study from the point immediately prior to the introduction of bad data. If, however, there are interspersed corruptions throughout the restart database (typical in a process without feedback, such as sampling), then the remove and remove_ids options of `dakota_restart_util` can be useful.

An example of the command syntax for the remove option is:

dakota_restart_util remove 2.e-04 dakota.rst dakota.rst.repaired

which results in a report similar to the following:

```
Writing new restart file dakota.rst.repaired
Restart repair completed: 65 evaluations retrieved, 2 removed, 63 saved.
```

where any evaluations in `dakota.rst` having an active response function value that matches `2.e-04` within machine precision are discarded when creating `dakota.rst.repaired`.

An example of the command syntax for the remove_ids option is:
dakota_restart_util remove_ids 12 15 23 44 57 dakota.rst dakota.rst.repaired

which results in a report similar to the following:

Writing new restart file dakota.rst.repaired
Restart repair completed: 65 evaluations retrieved, 5 removed, 60 saved.

where evaluation ids 12, 15, 23, 44, and 57 have been discarded when creating dakota.rst.repaired.

An important detail is that, unlike the -stop_restart option which operates on restart record numbers, the remove_ids option operates on evaluation ids. Thus, removal is not necessarily based on the order of appearance in the restart file. This distinction is important when removing restart records for a run that contained either asynchronous or duplicate evaluations, since the restart insertion order and evaluation ids may not correspond in these cases (asynchronous evaluations have ids assigned in the order of job creation but are inserted in the restart file in the order of job completion, and duplicate evaluations are not recorded which introduces offsets between evaluation id and record number). This can also be important if removing records from a concatenated restart file, since the same evaluation id could appear more than once. In this case, all evaluation records with ids matching the remove_ids list will be removed.

If neither of these removal options is sufficient to handle a particular restart repair need, then the fallback position is to resort to direct editing of a neutral file to perform the necessary modifications.
Chapter 3

Test Problems

This page contains additional information about two test problems that are used in Dakota examples throughout the Dakota manuals Textbook and Rosenbrock.

Many of these examples are also used as code verification tests. The examples are run periodically and the results are checked against known solutions. This ensures that the algorithms are correctly implemented.

Additional test problems are described in the User’s Manual.

3.1 Textbook

The two-variable version of the “textbook” test problem provides a nonlinearly constrained optimization test case. It is formulated as:

\[
\begin{align*}
\text{minimize} & \quad f = (x_1 - 1)^4 + (x_2 - 1)^4 \\
\text{subject to} & \quad g_1 = x_1^2 - \frac{x_2}{2} \leq 0 \\
& \quad g_2 = x_2^2 - \frac{x_1}{2} \leq 0 \\
& \quad 0.5 \leq x_1 \leq 5.8 \\
& \quad -2.9 \leq x_2 \leq 2.9
\end{align*}
\]

Contours of this test problem are illustrated in the next two figures.
CHAPTER 3. TEST PROBLEMS

Figure 3.1: Contours of the textbook problem on the [-3,4] x [-3,4] domain. The feasible region lies at the intersection of the two constraints $g_1$ (solid) and $g_2$ (dashed).

Figure 3.2: Contours of the textbook problem zoomed into an area containing the constrained optimum point $(x_1, x_2) = (0.5, 0.5)$. The feasible region lies at the intersection of the two constraints $g_1$ (solid) and $g_2$ (dashed).

For the textbook test problem, the unconstrained minimum occurs at $(x_1, x_2) = (1, 1)$. However, the inclusion of the constraints moves the minimum to $(x_1, x_2) = (0.5, 0.5)$. Equation textbookform presents the 2-dimensional
form of the textbook problem. An extended formulation is stated as

\[
\begin{align*}
\text{minimize } f & = \sum_{i=1}^{n} (x_i - 1)^4 \\
\text{subject to } g_1 &= x_1^2 - \frac{x_2}{2} \leq 0 \\
& \quad g_2 = x_2^2 - \frac{x_1}{2} \leq 0 \\
& \quad 0.5 \leq x_1 \leq 5.8 \\
& \quad -2.9 \leq x_2 \leq 2.9
\end{align*}
\]

where \( n \) is the number of design variables. The objective function is designed to accommodate an arbitrary number of design variables in order to allow flexible testing of a variety of data sets. Contour plots for the \( n = 2 \) case have been shown previously.

For the optimization problem given in Equation tbe, the unconstrained solution (num_nonlinear_inequality_constraints set to zero) for two design variables is:

\[
\begin{align*}
x_1 &= 1.0 \\
x_2 &= 1.0
\end{align*}
\]

with

\[
\begin{align*}
f^* &= 0.0 \\
g_1^* &= 0.0 \ \text{(active)}
\end{align*}
\]

The solution for the optimization problem constrained by \( g_1 \) (num_nonlinear_inequality_constraints set to one) is:

\[
\begin{align*}
x_1 &= 0.763 \\
x_2 &= 1.16
\end{align*}
\]

with

\[
\begin{align*}
f^* &= 0.00388 \\
g_1^* &= 0.0 \ \text{(active)}
\end{align*}
\]

The solution for the optimization problem constrained by \( g_1 \) and \( g_2 \) (num_nonlinear_inequality_constraints set to two) is:

\[
\begin{align*}
x_1 &= 0.500 \\
x_2 &= 0.500
\end{align*}
\]

with

\[
\begin{align*}
f^* &= 0.125 \\
g_1^* &= 0.0 \ \text{(active)} \\
g_2^* &= 0.0 \ \text{(active)}
\end{align*}
\]

Note that as constraints are added, the design freedom is restricted (the additional constraints are active at the solution) and an increase in the optimal objective function is observed.
3.2 Rosenbrock

The Rosenbrock function[34] is a well-known test problem for optimization algorithms. The standard formulation includes two design variables, and computes a single objective function. This problem can also be posed as a least-squares optimization problem with two residuals to be minimized because the objective function is the sum of squared terms.

**Standard Formulation**

The standard two-dimensional formulation can be stated as

\[
\text{minimize } f = 100(x_2 - x_1^2)^2 + (1 - x_1)^2
\]

(rosenstd)

Surface and contour plots for this function are shown in the Dakota User’s Manual. The optimal solution is:

\[
\begin{align*}
  x_1 &= 1.0 \\
  x_2 &= 1.0
\end{align*}
\]

with

\[
  f^* = 0.0
\]

**A Least-Squares Optimization Formulation**

This test problem may also be used to exercise least-squares solution methods by recasting the standard problem formulation into:

\[
\text{minimize } f = (f_1)^2 + (f_2)^2
\]

(rosenls)

where

\[
  f_1 = 10(x_2 - x_1^2)
\]

(rosenr1)

and

\[
  f_2 = 1 - x_1
\]

(rosenr2)

are residual terms.

The included analysis driver can handle both formulations. In the Dakota/test directory, the rosenbrock executable (compiled from Dakota_Source/test/rosenbrock.cpp) checks the number of response functions passed in the parameters file and returns either an objective function (as computed from Equation rosenstd) for use with optimization methods or two least squares terms (as computed from Equations rosenr1 - rosenr2) for use with least squares methods. Both cases support analytic gradients of the function set with respect to the design variables. See the User’s Manual for examples of both cases (search for Rosenbrock).
Chapter 4

Dakota Input Specification

Dakota input is specified in a text file, e.g., dakota_uq.in containing blocks of keywords that control program behavior. This section describes the format and admissible elements of an input file.

4.1 Dakota Keywords

Valid Dakota input keywords are dictated by dakota.xml, included in source and binary distributions of Dakota. This specification file is used with the NIDR[30] parser to validate user input and is therefore the definitive source for input syntax, capability options, and optional and required capability sub-parameters for any given Dakota version. A more readable variant of the specification dakota.input.summary is also distributed.

While complete, users may find dakota.input.summary overwhelming or confusing and will likely derive more benefit from adapting example input files to a particular problem. Some examples can be found here: Sample Input Files. Advanced users can master the many input specification possibilities by understanding the structure of the input specification file.

4.2 Input Spec Overview

Refer to the dakota.input.summary file, in Input Spec Summary, for all current valid input keywords.

- The summary describes every keyword including:
  - Whether it is required or optional
  - Whether it takes ARGUMENTS (always required) Additional notes about ARGUMENTS can be found here: Specifying Arguments.
  - Whether it has an ALIAS, or synonym
  - Which additional keywords can be specified to change its behavior

- Additional details and descriptions are described in Keywords Area

- For additional details on NIDR specification logic and rules, refer to[30] (Gay, 2008).

4.2.1 Common Specification Mistakes

Spelling mistakes and omission of required parameters are the most common errors. Some causes of errors are more obscure:
• Documentation of new capability sometimes lags its availability in source and executables, especially stable releases. When parsing errors occur that the documentation cannot explain, reference to the particular input specification `dakota.input.summary` used in building the executable, which is installed alongside the executable, will often resolve the errors.

• If you want to compare results with those obtained using an earlier version of Dakota (prior to 4.1), your input file for the earlier version must use backslashes to indicate continuation lines for Dakota keywords. For example, rather than

```plaintext
# Comment about the following "responses" keyword...
responses,
  objective_functions = 1
# Comment within keyword "responses"
  analytic_gradients
# Another comment within keyword "responses"
  no_hessians
```

you would need to write

```plaintext
# Comment about the following "responses" keyword...
responses,
  objective_functions = 1 \  
# Comment within keyword "responses"
  analytic_gradients \ 
# Another comment within keyword "responses"
  no_hessians
```

with no white space (blanks or tabs) after the `\` character.

In most cases, the Dakota parser provides error messages that help the user isolate errors in input files. Running `dakota -input dakota_study.in -check` will validate the input file without running the study.

### 4.2.2 Specifying Arguments

Some keywords, such as those providing bounds on variables, have an associated list of values or strings, referred to as arguments.

When the same value should be repeated several times in a row, you can use the notation `N*value` instead of repeating the value N times.

For example

```plaintext
lower_bounds  -2.0  -2.0  -2.0
upper_bounds  2.0   2.0   2.0
```

could also be written

```plaintext
lower_bounds  3*-2.0
upper_bounds  3*  2.0
```

(with optional spaces around the `*`).

Another possible abbreviation is for sequences: L:S:U (with optional spaces around the `:`) is expanded to L L+S L+2*S ... U, and L:U (with no second colon) is treated as L:1:U.

For example, in one of the test examples distributed with Dakota (test case 2 of `test/dakota_uq_textbook_sop_lhs.in`),

```plaintext
histogram_point = 2
  abscissas = 50. 60. 70. 80. 90.
  30. 40. 50. 60. 70.
  counts = 10 20 30 20 10
```

could also be written

```plaintext
histogram_point = 2
  abscissas = 50 : 10 : 90
         30 : 10 : 70
  counts = 10:10:30 20 10
         10:10:30 20 10
```

Count and sequence abbreviations can be used together. For example

```plaintext
response_levels =
  0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0
  0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0
```

can be abbreviated

```plaintext
response_levels =
2*0.0:0.1:1.0
```

### 4.3 Sample Input Files

A Dakota input file is a collection of fields from the dakota.input.summary file that describe the problem to be solved by Dakota. Several examples follow.

#### Sample 1: Optimization

The following sample input file shows single-method optimization of the Textbook Example (see Textbook) using DOT’s modified method of feasible directions. A similar file is available as Dakota/examples/users/textbook_opt_conmin.in.

```plaintext
# Dakota Input File: textbook_opt_conmin.in
environment
  graphics
  tabular_data
    tabular_data_file = 'textbook_opt_conmin.dat'
method
  # dot_mmfd #DOT performs better but may not be available
  conmin_mfd
    max_iterations = 50
    convergence_tolerance = 1e-4
variables
  continuous_design = 2
  initial_point 0.9 1.1
  upper_bounds  5.8 2.9
  lower_bounds  0.5 -2.9
  descriptors 'x1' 'x2'
interface
  direct
    analysis_driver = 'text_book'
responses
  objective_functions = 1
  nonlinear_inequality_constraints = 2
  numerical_gradients
    method_source dakota
    interval_type central
    fd_gradient_step_size = 1.e-4
  no_hessians
```
Sample 2: Least Squares (Calibration)
The following sample input file shows a nonlinear least squares (calibration) solution of the Rosenbrock Example (see Rosenbrock) using the NL2SOL method. A similar file is available as Dakota/examples/users/rosen_opt_nls.in

```dakota
# Dakota Input File: rosen_opt_nls.in
environment
graphics
tabular_data
tabular_data_file = 'rosen_opt_nls.dat'
method
max_iterations = 100
convergence_tolerance = 1e-4
nl2sol
model
single
variables
continuous_design = 2
initial_point -1.2 1.0
lower_bounds -2.0 -2.0
upper_bounds 2.0 2.0
descriptors 'x1' 'x2'
interface
analysis_driver = 'rosenbrock'
direct
responses
calibration_terms = 2
analytic_gradients
no_hessians
```

Sample 3: Nondeterministic Analysis
The following sample input file shows Latin Hypercube Monte Carlo sampling using the Textbook Example (see Textbook). A similar file is available as Dakota/test/dakota_uq_textbook_lhs.in.

```dakota
method,
sampling,
samples = 100 seed = 1
complementary_distribution
response_levels = 3.6e+11 4.0e+11 4.4e+11 6.0e+04 6.5e+04 7.0e+04 3.5e+05 4.0e+05 4.5e+05
sample_type lhs
variables,
normal_uncertain = 2
means = 248.89, 593.33
std_deviations = 12.4, 29.7
descriptors = 'TF1n' 'TF2n'
uniform_uncertain = 2
lower_bounds = 199.3, 474.63
upper_bounds = 298.5, 712.
descriptors = 'TF1u' 'TF2u'
weibull_uncertain = 2
alphas = 12., 30.
betas = 250., 590.
descriptors = 'TF1w' 'TF2w'
```
4.3. SAMPLE INPUT FILES

histogram_bin_uncertain = 2
num_pairs = 3 4
abscissas = 5 8 10 .1 .2 .3 .4
counts = 12 17 24 12 0
descriptors = 'TF1h' 'TF2h'

histogram_point_uncertain = 1
num_pairs = 2
abscissas = 3 4
counts = 1 1
descriptors = 'TF3h'

interface,
for asynchronous evaluation_concurrency = 5
analysis_driver = 'text_book'

responses,
response_functions = 3
no_gradients
no_hessians

Sample 4: Parameter Study
The following sample input file shows a 1-D vector parameter study using the Textbook Example (see Textbook). It makes use of the default environment and model specifications, so they can be omitted. A similar file is available in the test directory as Dakota/examples/users/rosen_ps_vector.in.

# Dakota Input File: rosen_ps_vector.in
environment
    graphics
    tabular_data
    tabular_data_file = 'rosen_ps_vector.dat'
method
    vector_parameter_study
    final_point = 1.1 1.3
    num_steps = 10
variables
    continuous_design = 2
    initial_point = -0.3 0.2
    descriptors = 'x1' 'x2'
interface
    analysis_driver = 'rosenbrock'
direct
responses
    objective_functions = 1
    no_gradients
    no_hessians

Sample 5: Hybrid Strategy
The following sample input file shows a hybrid environment using three methods. It employs a genetic algorithm, pattern search, and full Newton gradient-based optimization in succession to solve the Textbook Example (see Textbook). A similar file is available as Dakota/examples/users/textbook_hybrid_strat.in.

environment
    graphics
    hybrid sequential
    method_list = 'PS' 'PS2' 'NLP'
method
  id_method = 'PS'
  model_pointer = 'M1'
  coliny_pattern_search stochastic
  seed = 1234
  initial_delta = 0.1
  threshold_delta = 1.e-4
  solution_accuracy = 1.e-10
  exploratory_moves basic_pattern
  #verbose output

method
  id_method = 'PS2'
  model_pointer = 'M1'
  max_function_evaluations = 10
  coliny_pattern_search stochastic
  seed = 1234
  initial_delta = 0.1
  threshold_delta = 1.e-4
  solution_accuracy = 1.e-10
  exploratory_moves basic_pattern
  #verbose output

method
  id_method = 'NLP'
  model_pointer = 'M2'
    optpp_newton
    gradient_tolerance = 1.e-12
    convergence_tolerance = 1.e-15
  #verbose output

model
  id_model = 'M1'
  single
  variables_pointer = 'V1'
  interface_pointer = 'I1'
  responses_pointer = 'R1'

model
  id_model = 'M2'
  single
  variables_pointer = 'V1'
  interface_pointer = 'I1'
  responses_pointer = 'R2'

variables
  id_variables = 'V1'
  continuous_design = 2
  initial_point 0.6 0.7
  upper_bounds 5.8 2.9
  lower_bounds 0.5 -2.9
  descriptors 'x1' 'x2'

interface
  id_interface = 'I1'
  direct
    analysis_driver= 'text_book'

responses
  id_responses = 'R1'
  objective_functions = 1
  no_gradients
4.4. INPUT SPEC SUMMARY

Additional example input files, as well as the corresponding output and graphics, are provided in the Tutorial chapter of the Users Manual [4].

4.4 Input Spec Summary

This file is derived automatically from dakota.xml, which is used in the generation of parser system files that are compiled into the Dakota executable. Therefore, these files are the definitive source for input syntax, capability options, and associated data inputs. Refer to the Developers Manual information on how to modify the input specification and propagate the changes through the parsing system.

Key features of the input specification and the associated user input files include:

- In the input specification, required individual specifications simply appear, optional individual and group specifications are enclosed in [ ], required group specifications are enclosed in ( ), and either-or relationships are denoted by the | symbol. These symbols only appear in dakota.input.summary; they must not appear in actual user input files.

- Keyword specifications (i.e., environment, method, model, variables, interface, and responses) begin with the keyword possibly preceded by white space (blanks, tabs, and newlines) both in the input specifications and in user input files. For readability, keyword specifications may be spread across several lines. Earlier versions of Dakota (prior to 4.1) required a backslash character (\) at the ends of intermediate lines of a keyword. While such backslashes are still accepted, they are no longer required.

- Some of the keyword components within the input specification indicate that the user must supply INTEGER, REAL, STRING, INTEGERLIST, REALLIST, or STRINGLIST data as part of the specification. In a user input file, the "=" is optional, data in a LIST can be separated by commas or whitespace, and the STRING data are enclosed in single or double quotes (e.g., ‘text_book’ or "text_book").

- In user input files, input is largely order-independent (except for entries in lists of data), case insensitive, and white-space insensitive. Although the order of input shown in the Sample Input Files generally follows the order of options in the input specification, this is not required.

- In user input files, specifications may be abbreviated so long as the abbreviation is unique. For example, the npsol.sqp specification within the method keyword could be abbreviated as npsol, but dot.sqp should not be abbreviated as dot since this would be ambiguous with other DOT method specifications.

- In both the input specification and user input files, comments are preceded by #.

- ALIAS refers to synonymous keywords, which often exist for backwards compatability. Users are encouraged to use the most current keyword.

dakota.input.summary:

KEYWORD01 environment
    [ tabular_data ALIAS tabular_graphics_data
      [ tabular_data_file ALIAS tabular_graphics_file STRING ]
      [ annotated

```
(custom_annotated
  [header]
  [eval_id]
  [interface_id]
)

(output_file STRING)
(error_file STRING)
(read_restart STRING
  [stop_restart INTEGER >= 0])
(write_restart STRING)
(output_precision INTEGER >= 0)
(results_output
  [results_output_file STRING])

(graphics)
(check)
(pre_run
  [input STRING]
  [output STRING
    [annotated]
    (custom_annotated
      [header]
      [eval_id]
      [interface_id]
    )
    (freeform)
  ]
)
(run
  [input STRING]
  [output STRING])
(post_run
  [input STRING
    [annotated]
    (custom_annotated
      [header]
      [eval_id]
      [interface_id]
    )
    (freeform)
  ]
  [output STRING])
[top_method_pointer ALIAS method_pointer STRING]

KEYWORD12 method
[ id_method STRING]
[output
debug
| verbose
| normal
| quiet
4.4. INPUT SPEC SUMMARY

| silent
| |
| [ final_solutions INTEGER >= 0 ] ( hybrid
| sequential ALIAS uncoupled
| [ method_name_list STRINGLIST
| [ model_pointer_list STRING ]
| ] method_pointer_list STRINGLIST ) |
| [ embedded ALIAS coupled
| [ global_method_name STRING
| [ global_model_pointer STRING ]
| ] global_method_pointer STRING
| [ local_method_name STRING
| [ local_model_pointer STRING ]
| ] local_method_pointer STRING
| [ local_search_probability REAL ] )
| ]
| [ collaborative
| [ method_name_list STRINGLIST
| [ model_pointer_list STRING ]
| ] method_pointer_list STRINGLIST ) |
| [ iterator_servers INTEGER > 0 ] ( multi_start
| [ method_name STRING
| [ model_pointer STRING ]
| ] method_pointer STRING
| [ random_starts INTEGER
| [ seed INTEGER ]
| ] starting_points REALLIST ) |
| [ iterator_servers INTEGER > 0 ] ( pareto_set
| [ method_name ALIAS opt_method_name STRING
| [ model_pointer ALIAS opt_model_pointer STRING ]
| ] method_pointer ALIAS opt_method_pointer STRING
| [ random_weight_sets INTEGER
| [ seed INTEGER ]
| ]
| |
| |
[ weight_sets ALIAS multi_objective_weight_sets REALLIST ]
[ iterator_servers INTEGER > 0 ]
[ iterator_scheduling
  master
  peer ]
[ processors_per_iterator INTEGER > 0 ]
)

| branch_and_bound
  method_pointer STRING |
  ( method_name STRING
    [ model_pointer STRING ]
  )
  [ scaling ]
 |
| surrogate_based_local
  method_pointer ALIAS approx_method_pointer STRING
  [ method_name ALIAS approx_method_name STRING
    model_pointer ALIAS approx_model_pointer STRING
    [ soft_convergence_limit INTEGER ]
    [ truth_surrogate_bypass ]
    [ approx_subproblem
      original_primary
      | single_objective
      | augmented_lagrangian_objective
      | lagrangian_objective
      | linearized_constraints
      | no_constraints
    ]
  ]
  [ merit_function
    penalty_merit
    | adaptive_penalty_merit
    | lagrangian_merit
    | augmented_lagrangian_merit
  ]
  [ acceptance_logic
    tr_ratio
    | filter
  ]
  [ constraint_relax
    homotopy
  ]
  [ trust_region
    [ initial_size REALLIST ]
    [ minimum_size REAL ]
    [ contract_threshold REAL ]
    [ expand_threshold REAL ]
    [ contraction_factor REAL ]
    [ expansion_factor REAL ]
  ]
  [ max_iterations INTEGER >= 0 ]
  [ convergence_tolerance REAL ]
  [ constraint_tolerance REAL ]
  )

| surrogate_based_global
  method_pointer ALIAS approx_method_pointer STRING
  [ method_name ALIAS approx_method_name STRING

model_pointer ALIAS approx_model_pointer STRING
  [ replace_points ]
  [ max_iterations INTEGER >= 0 ]
}
|
  ( dot_frcg
    [ max_iterations INTEGER >= 0 ]
    [ convergence_tolerance REAL ]
    [ constraint_tolerance REAL ]
    [ speculative ]
    [ max_function_evaluations INTEGER >= 0 ]
    [ scaling ]
    [ model_pointer STRING ]
  )
  |
  ( dot_mmfd
  |
  )
  |
  ( dot_bfgs
  |
  )
  |
  ( dot_slp
  |
  )
  |
  ( dot_sqp
  |
  )
  |
  ( dot
    frcg
    |
    mmfd
    |
    bfgs
    |
    slp
    |
    sqp
    [ max_iterations INTEGER >= 0 ]
    [ convergence_tolerance REAL ]
    [ constraint_tolerance REAL ]
    [ speculative ]
    [ max_function_evaluations INTEGER >= 0 ]
    [ scaling ]
    [ model_pointer STRING ]
  )
  |
  ( conmin_frcg
    [ max_iterations INTEGER >= 0 ]
    [ convergence_tolerance REAL ]
    [ constraint_tolerance REAL ]
    [ speculative ]
    [ max_function_evaluations INTEGER >= 0 ]
    [ scaling ]
    [ model_pointer STRING ]
  )
  |
  ( conmin_mmfd
  |
  )
  |
  ( conmin
    frcg
    |
    mfd
    |
    bfgs
    |
    slp
    |
    sqp
    [ max_iterations INTEGER >= 0 ]
    [ convergence_tolerance REAL ]
    [ constraint_tolerance REAL ]
    [ speculative ]
    [ max_function_evaluations INTEGER >= 0 ]
    [ scaling ]
    [ model_pointer STRING ]
  )
  |
  ( dl_solver STRING
    [ max_function_evaluations INTEGER >= 0 ]
    [ scaling ]
    [ model_pointer STRING ]
  )
CHAPTER 4. DAKOTA INPUT SPECIFICATION

{ npsol_sqp
  [ verify_level INTEGER ]
  [ function_precision REAL ]
  [ linesearch_tolerance REAL ]
  [ convergence_tolerance REAL ]
  [ max_iterations INTEGER >= 0 ]
  [ constraint_tolerance REAL ]
  [ speculative ]
  [ max_function_evaluations INTEGER >= 0 ]
  [ scaling ]
  [ model_pointer STRING ]
}

{ nlssol_sqp
}

{ stanford
  npsol
  nlssol
  [ verify_level INTEGER ]
  [ function_precision REAL ]
  [ linesearch_tolerance REAL ]
  [ convergence_tolerance REAL ]
  [ max_iterations INTEGER >= 0 ]
  [ constraint_tolerance REAL ]
  [ speculative ]
  [ max_function_evaluations INTEGER >= 0 ]
  [ scaling ]
  [ model_pointer STRING ]
}

{ nlpql_sqp
  [ max_iterations INTEGER >= 0 ]
  [ convergence_tolerance REAL ]
  [ max_function_evaluations INTEGER >= 0 ]
  [ scaling ]
  [ model_pointer STRING ]
}

{ optpp_cg
  [ max_step REAL ]
  [ gradient_tolerance REAL ]
  [ max_iterations INTEGER >= 0 ]
  [ convergence_tolerance REAL ]
  [ speculative ]
  [ max_function_evaluations INTEGER >= 0 ]
  [ scaling ]
  [ model_pointer STRING ]
}

{ optpp_q_newton
  | optpp_fd_newton
  | optpp_g_newton
  | optpp_newton
  | search_method
    value_based_line_search
    | gradient_based_line_search
    | trust_region
    | tr_pds
  |
  | merit_function
    el_bakry
    | argaez_tapia


4.4. INPUT SPEC SUMMARY

| van_shanno |
| [ steplength_to_boundary REAL ] |
| [ centering_parameter REAL ] |
| [ max_step REAL ] |
| [ gradient_tolerance REAL ] |
| [ max_iterations INTEGER >= 0 ] |
| [ convergence_tolerance REAL ] |
| [ speculative ] |
| [ max_function_evaluations INTEGER >= 0 ] |
| [ scaling ] |
| [ model_pointer STRING ] |
|)
|
| ( optpp_pds |
| [ search_scheme_size INTEGER ] |
| [ max_iterations INTEGER >= 0 ] |
| [ convergence_tolerance REAL ] |
| [ max_function_evaluations INTEGER >= 0 ] |
| [ scaling ] |
| [ model_pointer STRING ] |
|)
|
| ( asynch_pattern_search ALIAS coliny_apps |
| [ initial_delta REAL ] |
| [ contraction_factor REAL ] |
| [ threshold_delta REAL ] |
| [ solution_target ALIAS solution_accuracy REAL ] |
| [ synchronization blocking |
| [ nonblocking ] |
| [ merit_function |
| merit_max |
| [ merit_max_smooth ] |
| [ merit1 ] |
| [ merit1_smooth ] |
| [ merit2 ] |
| [ merit2_smooth ] |
| [ merit2_squared ] |
| [ constraint_penalty REAL ] |
| [ smoothing_factor REAL ] |
| [ constraint_tolerance REAL ] |
| [ max_function_evaluations INTEGER >= 0 ] |
| [ scaling ] |
| [ model_pointer STRING ] |
|)
|
| ( mesh_adaptive_search |
| [ initial_delta REAL ] |
| [ threshold_delta REAL ] |
| [ function_precision REAL ] |
| [ seed INTEGER > 0 ] |
| [ history_file STRING ] |
| [ display_format STRING ] |
| [ variable_neighborhood_search REAL ] |
| [ neighbor_order INTEGER > 0 ] |
| [ display_all_evaluations ] |
| [ use_surrogate |
| inform_search |
| [ optimize ]
[ max_iterations INTEGER >= 0 ]
[ max_function_evaluations INTEGER >= 0 ]
[ scaling ]
[ model_pointer STRING ]
)

| ( nowpac
| trust_region
| [ initial_size REALLIST ]
| [ minimum_size REAL ]
| [ contract_threshold REAL ]
| [ expand_threshold REAL ]
| [ contraction_factor REAL ]
| [ expansion_factor REAL ]
| [ max_iterations INTEGER >= 0 ]
| [ max_function_evaluations INTEGER >= 0 ]
| [ scaling ]
| [ model_pointer STRING ]
)

| ( snowpac
| seed INTEGER > 0 ]
| trust_region
| [ initial_size REALLIST ]
| [ minimum_size REAL ]
| [ contract_threshold REAL ]
| [ expand_threshold REAL ]
| [ contraction_factor REAL ]
| [ expansion_factor REAL ]
| [ max_iterations INTEGER >= 0 ]
| [ max_function_evaluations INTEGER >= 0 ]
| [ scaling ]
| [ model_pointer STRING ]
)

| ( moga
| fitness_type
| layer_rank
| domination_count
| replacement_type
| elitist
| roulette_wheel
| unique_roulette_wheel
| [ below_limit REAL
| [ shrinkage_fraction ALIAS shrinkage_percentage REAL ]
| ]
| niching_type
| radial REALLIST
| [ distance REALLIST ]
| [ max_designs REALLIST
| [ num_designs INTEGER >= 2 ]
| ]
| convergence_type
| metric_tracker
4.4. INPUT SPEC SUMMARY

[ percent_change REAL ]
[ num_generations INTEGER >= 0 ]
]
[ postprocessor_type
  orthogonal_distance REALIST
]
[ max_iterations INTEGER >= 0 ]
[ max_function_evaluations INTEGER >= 0 ]
[ scaling ]
[ population_size INTEGER >= 0 ]
[ log_file STRING ]
[ print_each_pop ]
[ initialization_type
  simple_random
  | unique_random
  | flat_file STRING
]
[ crossover_type
  multi_point_binary INTEGER
  | multi_point_parameterized_binary INTEGER
  | multi_point_real INTEGER
  |
  [ shuffle_random
    [ num_parents INTEGER > 0 ]
    [ num_offspring INTEGER > 0 ]
  ]
  [ crossover_rate REAL ]
]
[ mutation_type
  bit_random
  | replace_uniform
  |
  [ offset_normal
    | offset_cauchy
    | offset_uniform
    [ mutation_scale REAL ]
  ]
  [ mutation_rate REAL ]
]
[ seed INTEGER > 0 ]
[ convergence_tolerance REAL ]
[ model_pointer STRING ]
]
|
[ soga
  [ fitness_type
    merit_function
    [ constraint_penalty REAL ]
  ]
  [ replacement_type
    elitist
    | favor_feasible
    | roulette_wheel
    | unique_roulette_wheel
  ]
  [ convergence_type
    [ best_fitness_tracker
      [ percent_change REAL ]
      [ num_generations INTEGER >= 0 ]
    ]
  ]
]
[ average_fitness_tracker
}
CHAPTER 4. DAKOTA INPUT SPECIFICATION

[ percent_change REAL ]
[ num_generations INTEGER >= 0 ]
)

[ max_iterations INTEGER >= 0 ]
[ max_function_evaluations INTEGER >= 0 ]
[ scaling ]
[ population_size INTEGER >= 0 ]
[ log_file STRING ]
[ print_each_pop ]
[ initialization_type
  simple_random
  unique_random
  flat_file STRING ]
[ crossover_type
  multi_point_binary INTEGER
  multi_point_parameterized_binary INTEGER
  multi_point_real INTEGER
  shuffle_random
  num_parents INTEGER > 0 ]
  num_offspring INTEGER > 0 ]
]
[ crossover_rate REAL ]
]
[ mutation_type
  bit_random
  replace_uniform
  offset_normal
  offset_cauchy
  offset_uniform
  mutation_scale REAL ]
]
[ mutation_rate REAL ]
]
[ seed INTEGER > 0 ]
[ convergence_tolerance REAL ]
[ model_pointer STRING ]
)

| coliny_pattern_search
  constant_penalty ]
  no_expansion ]
  expand_after_success INTEGER ]
[ pattern_basis
  coordinate
  simplex
 ]
[ stochastic ]
[ total_pattern_size INTEGER ]
[ exploratory_moves
  multi_step
  adaptive_pattern
  basic_pattern ]
[ synchronization
  blocking
  nonblocking
 ]
[ contraction_factor REAL ]
4.4. INPUT SPEC SUMMARY

```
[ constraint_penalty REAL ]
[ initial_delta REAL ]
[ threshold_delta REAL ]
[ solution_target ALIAS solution_accuracy REAL ]
[ seed INTEGER > 0 ]
[ show_m misc_options ]
[ misc_options STRINGLIST ]
[ max_iterations INTEGER >= 0 ]
[ convergence_tolerance REAL ]
[ max_function_evaluations INTEGER >= 0 ]
[ scaling ]
[ model_pointer STRING ]
|
| ( coliny_solis_wets

[ contract_after_failure INTEGER ]
[ no_expansion ]
[ expand_after_success INTEGER ]
[ constant_penalty ]
[ contraction_factor REAL ]
[ constraint_penalty REAL ]
[ initial_delta REAL ]
[ threshold_delta REAL ]
[ solution_target ALIAS solution_accuracy REAL ]
[ seed INTEGER > 0 ]
[ show_m misc_options ]
[ misc_options STRINGLIST ]
[ max_iterations INTEGER >= 0 ]
[ convergence_tolerance REAL ]
[ max_function_evaluations INTEGER >= 0 ]
[ scaling ]
[ model_pointer STRING ]
|
| ( coliny_cobyla

[ initial_delta REAL ]
[ threshold_delta REAL ]
[ solution_target ALIAS solution_accuracy REAL ]
[ seed INTEGER > 0 ]
[ show_m misc_options ]
[ misc_options STRINGLIST ]
[ max_iterations INTEGER >= 0 ]
[ convergence_tolerance REAL ]
[ max_function_evaluations INTEGER >= 0 ]
[ scaling ]
[ model_pointer STRING ]
|
| ( coliny_direct

[ division ]

[ major_dimension ]

[ all_dimensions ]

[ global_balance_parameter REAL ]
[ local_balance_parameter REAL ]
[ max_boxsize_limit REAL ]
[ min_boxsize_limit REAL ]
[ constraint_penalty REAL ]
[ solution_target ALIAS solution_accuracy REAL ]
[ seed INTEGER > 0 ]
[ show_m misc_options ]
[ misc_options STRINGLIST ]
```
[ max_iterations INTEGER >= 0 ]
[ convergence_tolerance REAL ]
[ max_function_evaluations INTEGER >= 0 ]
[ scaling ]
[ model_pointer STRING ]
)
|
{ coliny_ea
[ population_size INTEGER > 0 ]
[ initialization_type
  simple_random
  | unique_random
  | flat_file STRING
]
[ fitness_type
  linear_rank
  | merit_function
]
[ replacement_type
  random INTEGER
  | chc INTEGER
  | elitist INTEGER
  [ new_solutions_generated INTEGER ]
]
[ crossover_rate REAL ]
[ crossover_type
  two_point
  | blend
  | uniform
]
[ mutation_rate REAL ]
[ mutation_type
  replace_uniform
  |
    { offset_normal
    | offset_cauchy
    | offset_uniform
    [ mutation_scale REAL ]
    [ mutation_range INTEGER ]
  ]
  [ non_adaptive ]
]
[ constraint_penalty REAL ]
[ solution_target ALIAS solution_accuracy REAL ]
[ seed INTEGER > 0 ]
[ show_misc_options ]
[ misc_options STRINGLIST ]
[ max_iterations INTEGER >= 0 ]
[ convergence_tolerance REAL ]
[ max_function_evaluations INTEGER >= 0 ]
[ scaling ]
[ model_pointer STRING ]
)
|
{ coliny_beta
 beta_solver_name STRING
[ solution_target ALIAS solution_accuracy REAL ]
[ seed INTEGER > 0 ]
[ show_misc_options ]
[ misc_options STRINGLIST ]
[ max_iterations INTEGER >= 0 ]
[ convergence_tolerance REAL ]

4.4. INPUT SPEC SUMMARY

```
[ max_function_evaluations INTEGER >= 0 | scaling ]
[ model_pointer STRING ]
)

| nl2sol
[ function_precision REAL ]
[ absolute_conv_tol REAL ]
[ x_conv_tol REAL ]
[ singular_conv_tol REAL ]
[ singular_radius REAL ]
[ false_conv_tol REAL ]
[ initial_trust_radius REAL ]
[ covariance INTEGER ]
[ regression_diagnostics ]
[ convergence_tolerance REAL ]
[ max_iterations INTEGER >= 0 ]
[ speculative ]
[ max_function_evaluations INTEGER >= 0 ]
[ scaling ]
[ model_pointer STRING ]
)

| nonlinear_cg
[ misc_options STRINGLIST ]
[ convergence_tolerance REAL ]
[ max_iterations INTEGER >= 0 ]
[ scaling ]
[ model_pointer STRING ]
)

| ncsu_direct
[ solution_target ALIAS solution_accuracy REAL ]
[ min_boxsize_limit REAL ]
[ volume_boxsize_limit REAL ]
[ convergence_tolerance REAL ]
[ max_iterations INTEGER >= 0 ]
[ max_function_evaluations INTEGER >= 0 ]
[ scaling ]
[ model_pointer STRING ]
)

| genie_opt_darts
[ seed INTEGER > 0 |
[ max_function_evaluations INTEGER >= 0 ]
[ scaling ]
[ model_pointer STRING ]
)

| efficient_global
[ initial_samples INTEGER ]
[ seed INTEGER > 0 ]
[ max_iterations INTEGER >= 0 ]
[ gaussian_process ALIAS kriging ]
surfpack
[ dakota ]
[ use_derivatives ]
[ import_build_points_file ALIAS import_points_file STRING ]
[ annotated ]
```
{ custom_annotated
  [ header ]
  [ eval_id ]
  [ interface_id ]

  [ freeform
  [ active_only ]
]

[ export_approx_points_file ALIAS export_points_file STRING
  [ annotated
    |
    { custom_annotated
      [ header ]
      [ eval_id ]
      [ interface_id ]
    |
    { freeform
    ]
  ]

  [ model_pointer STRING ]
)

[ polynomial_chaos ALIAS nond_polynomial_chaos
  [ samples_on_emulator ALIAS samples INTEGER ]
  [ seed INTEGER > 0 ]
  [ fixed_seed ]
  [ max_refinement_iterations INTEGER >= 0 ]
  [ convergence_tolerance REAL ]
  [ final_moments
    none
    | standard
    | central
  ]
  [ p_refinement
    uniform
    |
    { dimension_adaptive
      sobol
      | decay
      | generalized
    ]
  ]
  [ askey
  | wiener ]
( quadrature_order_sequence INTEGERLIST
  [ dimension_preference REALLIST ]
  [ nested
  | non_nested ]
)

( sparse_grid_level_sequence INTEGERLIST
  [ restricted
  | unrestricted ]
  [ dimension_preference REALLIST ]
  [ nested
  | non_nested ]
)

| cubature_integrand INTEGER

( expansion_order_sequence INTEGERLIST
  [ dimension_preference REALLIST ]

  [ unrestricted
  | restricted ]
  [ dimension_preference REALLIST ]
  [ nested
  | non_nested ]
)
[ basis_type
tensor_product
| total_order
| |
| ( adapted
| advancements INTEGER ]
| soft_convergence_limit INTEGER ]
)
]

collocation_points_sequence INTEGERLIST
collocation_ratio REAL
collocation_ratio REAL ]
| { least_squares
| svd
| equality_constrained ]
|
| ( orthogonal_matching_pursuit ALIAS omp
| noise_tolerance REALLIST ]
|
| least_angle_regression ALIAS lars
| noise_tolerance REALLIST ]
|
| ( least_absolute_shrinkage ALIAS lasso
| noise_tolerance REALLIST ]
| l2_penalty REAL ]
|
cross_validation
| noise_only ]
|
| use_derivatives ]
tensor_grid ]
| reuse_points ALIAS reuse_samples ]
| max_iterations INTEGER >= 0 ]
| max_solver_iterations INTEGER >= 0 ]
)
]

expansion_samples_sequence INTEGERLIST
| reuse_points ALIAS reuse_samples ]
| incremental_lhs ]
)
]
import_build_points_file ALIAS import_points_file STRING
| annotated
| ( custom_annotated
| header ]
eval_id ]
| interface_id ]
|
| ( freeform
| active_only ]
)
( orthogonal_least_interpolation ALIAS least_interpolation ALIAS collocation_points_sequence INTEGERLIST
  [ tensor_grid INTEGERLIST ]
  [ reuse_points ALIAS reuse_samples ]
  [ import_build_points_file ALIAS import_points_file STRING
    [ annotated ]
    [ custom_annotated
      [ header ]
      [ eval_id ]
      [ interface_id ]
    ]
    [ freeform
      [ active_only ]
    ]
  ]
  [ import_expansion_file STRING
    [ variance_based_decomp
      [ interaction_order INTEGER > 0 ]
      [ drop_tolerance REAL ]
    ]
    [ diagonal_covariance
    [ full_covariance ]
    [ normalized ]
    [ sample_type
      lhs
      random
    ]
    [ probability_refinement ALIAS sample_refinement
      import
      [ adapt_import
        mm_adapt_import
        [ refinement_samples INTEGERLIST ]
      ]
    ]
  ]
  [ import_approx_points_file STRING
    [ annotated ]
    [ custom_annotated
      [ header ]
      [ eval_id ]
      [ interface_id ]
    ]
    [ freeform
      [ active_only ]
    ]
  ]
  [ export_approx_points_file ALIAS export_points_file STRING
    [ annotated ]
    [ custom_annotated
      [ header ]
      [ eval_id ]
      [ interface_id ]
    ]
    [ freeform
    ]
  ]
  [ export_expansion_file STRING ]
  [ reliability_levels REALLIST
    [ num_reliability_levels INTEGERLIST ]
  ])
4.4. INPUT SPEC SUMMARY

[ response_levels REALIST
  [ num_response_levels INTEGERLIST ]
  [ compute
    probabilities
    | reliabilities
    | gen_reliabilities
    [ system
      series
      | parallel
      ]
  ]
]

[ distribution
  cumulative
  | complementary
  ]

[ probability_levels REALIST
  [ num_probability_levels INTEGERLIST ]
]

[ gen_reliability_levels REALIST
  [ num_gen_reliability_levels INTEGERLIST ]
]

[ rng
  mt19937
  | rnum2
  ]

[ model_pointer STRING ]

[ stoch_collocation ALIAS nond_stoch_collocation
  [ samples_on_emulator ALIAS samples INTEGER ]
  [ seed INTEGER > 0 ]
  [ fixed_seed ]
  [ max_refinement_iterations INTEGER >= 0 ]
  [ convergence_tolerance REAL ]
  [ final_moments
    none
    | standard
    | central
  ]
  [ [ p_refinement
     uniform
     |
     ( dimension_adaptive
       sobol
     | generalized
     )
   ]
  ]
  [ h_refinement
    uniform
    |
    ( dimension_adaptive
      sobol
    | generalized
    )
    | local_adaptive
  ]
  [ piecewise
    | asky
    | wiener
  ]
  quadrature_order_sequence INTEGERLIST]
CHAPTER 4. DAKOTA INPUT SPECIFICATION

sparse_grid_level_sequence INTEGERLIST
  [ restricted
  | unrestricted ]
  [ nodal
  | hierarchical ]
)

use_derivatives

nested
| non_nested ]

variance_based_decomp
  [ interaction_order INTEGER > 0 ]
  [ drop_tolerance REAL ]
)

diagonal_covariance
| full_covariance ]

sample_type
  lhs
  | random ]

probability_refinement ALIAS sample_refinement

import
  | adapt_import
  | mm_adapt_import
  [ refinement_samples INTEGERLIST ]
)

import_approx_points_file STRING

[ annotated
  |
  { custom_annotated
    [ header ]
    [ eval_id ]
    [ interface_id ]
  ]
  |
  { freeform
    [ active_only ]
  ]

export_approx_points_file ALIAS export_points_file STRING

[ annotated
  |
  { custom_annotated
    [ header ]
    [ eval_id ]
    [ interface_id ]
  ]
  |
  { freeform
    [ reliability_levels REALLIST
      [ num_reliability_levels INTEGERLIST ]
    ]
  ]

response_levels REALLIST
  [ num_response_levels INTEGERLIST ]

[ compute
  probabilities
  | reliabilities
  | gen_reliabilities
  [ system
    series
  ]
  | parallel
4.4. INPUT SPEC SUMMARY

| [ distribution
cumulative
| complementary
|
| probability_levels REALLIST
| num_probability_levels INTEGERLIST ]
|
| gen_reliability_levels REALLIST
| num_gen_reliability_levels INTEGERLIST ]
|
| rng
| mt19937
| rnum2
|
| model_pointer STRING ]
|
| [ sampling ALIAS nond_sampling
| samples ALIAS initial_samples INTEGER ]
| seed INTEGER > 0 ]
| fixed_seed |
| sample_type
| lhs
| random
| incremental_lhs
| incremental_random
|
| refinement_samples INTEGERLIST ]
|
| d_optimal
| candidate_designs INTEGER > 0
| leja_oversample_ratio REAL ]
|
| variance_based_decomp
| drop_tolerance REAL ]
|
| backfill ]
| principal_components
| percent_variance_explained REAL ]
|
| wilks
| order INTEGER ]
| confidence_level REAL ]
| one_sided_lower ]
| one_sided_upper ]
| two_sided ]
|
| final_moments
| none
| standard
| central
|
| reliability_levels REALLIST
| num_reliability_levels INTEGERLIST ]
|
| response_levels REALLIST
| num_response_levels INTEGERLIST ]
| compute
| probabilities
| reliabilities
CHAPTER 4. DAKOTA INPUT SPECIFICATION

| gen_reliabilities
| system
| series
| parallel
|
| distribution
cumulative
| complementary
|
| probability_levels REALLIST
| num_probability_levels INTEGERLIST |
|
| gen_reliability_levels REALLIST
| num_gen_reliability_levels INTEGERLIST |
|
| rng
| mt19937
| rnum2
|
| model_pointer STRING |
|
| multilevel_sampling ALIAS multilevel_mc
| seed INTEGER > 0 |
| fixed_seed |
| pilot_samples INTEGERLIST |
| sample_type
| lhs |
| random |
| export_sample_sequence
| annotated |
| custom.annotated
| header |
| eval_id |
| interface_id |
|
| freeform |
|
| max_iterations INTEGER >= 0 |
| convergence_tolerance REAL |
| final_moments
| none |
| standard |
| central |
| distribution
cumulative
| complementary |
|
| probability_levels REALLIST
| num_probability_levels INTEGERLIST |
|
| gen_reliability_levels REALLIST
| num_gen_reliability_levels INTEGERLIST |
|
| rng
| mt19937
4.4. INPUT SPEC SUMMARY

| rnum2 |
| model_pointer STRING |

| ( importance_sampling ALIAS nond_importance_sampling |
| samples ALIAS initial_samples INTEGER |
| seed INTEGER > 0 |
| import |
| adapt_import |
| mm_adapt_import |
| refinement_samples INTEGERLIST |
| response_levels REALLIST |
| num_response_levels INTEGERLIST |
| compute |
| probabilities |
| gen_reliabilities |
| system |
| series |
| parallel |
| ) |
| ) |
| max_iterations INTEGER >= 0 |
| convergence_tolerance REAL |
| distribution |
| cumulative |
| complementary |
| ) |
| probability_levels REALLIST |
| num_probability_levels INTEGERLIST |
| ) |
| gen_reliability_levels REALLIST |
| num_gen_reliability_levels INTEGERLIST |
| ) |
| rng |
| mt19937 |
| rnum2 |
| ) |
| model_pointer STRING |
| ) |

| gpais ALIAS gaussian_process_adaptive_importance_sampling |
| build_samples ALIAS samples INTEGER |
| seed INTEGER > 0 |
| samples_on_emulator INTEGER |
| import_build_points_file ALIAS import_points_file STRING |
| annotated |
| ) |
| custom_annotated |
| header |
| eval_id |
| interface_id |
| ) |
| freeform |
| active_only |
| ) |
| export_approx_points_file ALIAS export_points_file STRING |
| annotated |
| ) |
| custom_annotated |
[ header ]
[ eval_id ]
[ interface_id ]
|
| ( freeform |
|)

[ response_levels REALLIST
[ num_response_levels INTEGERLIST ]
[ compute
  probabilities |
  gen_reliabilities
|
  system
  series |
  parallel |
]
|
[ max_iterations INTEGER >= 0 ]
[ distribution
cumulative
  | complementary ]
|
[ probability_levels REALLIST
[ num_probability_levels INTEGERLIST ]
]
|
[ gen_reliability_levels REALLIST
[ num_gen_reliability_levels INTEGERLIST ]
]
|
[ rng
  mt19937 |
  rnum2 |
  model_pointer STRING ]
)
|
| ( adaptive_sampling ALIAS nond_adaptive_sampling
|
  [ initial_samples ALIAS samples INTEGER ]
|
  [ seed INTEGER > 0 ]
|
  [ samples_on_emulator INTEGER ]
|
  [ fitness_metric
predicted_variance
  | distance |
  | gradient ]
|
| [ batch_selection
  naive
  | distance_penalty |
  | topology |
  | constant_liar ]
|
| [ refinement_samples INTEGERLIST ]
|
| [ import_build_points_file ALIAS import_points_file STRING
[ annotated |
|
  [ custom_annotated
  | header ]
|
  [ eval_id ]
|
  [ interface_id ]
]
|
| ( freeform |
4.4. INPUT SPEC SUMMARY

- active_only
- export_approx_points_file ALIAS export_points_file STRING
  - annotated
    - custom_annotated
      - header
      - eval_id
      - interface_id
  - freeform
- response_levels REALLIST
  - num_response_levels INTEGERLIST
  - compute
    - probabilities
      - gen_reliabilities
    - system
      - parallel
      - series
  - misc_options STRINGLIST
  - max_iterations INTEGER \geq 0
  - distribution
    - cumulative
      - complementary
      - probability_levels REALLIST
        - num_probability_levels INTEGERLIST
      - gen_reliability_levels REALLIST
        - num_gen_reliability_levels INTEGERLIST
      - rng
        - mt19937
        - rnum2
      - model_pointer STRING
  - pof_darts ALIAS nond_pof_darts
    - build_samples ALIAS samples INTEGER
      - seed INTEGER > 0
      - lipschitz
        - local
        - global
      - samples_on_emulator INTEGER
      - response_levels REALLIST
        - num_response_levels INTEGERLIST
        - compute
          - probabilities
            - gen_reliabilities
          - system
            - parallel
            - series
      }
[ distribution
  cumulative
  | complementary
] [ probability_levels REALLIST
  [ num_probability_levels INTEGERLIST ] ]
[ gen_reliability_levels REALLIST
  [ num_gen_reliability_levels INTEGERLIST ] ]
[ rng
  mt19937
  rnum2
] [ model_pointer STRING ]
)
}
(rkd_darts ALIAS nond_rkd_darts
build_samples ALIAS samples INTEGER
[ seed INTEGER > 0 ]
[ lipschitz
  local
  | global
] [ samples_on_emulator INTEGER ]
[ response_levels REALLIST
  [ num_response_levels INTEGERLIST ]
  [ compute
    probabilities
    | gen_reliabilities
    [ system
      series
      | parallel
    ]
  ]
]
[ distribution
  cumulative
  | complementary
] [ probability_levels REALLIST
  [ num_probability_levels INTEGERLIST ] ]
[ gen_reliability_levels REALLIST
  [ num_gen_reliability_levels INTEGERLIST ] ]
[ rng
  mt19937
  rnum2
] [ model_pointer STRING ]
)
)
(global_evidence ALIAS nond_global_evidence
[ samples INTEGER ]
[ seed INTEGER > 0 ]
[ sbo
  | ego
  [ gaussian_process ALIAS kriging
    surfpack
    | dakota
  ]}
[ use_derivatives ]
[ import_build_points_file ALIAS import_points_file STRING
  [ annotated
    | ( custom_annotated
      [ header ]
      [ eval_id ]
      [ interface_id ]
    )
    | ( freeform
      [ active_only ]
    )
  ]
[ export_approx_points_file ALIAS export_points_file STRING
  [ annotated
    | ( custom_annotated
      [ header ]
      [ eval_id ]
      [ interface_id ]
    )
    | ( freeform
      [ ]
    )
  ]
[ ea
  | lhs ]
[ response_levels REALLIST
  [ num_response_levels INTEGERLIST ]
  [ compute
    probabilities
    | gen_reliabilities
      [ system
        [ series
          | parallel
        ]
      ]
    ]
  [ distribution
    cumulative
    | complementary
  ]
[ probability_levels REALLIST
  [ num_probability_levels INTEGERLIST ]
  [ gen_reliability_levels REALLIST
    [ num_gen_reliability_levels INTEGERLIST ]
  ]
[ rng
  mt19937
  | rnum2
]
[ model_pointer STRING ]
]
[ global_interval_est ALIAS nond_global_interval_est
  [ samples INTEGER ]
  [ seed INTEGER > 0 ]
  [ max_iterations INTEGER >= 0 ]
  [ convergence_tolerance REAL ]
  [ max_function_evaluations INTEGER >= 0 ]
  [ sbo ]
CHAPTER 4. DAKOTA INPUT SPECIFICATION

| ego |
| gaussian_process ALIAS kriging |
| surfpack |
| dakota |
| use_derivatives |
| import_build_points_file ALIAS import_points_file STRING |
| annotated |
| custom_annotated |
| header |
| eval_id |
| interface_id |
| freeform |
| active_only |

| export_approx_points_file ALIAS export_points_file STRING |
| annotated |
| custom_annotated |
| header |
| eval_id |
| interface_id |
| freeform |

| ea |
| lhs |
| rng |
| mt19937 |
| rnum2 |

| model_pointer STRING |

| bayes_calibration ALIAS nond_bayes_calibration |
| queso |
| chain_samples ALIAS samples INTEGER |
| seed INTEGER > 0 |
| emulator |
| gaussian_process ALIAS kriging |
| surfpack |
| dakota |
| build_samples INTEGER |
| posterior_adaptive |
| import_build_points_file ALIAS import_points_file STRING |
| annotated |
| custom_annotated |
| header |
| eval_id |
| interface_id |
| freeform |
| active_only |
4.4. INPUT SPEC SUMMARY

| ( pce
sparse_grid_level_sequence INTEGERLIST
| | ( expansion_order_sequence INTEGERLIST
collocation_points_sequence INTEGERLIST
| collocation_ratio REAL
| ( cross_validation |
| posterior_adaptive |
| import_build_points_file ALIAS import_points_file STRING
| ( annotated |
| ( custom_annotated |
| ( header |
| ( eval_id |
| ( interface_id |
| |
| ( freeform |
| ( active_only |
| )
|
| ( orthogonal_least_interpolation
collocation_points_sequence INTEGERLIST
| posterior_adaptive |
| import_build_points_file ALIAS import_points_file STRING
| ( annotated |
| ( custom_annotated |
| ( header |
| ( eval_id |
| ( interface_id |
| |
| ( freeform |
| ( active_only |
| )
|
| ( sc
sparse_grid_level_sequence INTEGERLIST
) |
| ( use_derivatives |
| ) |
| ( standardized_space |
| ( logit_transform |
| export_chain_points_file STRING
| ( annotated |
| ( custom_annotated |
| ( header |
| ( eval_id |
| ( interface_id |
| |
| ( freeform |
| )
dram
| delayed_rejection
| adaptive_metropolis
CHAPTER 4. DAKOTA INPUT SPECIFICATION

| metropolis_hastings
| multilevel |
| rng
| mt19937
| rnum2
|
| pre_solve
| sqp
| nip
| none
|
| proposal_covariance
| ( derivatives
| proposal_updates INTEGER )
| prior
|
| ( values REALIST
diagonal
| matrix
)
|
| ( filename STRING
diagonal
| matrix
)
|
| gpmsa
| chain_samples ALIAS samples INTEGER
| seed INTEGER > 0 |
| build_samples INTEGER
| import_build_points_file ALIAS import_points_file STRING
| annotated
|
| ( custom_annotated
| header ]
| eval_id ]
| interface_id ]
|
| ( freeform
|
| standardized_space ]
| logit_transform ]
| gpmsa_normalize ]
| export_chain_points_file STRING
| annotated
|
| ( custom_annotated
| header ]
| eval_id ]
| interface_id ]
|
| ( freeform
|
| dram
| delayed_rejection
| adaptive_metropolis
| metropolis_hastings ]
4.4. INPUT SPEC SUMMARY

```plaintext
[ rng
  mt19937
  | rnum2
 ]
[ proposal_covariance
  ( derivatives
  [ proposal_updates INTEGER ]
 )
  | prior
  |
  ( values REALIST
diagonal
  | matrix
  )
  |
  ( filename STRING
diagonal
  | matrix
  )
]
[ options_file STRING ]
)
)

| wasabi
[ seed INTEGER > 0 ]
[ emulator
  ( gaussian_process ALIAS kriging
   surfpack
   | dakota
  [ build_samples INTEGER ]
  [ posterior_adaptive ]
  [ import_build_points_file ALIAS import_points_file STRING
    [ annotated
      |
      ( custom_annotated
        [ header ]
        [ eval_id ]
        [ interface_id ]
      )
    ]
    |
    ( freeform
      [ active_only ]
    )
  ]
  )
)
)
| pce
sparse_grid_level_sequence INTEGERLIST
|
{ expansion_order_sequence INTEGERLIST
collocation_points_sequence INTEGERLIST
 | collocation_ratio REAL
| cross_validation |
| posterior_adaptive |
| import_build_points_file ALIAS import_points_file STRING
 | annotated
 | |
| { custom_annotated
  | header ]
  | eval_id ]
  | interface_id ]
| |
| |
```
CHAPTER 4. DAKOTA INPUT SPECIFICATION

{ freeform
  [ active_only ]
}

{ orthogonal_least_interpolation
  collocation_points_sequence INTEGERLIST
  [ posterior_adaptive ]
  [ import_build_points_file ALIAS import_points_file STRING
    [ annotated
      
      [ custom.annotated
        [ header ]
        [ eval_id ]
        [ interface_id ]
      ]
    ]
    [ freeform
      [ active_only ]
    ]
  ]
}

{ sc
  sparse_grid_level_sequence INTEGERLIST
  [ use_derivatives ]
}

{ standardized_space
  data_distribution
  [ gaussian
    means REALLIST
    [ covariance REALLIST
      diagonal
      | matrix
    ]
  ]
}

[ obs_data_filename STRING ]
[ posterior_density_export_filename STRING ]
[ posterior_samples_export_filename STRING ]
[ posterior_samples_import_filename STRING ]
[ generate_posterior_samples ]
[ evaluate_posterior_samples ]

{ dream
  chain_samples ALIAS samples INTEGER
  [ seed INTEGER > 0 ]
  [ chains INTEGER >= 3 ]
  [ num_or INTEGER >= 1 ]
  [ crossover_chain_pairs INTEGER >= 0 ]
  [ gr_threshold REAL > 0.0 ]
  [ jump_step INTEGER >= 0 ]
  [ emulator
    [ gaussian_process ALIAS kriging
      surfpack
      ]
  ]
  [ dakota
    [ build_samples INTEGER ]
    [ posterior_adaptive ]
    [ import_build_points_file ALIAS import_points_file STRING ]
  ]
}
4.4. INPUT SPEC SUMMARY

[ annotated
| ( custom_annotated
  [ header ]
  [ eval_id ]
  [ interface_id ]
 ]
| ( freeform
  [ active_only ]
 ]
)

| ( pce
sparse_grid_level_sequence INTEGERLIST
| ( expansion_order_sequence INTEGERLIST
collocation_points_sequence INTEGERLIST
| collocation_ratio REAL
| ( cross_validation
  [ posterior_adaptive ]
  [ import_build_points_file ALIAS import_points_file STRING
  [ annotated
  | ( custom_annotated
    [ header ]
    [ eval_id ]
    [ interface_id ]
  ]
  | ( freeform
    [ active_only ]
  ]
)
| ( orthogonal_least_interpolation
collocation_points_sequence INTEGERLIST
| posterior_adaptive
| [ import_build_points_file ALIAS import_points_file STRING
  [ annotated
  | ( custom_annotated
    [ header ]
    [ eval_id ]
    [ interface_id ]
  ]
  | ( freeform
    [ active_only ]
  ]
)
)
| ( sc
sparse_grid_level_sequence INTEGERLIST
)
| ( use_derivatives ]
)
| ( standardized_space ]
| export_chain_points_file STRING
| ( annotated
| |
( custom_annotated
  [ header ]
  [ eval_id ]
  [ interface_id ]
)
|
( freeform
|
)
[ experimental_design
  initial_samples ALIAS samples INTEGER
  num_candidates INTEGER > 0
  [ max_hifi_evaluations INTEGER >= 0 ]
  [ import_candidate_points_file STRING
    [ annotated
    ]
    [ custom_annotated
      [ header ]
      [ eval_id ]
      [ interface_id ]
    ]
    |
    ( freeform
    )
  ]
  [ calibrate_error_multipliers
    one
    | per_experiment
    | per_response
    | both
    [ hyperprior_alphas REALLIST
      hyperprior_betas REALLIST
    ]
  ]
  [ burn_in_samples INTEGER ]
  [ posterior_stats
    [ kl_divergence ]
    [ mutual_info ]
  ]
  [ model_discrepancy
    [ discrepancy_type
      gaussian_process ALIAS kriging
      | polynomial
    ]
    [ correction_order
      constant
      | linear
      | quadratic
    ]
  ]
  [ num_prediction_configs INTEGER >= 0 ]
  [ prediction_configs REALLIST ]
  [ import_prediction_configs STRING
    [ annotated
    ]
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      [ interface_id ]
    ]
    |
    ( freeform
    )
4.4. INPUT SPEC SUMMARY

[ export_discrepancy_file STRING
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      [ interface_id ]
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    | ( freeform
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  ]
  [ export_corrected_model_file STRING
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      | ( custom_annotated
      [ header ]
      [ eval_id ]
      [ interface_id ]
    )
    | ( freeform
    ]
  ]
  [ export_corrected_variance_file STRING
    [ annotated
      | ( custom_annotated
      [ header ]
      [ eval_id ]
      [ interface_id ]
    )
    | ( freeform
    ]
  ]
  [ sub_sampling_period INTEGER ]
  [ probability_levels REALLIST
    [ num_probability_levels INTEGERLIST ]
  ]
  [ convergence_tolerance REAL ]
  [ max_iterations INTEGER >= 0 ]
  [ model_pointer STRING ]
]
]
]
]
]
[dace
  grid
  | random
  | oas
  | lhs
  | oa_lhs
  | box_behnken
  | central_composite
  | samples INTEGER ]
  | seed INTEGER > 0 ]
  | main_effects ]
  | quality_metrics ]
  | variance_based_decomp
    [ drop_tolerance REAL ]
  ]
  [ fixed_seed ]
  [ symbols INTEGER ]
  [ model_pointer STRING ]
]
| fsu_cvt
| [ samples INTEGER ]
| [ seed INTEGER > 0 ]
| [ latinize ]
| [ quality_metrics ]
| [ variance_based_decomp
| [ drop_tolerance REAL ]
| ]
| [ fixed_seed ]
| [ trial_type
| [ grid
| [ halton
| [ random
| ]
| [ num_trials INTEGER ]
| [ max_iterations INTEGER >= 0 ]
| [ model_pointer STRING ]
| ]

| psuade_moat
| [ partitions INTEGERLIST ]
| [ samples INTEGER ]
| [ seed INTEGER > 0 ]
| [ model_pointer STRING ]
| ]

| local_evidence ALIAS nond_local_evidence
| [ sqp
| [ nip ]
| [ response_levels REALLIST
| [ num_response_levels INTEGERLIST ]
| [ compute
| probabilities
| [ gen_reliabilities
| [ system
| series
| parallel
| ]
| ]
| [ probability_levels REALLIST
| [ num_probability_levels INTEGERLIST ]
| ]
| [ gen_reliability_levels REALLIST
| [ num_gen_reliability_levels INTEGERLIST ]
| ]
| [ distribution
| cumulative
| complementary
| ]
| [ model_pointer STRING ]
| ]

| local_interval_est ALIAS nond_local_interval_est
| [ sqp
| [ nip ]
| [ convergence_tolerance REAL ]
| [ model_pointer STRING ]
| ]

| local_reliability ALIAS nond_local_reliability
4.4. INPUT SPEC SUMMARY

[ mpp_search
  x_taylor_mean
  | u_taylor_mean
  | x_taylor_mpp
  | u_taylor_mpp
  | x_two_point
  | u_two_point
  | no_approx
  | sqp
  | nip |
[ integration
  | first_order
  | second_order
  [ probability_refinement ALIAS sample_refinement
import
  | adapt_import
  | mm_adapt_import
  [ refinement_samples INTEGERLIST |
  | seed INTEGER > 0 |
  ]
  ]
[ response_levels REALLIST
  | num_response_levels INTEGERLIST |
[ compute
  | probabilities
  | reliabilities
  | gen_reliabilities
  [ system
  series
  | parallel
  ]
  ]
[ reliability_levels REALLIST
  | num_reliability_levels INTEGERLIST |
  ]
  [ max_iterations INTEGER >= 0 |
[ convergence_tolerance REAL |
[ final_moments
  none
  | standard
  | central |
  ]
  [ distribution
  cumulative
  | complementary
  | |
  ]
[ probability_levels REALLIST
  | num_probability_levels INTEGERLIST |
  ]
[ gen_reliability_levels REALLIST
  | num_gen_reliability_levels INTEGERLIST |
  ]
  [ model_pointer STRING |
  ]
  ]
[ global_reliability ALIAS nond_global_reliability
  | initial_samples INTEGER |
  x_gaussian_process ALIAS x_kriging
  | u_gaussian_process ALIAS u_kriging
  | surfpack
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<td>max_iterations INTEGER &gt;= 0</td>
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<td>hammersley</td>
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<td>quality_metrics</td>
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<td>variance_based_decomp</td>
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</table>
4.4. INPUT SPEC SUMMARY

[ drop_tolerance REAL ]
[ samples INTEGER ]
[ fixed_sequence ]
[ sequence_start INTEGERLIST ]
[ sequence_leap INTEGERLIST ]
[ prime_base INTEGERLIST ]
[ max_iterations INTEGER >= 0 ]
[ model_pointer STRING ]
)
|
( vector_parameter_study
  final_point REALLIST
  step_vector REALLIST
  num_steps INTEGER
  [ model_pointer STRING ]
)
|
( list_parameter_study
  list_of_points REALLIST
  [ import_points_file STRING
    [ annotated
      [ custom_annotated
        [ header ]
        [ eval_id ]
        [ interface_id ]
      ]
    ]
    [ freeform
      [ active_only ]
    ]
    [ model_pointer STRING ]
  )
)
|
( centered_parameter_study
  step_vector REALLIST
  steps_per_variable ALIAS deltas_per_variable INTEGERLIST
  [ model_pointer STRING ]
)
|
( multidim_parameter_study
  partitions INTEGERLIST
  [ model_pointer STRING ]
)
|
( richardson_extrap
  estimate_order
  converge_order
  converge_qoi
  [ refinement_rate REAL ]
  [ convergence_tolerance REAL ]
  [ max_iterations INTEGER >= 0 ]
  [ model_pointer STRING ]
)

KEYWORD model
[ id_model STRING ]
( single ALIAS simulation
  [ interface_pointer STRING ]
  [ solution_level_control STRING ]
CHAPTER 4. DAKOTA INPUT SPECIFICATION

```
solution_level_cost REALLIST

{ surrogate
  [ id_surrogates INTEGERLIST ]

  { global
    { gaussian_process ALIAS kriging
      { dakota
        [ point_selection ]
        [ trend
          constant
          | linear
          | reduced_quadratic
          |
        ]
      }
    }
    { surfpack
      [ trend
        constant
        | linear
        | reduced_quadratic
        | quadratic
        |
      ]
      { optimization_method STRING ]
      { max_trials INTEGER > 0 ]
      { nugget REAL > 0 ]
      { find_nugget INTEGER ]
      { correlation_lengths REALLIST ]
      export_model
      [ filename_prefix STRING ]
      [ formats
        [ text_archive ]
        [ binary_archive ]
        [ algebraic_file ]
        [ algebraic_console ]
      ]
    }
  }
  }

  { mars
    [ max_bases INTEGER ]
    [ interpolation
      linear
      | cubic
      ]
    [ export_model
      [ filename_prefix STRING ]
      [ formats
        [ text_archive ]
        [ binary_archive ]
      ]
    ]
  }

  { moving_least_squares
    [ basis_order ALIAS poly_order INTEGER >= 0 ]
    [ weight_function INTEGER ]
    [ export_model
      [ filename_prefix STRING ]
      [ formats
```
4.4. INPUT SPEC SUMMARY

```
[ text_archive ]
[ binary_archive ]
)
)
(neural_network
  [ max_nodes ALIAS nodes INTEGER ]
  [ range REAL ]
  [ random_weight INTEGER ]
  [ export_model
    [ filename_prefix STRING ]
    [ formats
      [ text_archive ]
      [ binary_archive ]
      [ algebraic_file ]
      [ algebraic_console ]
    )
  ]
)
(radial_basis
  [ bases INTEGER ]
  [ max_pts INTEGER ]
  [ min_partition INTEGER ]
  [ max_subsets INTEGER ]
  [ export_model
    [ filename_prefix STRING ]
    [ formats
      [ text_archive ]
      [ binary_archive ]
      [ algebraic_file ]
      [ algebraic_console ]
    )
  ]
)
(polynomial
  basis_order INTEGER >= 0
  | linear
  | quadratic
  | cubic
  [ export_model
    [ filename_prefix STRING ]
    [ formats
      [ text_archive ]
      [ binary_archive ]
      [ algebraic_file ]
      [ algebraic_console ]
    )
  ]
)
(domain_decomposition
  [ cell_type STRING ]
  [ support_layers INTEGER ]
  [ discontinuity_detection
    jump_threshold REAL
    | gradient_threshold REAL
  ]
)
[ total_points INTEGER
  | minimum_points
```
CHAPTER 4. DAKOTA INPUT SPECIFICATION

| recommended_points |
| ( dace_method_pointer STRING |
| auto_refinement |
| [ max_iterations INTEGER > 0 ] |
| [ max_function_evaluations INTEGER > 0 ] |
| [ convergence_tolerance REAL ] |
| [ soft_convergence_limit INTEGER >= 0 ] |
| [ cross_validation_metric STRING |
| [ folds INTEGER > 0 ] |
| ] |
| ) |
| actual_model_pointer STRING |
| [ reuse_points ALIAS reuse_samples |
| all |
| region |
| none |
| ] |
| import_build_points_file ALIAS import_points_file ALIAS samples_file STRING |
| [ annotated |
| ] |
| [ custom_annotated |
| header ] |
| [ eval_id ] |
| [ interface_id ] |
| ] |
| [ freeform |
| active_only ] |
| ] |
| export_approx_points_file ALIAS export_points_file STRING |
| [ annotated |
| ] |
| [ custom_annotated |
| header ] |
| [ eval_id ] |
| [ interface_id ] |
| ] |
| [ freeform |
| ] |
| use_derivatives |
| [ correction |
| zeroth_order |
| first_order |
| second_order |
| additive |
| multiplicative |
| combined |
| ] |
| metrics ALIAS diagnostics STRINGLIST |
| [ cross_validation |
| [ folds INTEGER |
| percent REAL ] |
| ] |
| [ press ] |
| ] |
| import_challenge_points_file ALIAS challenge_points_file STRING |
| [ annotated |
| ] |
| [ custom_annotated |
| header ] |
4.4. INPUT SPEC SUMMARY

[ eval_id ]
[ interface_id ]
]
|
| freeform
| active_only |
]
|
| multipoint
| tana
| actual_model_pointer STRING |
]
|
| local
| taylor_series
| actual_model_pointer STRING |
]
|
| hierarchical
| ordered_model_fidelities ALIAS model_fidelity_sequence STRINGLIST |
| correction
| zeroth_order
| first_order
| second_order
| additive
| multiplicative
| combined |
]
|
| nested
| [ optional_interface_pointer STRING |
| [ optional_interface_responses_pointer STRING ] |
|
| sub_method_pointer STRING |
| [ iterator_servers INTEGER > 0 ] |
| [ iterator_scheduling |
| master |
| peer |
| [ processors_per_iterator INTEGER > 0 ] |
| [ primary_variable_mapping STRINGLIST ] |
| [ secondary_variable_mapping STRINGLIST ] |
| [ primary_response_mapping REALLIST ] |
| [ secondary_response_mapping REALLIST ] |
]
|
| active_subspace ALIAS subspace
| actual_model_pointer STRING |
| [ initial_samples INTEGER ] |
| [ sample_type |
| lha |
| random |
| ] |
| truncation_method |
| [ bing_li ] |
| [ constantine ] |
| [ energy |
| [ truncation_tolerance REAL ] |
| { cross_validation
|   [ minimum
|     relative
|     decrease ]
|   [ relative_tolerance REAL ]
|   [ decrease_tolerance REAL ]
|   [ max_rank INTEGER ]
|   [ exhaustive ]
| }
| { dimension INTEGER ]
| { bootstrap_samples INTEGER ]
| { build_surrogate
|   [ refinement_samples INTEGERLIST ]
| }
| { normalization
|   mean_value
|   | mean_gradient
|   | local_gradient
| }
| { adapted_basis
| actual_model_pointer STRING
| sparse_grid_level INTEGER
| { expansion_order INTEGER
|   collocation_ratio REAL
| }
| { random_field
|   [ build_source
|     rf_data_file STRING
|     dace_method_pointer STRING
|   ]
|   [ analytic_covariance
|     squared_exponential
|     exponential
|   ]
| { expansion_form
|     karhunen_loeve
|     | principal_components
|   ]
| { expansion_bases INTEGER ]
| { truncation_tolerance REAL ]
| propagation_model_pointer STRING
| }
| { variables_pointer STRING ]
| { responses_pointer STRING ]
| { hierarchical_tagging ]

KEYWORD12 variables
| { id_variables STRING ]
| { active
|   all
|   | design
|   | uncertain
|   | aleatory
|   | epistemic
### 4.4. INPUT SPEC SUMMARY

- **state**
  - mixed
  - relaxed
- **continuous_design**
  - initial_point ALIAS cdv_initial_point REALLIST
  - lower_bounds ALIAS cdv_lower_bounds REALLIST
  - upper_bounds ALIAS cdv_upper_bounds REALLIST
  - scale_types ALIAS cdv_scale_types STRINGLIST
  - scales ALIAS cdv_scales REALLIST
  - descriptors ALIAS cdv_descriptors STRINGLIST
- **discrete_design_range**
  - initial_point ALIAS ddv_initial_point INTEGERLIST
  - lower_bounds ALIAS ddv_lower_bounds INTEGERLIST
  - upper_bounds ALIAS ddv_upper_bounds INTEGERLIST
  - descriptors ALIAS ddv_descriptors STRINGLIST
- **discrete_design_set**
  - integer ALIAS num_set_values INTEGERLIST
  - elements ALIAS set_values INTEGERLIST
  - adjacency_matrix ALIAS STRINGLIST
  - initial_point INTEGERLIST
  - descriptors STRINGLIST
- **string**
  - elements_per_variable ALIAS num_set_values INTEGERLIST
  - elements ALIAS set_values STRINGLIST
  - adjacency_matrix ALIAS STRINGLIST
  - initial_point STRINGLIST
  - descriptors STRINGLIST
- **real**
  - elements_per_variable ALIAS num_set_values INTEGERLIST
  - elements ALIAS set_values REALLIST
  - adjacency_matrix ALIAS STRINGLIST
  - initial_point REALLIST
  - descriptors STRINGLIST
- **normal_uncertain**
  - means ALIAS nuv_means REALLIST
  - std_deviations ALIAS nuv_std_deviations REALLIST
  - lower_bounds ALIAS nuv_lower_bounds REALLIST
  - upper_bounds ALIAS nuv_upper_bounds REALLIST
  - initial_point REALLIST
  - descriptors ALIAS nuv_descriptors STRINGLIST
- **lognormal_uncertain**
  - lambdas ALIAS lnuv_lambdas REALLIST
  - zetas ALIAS lnuv_zetas REALLIST
  - means ALIAS lnuv_means REALLIST
  - std_deviations ALIAS lnuv_std_deviations REALLIST
  - error_factors ALIAS lnuv_error_factors REALLIST
[ lower_bounds ALIAS lnuv_lower_bounds REALLIST ]
[ upper_bounds ALIAS lnuv_upper_bounds REALLIST ]
[ initial_point REALLIST ]
[ descriptors ALIAS lnuv_descriptors STRINGLIST ]
]

[ uniform_uncertain INTEGER > 0
lower_bounds ALIAS uuv_lower_bounds REALLIST
upper_bounds ALIAS uuv_upper_bounds REALLIST
[ initial_point REALLIST ]
[ descriptors ALIAS uuv_descriptors STRINGLIST ]
]

[ loguniform_uncertain INTEGER > 0
lower_bounds ALIAS luuv_lower_bounds REALLIST
upper_bounds ALIAS luuv_upper_bounds REALLIST
[ initial_point REALLIST ]
[ descriptors ALIAS luuv_descriptors STRINGLIST ]
]

[ triangular_uncertain INTEGER > 0
modes ALIAS tuv_modes REALLIST
lower_bounds ALIAS tuv_lower_bounds REALLIST
upper_bounds ALIAS tuv_upper_bounds REALLIST
[ initial_point REALLIST ]
[ descriptors ALIAS tuv_descriptors STRINGLIST ]
]

[ exponential_uncertain INTEGER > 0
betas ALIAS euv_betas REALLIST
[ initial_point REALLIST ]
[ descriptors ALIAS euv_descriptors STRINGLIST ]
]

[ beta_uncertain INTEGER > 0
alphas ALIAS buv_alphas REALLIST
betas ALIAS buv_betas REALLIST
lower_bounds ALIAS buv_lower_bounds REALLIST
upper_bounds ALIAS buv_upper_bounds REALLIST
[ initial_point REALLIST ]
[ descriptors ALIAS buv_descriptors STRINGLIST ]
]

[ gamma_uncertain INTEGER > 0
alphas ALIAS gauv_alphas REALLIST
betas ALIAS gauv_betas REALLIST
[ initial_point REALLIST ]
[ descriptors ALIAS gauv_descriptors STRINGLIST ]
]

[ gumbel_uncertain INTEGER > 0
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betas ALIAS guuv_betas REALLIST
[ initial_point REALLIST ]
[ descriptors ALIAS guuv_descriptors STRINGLIST ]
]

[ frechet_uncertain INTEGER > 0
alphas ALIAS fuv_alphas REALLIST
betas ALIAS fuv_betas REALLIST
[ initial_point REALLIST ]
[ descriptors ALIAS fuv_descriptors STRINGLIST ]
]

[ weibull_uncertain INTEGER > 0
alphas ALIAS wuv_alphas REALLIST
betas ALIAS wuv_betas REALLIST
[ initial_point REALLIST ]
[ descriptors ALIAS wuv_descriptors STRINGLIST ]
]

[ histogram_bin_uncertain INTEGER > 0
4.4. INPUT SPEC SUMMARY

[ pairs_per_variable ALIAS num_pairs INTEGERLIST ]
abscissas ALIAS huv_bin_abscissas REALLIST
ordinates ALIAS huv_bin_ordinates REALLIST
[ counts ALIAS huv_bin_counts REALLIST
  [ initial_point REALLIST ]
  [ descriptors ALIAS huv_bin_descriptors STRINGLIST ]
]

[ poisson_uncertain INTEGER > 0
  lambdas REALLIST
  [ initial_point INTEGERLIST ]
  [ descriptors STRINGLIST ]
]

[ binomial_uncertain INTEGER > 0
  probability_per_trial ALIAS prob_per_trial REALLIST
  num_trials INTEGERLIST
  [ initial_point INTEGERLIST ]
  [ descriptors STRINGLIST ]
]

[ negative_binomial_uncertain INTEGER > 0
  probability_per_trial ALIAS prob_per_trial REALLIST
  num_trials INTEGERLIST
  [ initial_point INTEGERLIST ]
  [ descriptors STRINGLIST ]
]

[ geometric_uncertain INTEGER > 0
  probability_per_trial ALIAS prob_per_trial REALLIST
  [ initial_point INTEGERLIST ]
  [ descriptors STRINGLIST ]
]

[ hypergeometric_uncertain INTEGER > 0
  total_population INTEGERLIST
  selected_population INTEGERLIST
  num_drawn INTEGERLIST
  [ initial_point INTEGERLIST ]
  [ descriptors STRINGLIST ]
]

[ histogram_point_uncertain
  [ pairs_per_variable ALIAS num_pairs INTEGERLIST ]
  abscissas INTEGERLIST
  counts REALLIST
  [ initial_point INTEGERLIST ]
  [ descriptors STRINGLIST ]
]

[ string INTEGER > 0
  [ pairs_per_variable ALIAS num_pairs INTEGERLIST ]
  abscissas STRINGLIST
  counts REALLIST
  [ initial_point STRINGLIST ]
  [ descriptors STRINGLIST ]
]

[ real INTEGER > 0
  [ pairs_per_variable ALIAS num_pairs INTEGERLIST ]
  abscissas REALLIST
  counts REALLIST
  [ initial_point REALLIST ]
  [ descriptors STRINGLIST ]
]

[ uncertain_correlation_matrix REALLIST ]
[ continuous_interval_uncertain ALIAS interval_uncertain INTEGER > 0
  [ num_intervals ALIAS iuv_num_intervals INTEGERLIST ]
]
CHAPTER 4. DAKOTA INPUT SPECIFICATION

[ interval_probabilities ALIAS interval_probs ALIAS iuv_interval_probs REALLIST ]
lower_bounds REALLIST
upper_bounds REALLIST
[ initial_point REALLIST ]
[ descriptors ALIAS iuv_descriptors STRINGLIST ]
)
[ discrete_interval_uncertain ALIAS discrete_uncertain_range INTEGER > 0
[ num_intervals INTEGERLIST ]
[ interval_probabilities ALIAS interval_probs ALIAS range_probabilities ALIAS range_probs REALLIST ]
lower_bounds INTEGERLIST
upper_bounds INTEGERLIST
[ initial_point INTEGERLIST ]
[ descriptors STRINGLIST ]
)
[ discrete_uncertain_set
[ integer INTEGER > 0
[ elements_per_variable ALIAS num_set_values INTEGERLIST ]
elements ALIAS set_values INTEGERLIST
[ categorical STRINGLIST ]
[ initial_point INTEGERLIST ]
[ descriptors STRINGLIST ]
)
[ string INTEGER > 0
[ elements_per_variable ALIAS num_set_values INTEGERLIST ]
elements ALIAS set_values STRINGLIST
[ categorical STRINGLIST ]
[ initial_point STRINGLIST ]
[ descriptors STRINGLIST ]
)
[ real INTEGER > 0
[ elements_per_variable ALIAS num_set_values INTEGERLIST ]
elements ALIAS set_values REALLIST
[ categorical STRINGLIST ]
[ initial_point REALLIST ]
[ descriptors STRINGLIST ]
)
[ continuous_state INTEGER > 0
[ initial_state ALIAS csv_initial_state REALLIST ]
lower_bounds ALIAS csv_lower_bounds REALLIST
upper_bounds ALIAS csv_upper_bounds REALLIST
[ descriptors ALIAS csv_descriptors STRINGLIST ]
)
[ discrete_state_range INTEGER > 0
[ initial_state ALIAS dsv_initial_state INTEGERLIST ]
lower_bounds ALIAS dsv_lower_bounds INTEGERLIST
upper_bounds ALIAS dsv_upper_bounds INTEGERLIST
[ descriptors ALIAS dsv_descriptors STRINGLIST ]
)
[ discrete_state_set
[ integer INTEGER > 0
[ elements_per_variable ALIAS num_set_values INTEGERLIST ]
elements ALIAS set_values INTEGERLIST
[ categorical STRINGLIST ]
[ initial_state INTEGERLIST ]
[ descriptors STRINGLIST ]
]
[ string INTEGER > 0
[ elements_per_variable ALIAS num_set_values INTEGERLIST ]
elements ALIAS set_values STRINGLIST
4.4. INPUT SPEC SUMMARY

[ initial_state STRINGLIST ]
[ descriptors STRINGLIST ]
]
[ real INTEGER > 0
[ elements_per_variable ALIAS num_set_values INTEGERLIST ]
elements ALIAS set_values REALLIST
[ categorical STRINGLIST ]
[ initial_state REALLIST ]
[ descriptors STRINGLIST ]
]
]
[ linear_inequality_constraint_matrix REALLIST ]
[ linear_inequality_lower_bounds REALLIST ]
[ linear_inequality_upper_bounds REALLIST ]
[ linear_inequality_scale_types STRINGLIST ]
[ linear_inequality_scales REALLIST ]
[ linear_equality_constraint_matrix REALLIST ]
[ linear_equality_targets REALLIST ]
[ linear_equality_scale_types STRINGLIST ]
[ linear_equality_scales REALLIST ]

KEYWORD12 interface
[ id_interface STRING ]
[ analysis_drivers STRINGLIST ]
[ input_filter STRING ]
[ output_filter STRING ]
( system
[ parameters_file STRING ]
[ results_file STRING ]
[ file_tag ]
[ file_save ]
[ labeled ]
[ aprepro ALIAS dprepro ]
[ work_directory
[ named STRING ]
[ directory_tag ALIAS dir_tag ]
[ directory_save ALIAS dir_save ]
[ link_files STRINGLIST ]
[ copy_files STRINGLIST ]
[ replace ]
]
[ allow_existing_results ]
[ verbatim ]
)
)

[ fork
[ parameters_file STRING ]
[ results_file STRING ]
[ file_tag ]
[ file_save ]
[ labeled ]
[ aprepro ALIAS dprepro ]
[ work_directory
[ named STRING ]
[ directory_tag ALIAS dir_tag ]
[ directory_save ALIAS dir_save ]
[ link_files STRINGLIST ]
[ copy_files STRINGLIST ]
[ replace ]
]
[ allow_existing_results ]
[ verbatim ]
]


) |  
  ( direct  
    [ processors_per_analysis INTEGER > 0 ]  
  ) |  
  matlab  
  |  
  ( python  
    [ numpy ]  
  ) |  
  scilab  
  |  
  grid  
    [ analysis_components STRINGLIST ]  
  ) ]  
  [ algebraic_mappings STRING ]  
  [ failure_capture  
    abort  
    | retry INTEGER  
    | recover REALIST  
    | continuation  
  ) |  
  [ deactivate  
    [ active_set_vector ]  
    [ evaluation_cache ]  
    [ strict_cache_equality  
      [ cache_tolerance REAL ]  
    ] |  
    [ restart_file ]  
  ) ]  
  [ asynchronous  
    [ evaluation_concurrency INTEGER > 0 ]  
    [ local_evaluation_scheduling  
      dynamic  
      | static  
    ] |  
    [ analysis_concurrency INTEGER > 0 ]  
  ) ]  
  [ evaluation_servers INTEGER > 0 ]  
  [ evaluation_scheduling  
    master  
    | ( peer  
      dynamic  
      | static  
    )  
  ] ]  
  [ processors_per_evaluation INTEGER > 0 ]  
  [ analysis_servers INTEGER > 0 ]  
  [ analysis_scheduling  
    master  
    | peer  
  ] ]  

KEYWORD12 responses 
  [ id_responses STRING ]  
  [ descriptors ALIAS response_descriptors STRINGLIST ]  
  [ objective_functions ALIAS num_objective_functions INTEGER >= 0  
    [ sense STRINGLIST ]  
    [ primary_scale_types ALIAS objective_function_scale_types STRINGLIST ]  
    [ primary_scales ALIAS objective_function_scales REALLIST ]  
    [ weights ALIAS multi_objective_weights REALLIST ]  
    [ nonlinear_inequality_constraints ALIAS num_nonlinear_inequality_constraints INTEGER >= 0  


4.4. INPUT SPEC SUMMARY

[ lower_bounds ALIAS nonlinear_inequality_lower_bounds REALLIST ]
[ upper_bounds ALIAS nonlinear_inequality_upper_bounds REALLIST ]
[ scale_types ALIAS nonlinear_inequality_scale_types STRINGLIST ]
[ scales ALIAS nonlinear_inequality_scales REALLIST ]

[ nonlinear_inequality_constraints ALIAS num_nonlinear_inequality_constraints INTEGER >= 0
[ targets ALIAS nonlinear_inequality_targets REALLIST ]
[ scale_types ALIAS nonlinear_inequality_scale_types STRINGLIST ]
[ scales ALIAS nonlinear_inequality_scales REALLIST ]

[ scalar_objectives ALIAS num_scalar_objectives INTEGER >= 0 ]
[ field_objectives ALIAS num_field_objectives INTEGER >= 0
lengths INTEGERLIST
[ num_coordinates_per_field INTEGERLIST ]
[ read_field_coordinates ]
]

[ calibration_terms ALIAS least_squares_terms ALIAS num_least_squares_terms INTEGER >= 0
[ scalar_calibration_terms INTEGER >= 0 ]
[ field_calibration_terms INTEGER >= 0
lengths INTEGERLIST
[ num_coordinates_per_field INTEGERLIST ]
[ read_field_coordinates ]
]

[ primary_scale_types ALIAS calibration_term_scale_types ALIAS least_squares_term_scale_types STRINGLIST ]
[ primary_scales ALIAS calibration_term_scales ALIAS least_squares_term_scales REALLIST ]
[ weights ALIAS calibration_weights ALIAS least_squares_weights REALLIST ]

[ calibration_data
[ num_experiments INTEGER >= 0 ]
[ num_config_variables INTEGER >= 0 ]
[ variance_type STRINGLIST ]
[ scalar_data_file STRING
annotated
]
[ custom_annotated
[ header ]
[ exp_id ]
]
[ freeform
[ interpolate ]
]

[ calibration_data_file ALIAS least_squares_data_file STRING
annotated
]
[ custom_annotated
[ header ]
[ exp_id ]
]
[ freeform
[ num_experiments INTEGER >= 0 ]
[ num_config_variables INTEGER >= 0 ]
[ variance_type STRINGLIST ]
]

[ nonlinear_inequality_constraints ALIAS num_nonlinear_inequality_constraints INTEGER >= 0
[ lower_bounds ALIAS nonlinear_inequality_lower_bounds REALLIST ]
[ upper_bounds ALIAS nonlinear_inequality_upper_bounds REALLIST ]
[ scale_types ALIAS nonlinear_inequality_scale_types STRINGLIST ]

[ scales ALIAS nonlinear_inequality_scales REALLIST ]

[ nonlinear_inequality_constraints ALIAS num_nonlinear_inequality_constraints INTEGER >= 0
  [ targets ALIAS nonlinear_inequality_targets REALLIST ]
  [ scale_types ALIAS nonlinear_inequality_scale_types STRINGLIST ]
  [ scales ALIAS nonlinear_inequality_scales REALLIST ]
]

| response_functions ALIAS num_response_functions INTEGER >= 0
| scalar_responses ALIAS num_scalar_responses INTEGER >= 0
| field_responses ALIAS num_field_responses INTEGER >= 0
  lengths INTEGERLIST
  [ num_coordinates_per_field INTEGERLIST ]
  [ read_field_coordinates ]
|
no_gradients
| analytic_gradients
| mixed_gradients
  id_numerical_gradients INTEGERLIST
  id_analytic_gradients INTEGERLIST
    [ method_source ]
    [ { dakota
      [ ignore_bounds ]
      [ relative
      | absolute
      | bounds ]
    ]
    | vendor ]
    [ interval_type ]
    [ forward
    | central ]
    [ fd_step_size ALIAS fd_gradient_step_size REALLIST ]
  )
|
( numerical_gradients
  [ method_source ]
  [ { dakota
    [ ignore_bounds ]
    [ relative
    | absolute
    | bounds ]
  ]
  | vendor ]
  [ interval_type ]
  [ forward
  | central ]
  [ fd_step_size ALIAS fd_gradient_step_size REALLIST ]
)
no_hessians
| numerical_hessians
  [ fd_step_size ALIAS fd_hessian_step_size REALLIST ]
  [ relative
  | absolute
  | bounds ]
  [ forward
  | central ]
)
4.4. INPUT SPEC SUMMARY

```plaintext
( quasi_hessians
  ( bfgs
    ( damped )
  )
  | sr1
 )
| analytic_hessians
|)
( mixed_hessians
  [ id_numerical_hessians INTEGERLIST
    [ fd_step_size ALIAS fd_hessian_step_size REALLIST ]
  ]
  [ relative
    | absolute
    | bounds ]
  [ forward
    | central ]
  [ id_quasi_hessians INTEGERLIST
    [ bfgs
      ( damped )
    ]
    | sr1
  ]
  [ id_analytic_hessians INTEGERLIST ]
)
```
Chapter 5

Topics Area

This page introduces the user to the topics used to organize keywords.

- admin
- dakota.IO
- dakota_concepts
- models
- variables
- responses
- interface
- methods
- advanced_topics
- packages

5.1 admin

Description
This is only for management while ref man is under construction

Related Topics
- empty
- problem
- not_yet_reviewed
Related Keywords
5.1.1 empty
Description
This topic tracks the keywords which do not have content in the reference manual

Related Topics
Related Keywords
5.1.2 problem
Description
empty

Related Topics
Related Keywords
5.1.3 not_yet_reviewed
Description
Not yet reviewed.

Related Topics
Related Keywords
5.2 dakota_IO
Description
Keywords and Concepts relating inputs to Dakota and outputs from Dakota

Related Topics
- dakota_inputs
- dakota_output
- file_formats

Related Keywords
- error_file : Base filename for error redirection
- output_file : Base filename for output redirection
- input : Base filename for post-run mode data input
5.2. DAKOTA.IO

- **output**: Base filename for post-run mode data output
- **input**: Base filename for pre-run mode data input
- **output**: Base filename for pre-run mode data output
- **read_restart**: Base filename for restart file read
- **stop_restart**: Evaluation ID number at which to stop reading restart file
- **input**: Base filename for run mode data input
- **output**: Base filename for run mode data output
- **write_restart**: Base filename for restart file write

5.2.1 dakota_inputs

Description
empty

Related Topics
- **block**
- **data_import_capabilities**

Related Keywords

5.2.2 block

Description
A block is the highest level of keyword organization in Dakota. There are currently 6 blocks in the Dakota input spec:

Related Topics
- **block_identifier**
- **block_pointer**

Related Keywords
- **environment**: Top-level settings for Dakota execution
- **interface**: Specifies how function evaluations will be performed in order to map the variables into the responses.
- **method**: Begins Dakota method selection and behavioral settings.
- **model**: Specifies how variables are mapped into a set of responses
- **responses**: Description of the model output data returned to Dakota upon evaluation of an interface.
- **variables**: Specifies the parameter set to be iterated by a particular method.
block_identifier

Description
empty

Related Topics

Related Keywords
- id_interface : Name the interface block; helpful when there are multiple
- id_method : Name the method block; helpful when there are multiple
- id_model : Give the model block an identifying name, in case of multiple model blocks
- id_responses : Name the responses block; helpful when there are multiple
- id_variables : Name the variables block; helpful when there are multiple

block_pointer

Description
See block_pointer for details about pointers.

Related Topics

Related Keywords
- top_method_pointer : Identify which method leads the Dakota study
- model_pointer : Identifier for model block to be used by a method
- model_pointer : Identifier for model block to be used by a method
- model_pointer : Identifier for model block to be used by a method
- model_pointer : Identifier for model block to be used by a method
- model_pointer : Identifier for model block to be used by a method
- model_pointer : Pointer to sub-method to apply to a surrogate or branch-and-bound sub-problem
- model_pointer : Identifier for model block to be used by a method
- model_pointer : Identifier for model block to be used by a method
- model_pointer : Identifier for model block to be used by a method
- model_pointer : Identifier for model block to be used by a method
- model_pointer : Identifier for model block to be used by a method
5.2. DAKOTA_IO

- `model_pointer` : Identifier for model block to be used by a method
- `model_pointer` : Identifier for model block to be used by a method
- `model_pointer` : Identifier for model block to be used by a method
- `model_pointer` : Identifier for model block to be used by a method
- `model_pointer` : Identifier for model block to be used by a method
- `model_pointer` : Identifier for model block to be used by a method
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- `model_pointer` : Identifier for model block to be used by a method
- `model_pointer` : Identifier for model block to be used by a method
- `model_pointer` : Identifier for model block to be used by a method
- `model_pointer` : Identifier for model block to be used by a method
- `model_pointer` : Identifier for model block to be used by a method
- `model_pointer` : Identifier for model block to be used by a method
- `model_pointer_list` : Associate models with method names
- `method_pointer_list` : Pointers to methods to execute sequentially or collaboratively
- `global_model_pointer` : Pointer to model used by global method
- `global_method_pointer` : Pointer to global method
- `local_model_pointer` : Pointer to model used by local method
- `local_method_pointer` : Pointer to local method
- `model_pointer_list` : Associate models with method names
- `method_pointer_list` : Pointers to methods to execute sequentially or collaboratively
• `model_pointer` : Identifier for model block to be used by a method
• `model_pointer` : Identifier for model block to be used by a method
• `model_pointer` : Identifier for model block to be used by a method
• `model_pointer` : Identifier for model block to be used by a method
• `model_pointer` : Identifier for model block to be used by a method
• `method_pointer` : Pointer to sub-method to run from each starting point
• `model_pointer` : Identifier for model block to be used by a method
• `model_pointer` : Identifier for model block to be used by a method
• `model_pointer` : Identifier for model block to be used by a method
• `model_pointer` : Identifier for model block to be used by a method
• `model_pointer` : Identifier for model block to be used by a method
• `model_pointer` : Identifier for model block to be used by a method
• `model_pointer` : Identifier for model block to be used by a method
• `model_pointer` : Identifier for model block to be used by a method
• `model_pointer` : Identifier for model block to be used by a method
• `model_pointer` : Identifier for model block to be used by a method
• `model_pointer` : Identifier for model block to be used by a method
• `model_pointer` : Identifier for model block to be used by a method
• `model_pointer` : Identifier for model block to be used by a method
• `model_pointer` : Identifier for model block to be used by a method
• `method_pointer` : Pointer to optimization or least-squares sub-method
• `model_pointer` : Identifier for model block to be used by a method
• `model_pointer` : Identifier for model block to be used by a method
• `model_pointer` : Identifier for model block to be used by a method
• `model_pointer` : Identifier for model block to be used by a method
• `model_pointer` : Identifier for model block to be used by a method
• `model_pointer` : Identifier for model block to be used by a method
• `model_pointer` : Identifier for model block to be used by a method
• `model_pointer` : Identifier for model block to be used by a method
• `model_pointer` : Identifier for model block to be used by a method
• `model_pointer` : Identifier for model block to be used by a method
• `model_pointer` : Identifier for model block to be used by a method
• `model_pointer` : Identifier for model block to be used by a method
• `model_pointer` : Identifier for model block to be used by a method
5.2. **DAKOTA IO**

- `model_pointer`: Identifier for model block to be used by a method
- `model_pointer`: Identifier for model block to be used by a method
- `model_pointer`: Identifier for model block to be used by a method
- `method_pointer`: Pointer to sub-method to apply to a surrogate or branch-and-bound sub-problem
- `model_pointer`: Identifier for model block to be used by a method
- `method_pointer`: Pointer to sub-method to apply to a surrogate or branch-and-bound sub-problem
- `model_pointer`: Identifier for model block to be used by a method
- `model_pointer`: Identifier for model block to be used by a method
- `actual_model_pointer`: Pointer to specify a full-space model, from which to construct a lower dimensional surrogate
- `actual_model_pointer`: Pointer to specify a "truth" model, from which to construct a surrogate
- `optional_interface_pointer`: Pointer to interface that provides non-nested responses
- `optional_interface_responses_pointer`: Pointer to responses block that defines non-nested responses
- `sub_method_pointer`: The `sub_method_pointer` specifies the method block for the sub-iterator
- `responses_pointer`: Specify which responses block will be used by this model block
- `interface_pointer`: Interface block pointer for the single model type
- `dace_method_pointer`: Specify a method to gather training data
- `actual_model_pointer`: Pointer to specify a "truth" model, from which to construct a surrogate
- `actual_model_pointer`: Pointer to specify a "truth" model, from which to construct a surrogate
- `variables_pointer`: Specify which variables block will be included with this model block

### 5.2.3 data_import_capabilities

**Description**

empty

**Related Topics**

**Related Keywords**

### 5.2.4 dakota_output

**Description**

empty
CHAPTER 5. TOPICS AREA

Related Topics

Related Keywords

- **graphics**: Display a 2D graphics window of variables and responses
- **output_precision**: Control the output precision
- **results_output**: (Experimental) Write a summary file containing the final results
- **results_output_file**: The base file name of the results file
- **tabular_data**: Write a tabular results file with variable and response history
- **tabular_data_file**: File name for tabular data output
- **output**: Control how much method information is written to the screen and output file

5.2.5 file formats

Description

See sections "Inputs to Dakota" and "Outputs from Dakota" in the Dakota User’s Manual[4].

Related Topics

Related Keywords

- **annotated**: Selects annotated tabular file format
- **custom_annotated**: Selects custom-annotated tabular file format
- **freeform**: Selects freeform file format
- **annotated**: Selects annotated tabular file format
- **custom_annotated**: Selects custom-annotated tabular file format
- **freeform**: Selects freeform file format
- **annotated**: Selects annotated tabular file format
- **custom_annotated**: Selects custom-annotated tabular file format
- **freeform**: Selects freeform file format
- **aprepro**: Write parameters files in APREPRO syntax
- **labeled**: Requires correct function value labels in results file
- **aprepro**: Write parameters files in APREPRO syntax
- **labeled**: Requires correct function value labels in results file
- **annotated**: Selects annotated tabular file format
- **custom_annotated**: Selects custom-annotated tabular file format
5.2. **DAKOTA_IO**

- **freeform**: Selects freeform file format
- **active_only**: Import only active variables from tabular data file
- **annotated**: Selects annotated tabular file format
- **custom_annotated**: Selects custom-annotated tabular file format
- **freeform**: Selects freeform file format
- **active_only**: Import only active variables from tabular data file
- **annotated**: Selects annotated tabular file format
- **custom_annotated**: Selects custom-annotated tabular file format
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- **active_only**: Import only active variables from tabular data file
- **annotated**: Selects annotated tabular file format
- **custom_annotated**: Selects custom-annotated tabular file format
- **freeform**: Selects freeform file format
- **active_only**: Import only active variables from tabular data file
- **annotated**: Selects annotated tabular file format
- **custom_annotated**: Selects custom-annotated tabular file format
- **freeform**: Selects freeform file format
- `custom_annotated`: Selects custom-annotated tabular file format
- `freeform`: Selects freeform file format
- `annotated`: Selects annotated tabular file format
- `custom_annotated`: Selects custom-annotated tabular file format
- `freeform`: Selects freeform file format
- `annotated`: Selects annotated tabular file format
- `custom_annotated`: Selects custom-annotated tabular file format
- `freeform`: Selects freeform file format
- `annotated`: Selects annotated tabular file format
- `custom_annotated`: Selects custom-annotated tabular file format
- `freeform`: Selects freeform file format
- `active_only`: Import only active variables from tabular data file
- `annotated`: Selects annotated tabular file format
- `custom_annotated`: Selects custom-annotated tabular file format
- `freeform`: Selects freeform file format
- `active_only`: Import only active variables from tabular data file
- `annotated`: Selects annotated tabular file format
- `custom_annotated`: Selects custom-annotated tabular file format
- `freeform`: Selects freeform file format
- `annotated`: Selects annotated tabular file format
- `custom_annotated`: Selects custom-annotated tabular file format
- `freeform`: Selects freeform file format
- `annotated`: Selects annotated tabular file format
- `custom_annotated`: Selects custom-annotated tabular file format
- `freeform`: Selects freeform file format
- `annotated`: Selects annotated tabular file format
- `custom_annotated`: Selects custom-annotated tabular file format
- `freeform`: Selects freeform file format
- `annotated`: Selects annotated tabular file format
- `custom_annotated`: Selects custom-annotated tabular file format
- `freeform`: Selects freeform file format
- `annotated`: Selects annotated tabular file format
- `custom_annotated`: Selects custom-annotated tabular file format
- `freeform`: Selects freeform file format
- `annotated`: Selects annotated tabular file format
- `custom_annotated`: Selects custom-annotated tabular file format
- `freeform`: Selects freeform file format
5.2. **DAKOTA_IO**

- **active_only**: Import only active variables from tabular data file
- **annotated**: Selects annotated tabular file format
- **custom_annotated**: Selects custom-annotated tabular file format
- **freeform**: Selects freeform file format
- **active_only**: Import only active variables from tabular data file
- **annotated**: Selects annotated tabular file format
- **custom_annotated**: Selects custom-annotated tabular file format
- **freeform**: Selects freeform file format
- **annotated**: Selects annotated tabular file format
- **custom_annotated**: Selects custom-annotated tabular file format
- **freeform**: Selects freeform file format
- **annotated**: Selects annotated tabular file format
- **custom_annotated**: Selects custom-annotated tabular file format
- **freeform**: Selects freeform file format
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- **freeform**: Selects freeform file format
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- **custom_annotated**: Selects custom-annotated tabular file format
- **freeform**: Selects freeform file format
- **annotated**: Selects annotated tabular file format
- `custom_annotated`: Selects custom-annotated tabular file format
- `freeform`: Selects freeform file format
- `active_only`: Import only active variables from tabular data file
- `annotated`: Selects annotated tabular file format
- `custom_annotated`: Selects custom-annotated tabular file format
- `freeform`: Selects freeform file format
- `annotated`: Selects annotated tabular file format
- `custom_annotated`: Selects custom-annotated tabular file format
- `freeform`: Selects freeform file format
- `annotated`: Selects annotated tabular file format
5.2. **DAKOTA_IO**

- **freeform**: Selects freeform file format
- **active_only**: Import only active variables from tabular data file
- **annotated**: Selects annotated tabular file format
- **custom_annotated**: Selects custom-annotated tabular file format
- **freeform**: Selects freeform file format
- **annotated**: Selects annotated tabular file format
- **custom_annotated**: Selects custom-annotated tabular file format
- **freeform**: Selects freeform file format
- **active_only**: Import only active variables from tabular data file
- **annotated**: Selects annotated tabular file format
- **custom_annotated**: Selects custom-annotated tabular file format
- **freeform**: Selects freeform file format
- **active_only**: Import only active variables from tabular data file
- **annotated**: Selects annotated tabular file format
- **custom_annotated**: Selects custom-annotated tabular file format
- **freeform**: Selects freeform file format
- **annotated**: Selects annotated tabular file format
- **custom_annotated**: Selects custom-annotated tabular file format
- **freeform**: Selects freeform file format
- **active_only**: Import only active variables from tabular data file
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- **custom_annotated**: Selects custom-annotated tabular file format
- **freeform**: Selects freeform file format
- **annotated**: Selects annotated tabular file format
- **custom_annotated**: Selects custom-annotated tabular file format
- **freeform**: Selects freeform file format
- **active_only**: Import only active variables from tabular data file
• active_only : Import only active variables from tabular data file
• annotated : Selects annotated tabular file format
• custom_annotated : Selects custom-annotated tabular file format
• freeform : Selects freeform file format
• annotated : Selects annotated tabular file format for experiment data
• custom_annotated : Selects custom-annotated tabular file format for experiment data
• freeform : Selects free-form tabular file format for experiment data
• annotated : Selects annotated tabular file format for experiment data
• custom_annotated : Selects custom-annotated tabular file format for experiment data
• freeform : Selects free-form tabular file format for experiment data

5.3  dakota_concepts

Description
Miscellaneous concepts related to Dakota operation

Related Topics
• method_independent_controls
• block
• strategies
• command_line_options
• restarts
• pointers

Related Keywords

5.3.1  method_independent_controls

Description
The <method independent controls> are those controls which are valid for a variety of methods. In some cases, these controls are abstractions which may have slightly different implementations from one method to the next. While each of these controls is not valid for every method, the controls are valid for enough methods that it was reasonable to consolidate the specifications.
5.3. **DAKOTA_CONCEPTS**

**Related Topics**

**Related Keywords**

- `max_iterations`: Number of iterations allowed for optimizers and adaptive UQ methods
- `constraint_tolerance`: The maximum allowable value of constraint violation still considered to be feasible
- `max_function_evaluations`: Number of function evaluations allowed for optimizers
- `scaling`: Turn on scaling for variables, responses, and constraints
- `convergence_tolerance`: Stopping criterion based on convergence of the objective function or statistics
- `max_iterations`: Number of iterations allowed for optimizers and adaptive UQ methods
- `scaling`: Turn on scaling for variables, responses, and constraints
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- `scaling`: Turn on scaling for variables, responses, and constraints
- `convergence_tolerance`: Stopping criterion based on convergence of the objective function or statistics
• **max_function_evaluations**: Number of function evaluations allowed for optimizers
• **max_iterations**: Number of iterations allowed for optimizers and adaptive UQ methods
• **scaling**: Turn on scaling for variables, responses, and constraints
• **constraint_tolerance**: The maximum allowable value of constraint violation still considered to be feasible
• **convergence_tolerance**: Stopping criterion based on convergence of the objective function or statistics
• **max_function_evaluations**: Number of function evaluations allowed for optimizers
• **max_iterations**: Number of iterations allowed for optimizers and adaptive UQ methods
• **scaling**: Turn on scaling for variables, responses, and constraints
• **speculative**: Compute speculative gradients
• **constraint_tolerance**: The maximum allowable value of constraint violation still considered to be feasible
• **convergence_tolerance**: Stopping criterion based on convergence of the objective function or statistics
• **max_function_evaluations**: Number of function evaluations allowed for optimizers
• **max_iterations**: Number of iterations allowed for optimizers and adaptive UQ methods
• **scaling**: Turn on scaling for variables, responses, and constraints
• **speculative**: Compute speculative gradients
• **max_function_evaluations**: Number of function evaluations allowed for optimizers
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• **max_iterations**: Number of iterations allowed for optimizers and adaptive UQ methods
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• **speculative**: Compute speculative gradients
• **constraint_tolerance**: The maximum allowable value of constraint violation still considered to be feasible
• **convergence_tolerance**: Stopping criterion based on convergence of the objective function or statistics
• **max_function_evaluations**: Number of function evaluations allowed for optimizers
• **max_iterations**: Number of iterations allowed for optimizers and adaptive UQ methods
• **scaling**: Turn on scaling for variables, responses, and constraints
• **speculative**: Compute speculative gradients
• **max_iterations**: Number of iterations allowed for optimizers and adaptive UQ methods
• **final_solutions** : Number of designs returned as the best solutions
• **max_iterations** : Number of iterations allowed for optimizers and adaptive UQ methods
• **max_iterations** : Number of iterations allowed for optimizers and adaptive UQ methods
• **max_function_evaluations** : Number of function evaluations allowed for optimizers
• **scaling** : Turn on scaling for variables, responses, and constraints
• **max_function_evaluations** : Number of function evaluations allowed for optimizers
• **scaling** : Turn on scaling for variables, responses, and constraints
• **convergence_tolerance** : Stopping criterion based on convergence of the objective function or statistics
• **max_function_evaluations** : Number of function evaluations allowed for optimizers
• **max_iterations** : Number of iterations allowed for optimizers and adaptive UQ methods
• **convergence_tolerance** : Stopping criterion based on convergence of the objective function or statistics
• **max_iterations** : Number of iterations allowed for optimizers and adaptive UQ methods
• **max_iterations** : Number of iterations allowed for optimizers and adaptive UQ methods
• **id_method** : Name the method block; helpful when there are multiple
• **convergence_tolerance** : Stopping criterion based on convergence of the objective function or statistics
• **max_iterations** : Number of iterations allowed for optimizers and adaptive UQ methods
• **convergence_tolerance** : Stopping criterion based on convergence of the objective function or statistics
• **max_iterations** : Number of iterations allowed for optimizers and adaptive UQ methods
• **max_function_evaluations** : Number of function evaluations allowed for optimizers
• **max_iterations** : Number of iterations allowed for optimizers and adaptive UQ methods
• **scaling** : Turn on scaling for variables, responses, and constraints
• **convergence_tolerance** : Stopping criterion based on convergence of the objective function or statistics
• **max_function_evaluations** : Number of function evaluations allowed for optimizers
• **max_iterations** : Number of iterations allowed for optimizers and adaptive UQ methods
• **scaling** : Turn on scaling for variables, responses, and constraints
5.3. DAKOTA_CONCEPTS

- **convergence_tolerance**: Stopping criterion based on convergence of the objective function or statistics
- **max_function_evaluations**: Number of function evaluations allowed for optimizers
- **max_iterations**: Number of iterations allowed for optimizers and adaptive UQ methods
- **scaling**: Turn on scaling for variables, responses, and constraints
- **speculative**: Compute speculative gradients
- **convergence_tolerance**: Stopping criterion based on convergence of the objective function or statistics
- **max_function_evaluations**: Number of function evaluations allowed for optimizers
- **max_iterations**: Number of iterations allowed for optimizers and adaptive UQ methods
- **scaling**: Turn on scaling for variables, responses, and constraints
- **constraint_tolerance**: The maximum allowable value of constraint violation still considered to be feasible
- **convergence_tolerance**: Stopping criterion based on convergence of the objective function or statistics
- **max_function_evaluations**: Number of function evaluations allowed for optimizers
- **max_iterations**: Number of iterations allowed for optimizers and adaptive UQ methods
- **scaling**: Turn on scaling for variables, responses, and constraints
- **speculative**: Compute speculative gradients
- **convergence_tolerance**: Stopping criterion based on convergence of the objective function or statistics
- **max_iterations**: Number of iterations allowed for optimizers and adaptive UQ methods
- **scaling**: Turn on scaling for variables, responses, and constraints
- **max_function_evaluations**: Number of function evaluations allowed for optimizers
- **max_iterations**: Number of iterations allowed for optimizers and adaptive UQ methods
- **scaling**: Turn on scaling for variables, responses, and constraints
- **speculative**: Compute speculative gradients
- **convergence_tolerance**: Stopping criterion based on convergence of the objective function or statistics
- **max_function_evaluations**: Number of function evaluations allowed for optimizers
- **max_iterations**: Number of iterations allowed for optimizers and adaptive UQ methods
- **scaling**: Turn on scaling for variables, responses, and constraints
- **speculative**: Compute speculative gradients
- **convergence_tolerance**: Stopping criterion based on convergence of the objective function or statistics
- **max_function_evaluations**: Number of function evaluations allowed for optimizers
- **max_iterations**: Number of iterations allowed for optimizers and adaptive UQ methods
- **scaling**: Turn on scaling for variables, responses, and constraints
• **scaling**: Turn on scaling for variables, responses, and constraints
• **speculative**: Compute speculative gradients
• **convergence\_tolerance**: Stopping criterion based on convergence of the objective function or statistics
• **max\_function\_evaluations**: Number of function evaluations allowed for optimizers
• **max\_iterations**: Number of iterations allowed for optimizers and adaptive UQ methods
• **scaling**: Turn on scaling for variables, responses, and constraints
• **speculative**: Compute speculative gradients
• **convergence\_tolerance**: Stopping criterion based on convergence of the objective function or statistics
• **max\_function\_evaluations**: Number of function evaluations allowed for optimizers
• **max\_iterations**: Number of iterations allowed for optimizers and adaptive UQ methods
• **scaling**: Turn on scaling for variables, responses, and constraints
• **speculative**: Compute speculative gradients
• **convergence\_tolerance**: Stopping criterion based on convergence of the objective function or statistics
• **max\_function\_evaluations**: Number of function evaluations allowed for optimizers
• **max\_iterations**: Number of iterations allowed for optimizers and adaptive UQ methods
• **scaling**: Turn on scaling for variables, responses, and constraints
• **speculative**: Compute speculative gradients
• **output**: Control how much method information is written to the screen and output file
• **convergence\_tolerance**: Stopping criterion based on convergence of the objective function or statistics
• **max\_iterations**: Number of iterations allowed for optimizers and adaptive UQ methods
5.3. DAKOTA CONCEPTS

- convergence_tolerance: Stopping criterion based on convergence of the objective function or statistics
- max_iterations: Number of iterations allowed for optimizers and adaptive UQ methods
- max_function_evaluations: Number of function evaluations allowed for optimizers
- max_iterations: Number of iterations allowed for optimizers and adaptive UQ methods
- scaling: Turn on scaling for variables, responses, and constraints
- convergence_tolerance: Stopping criterion based on convergence of the objective function or statistics
- max_function_evaluations: Number of function evaluations allowed for optimizers
- max_iterations: Number of iterations allowed for optimizers and adaptive UQ methods
- scaling: Turn on scaling for variables, responses, and constraints
- constraint_tolerance: The maximum allowable value of constraint violation still considered to be feasible
- convergence_tolerance: Stopping criterion based on convergence of the objective function or statistics
- max_function_evaluations: Number of function evaluations allowed for optimizers
- max_iterations: Number of iterations allowed for optimizers and adaptive UQ methods
- scaling: Turn on scaling for variables, responses, and constraints
- speculative: Compute speculative gradients
- convergence_tolerance: Stopping criterion based on convergence of the objective function or statistics
- max_iterations: Number of iterations allowed for optimizers and adaptive UQ methods
- constraint_tolerance: The maximum allowable value of constraint violation still considered to be feasible
- convergence_tolerance: Stopping criterion based on convergence of the objective function or statistics
- max_iterations: Number of iterations allowed for optimizers and adaptive UQ methods
- max_function_evaluations: Number of function evaluations allowed for optimizers
- max_iterations: Number of iterations allowed for optimizers and adaptive UQ methods

5.3.2 block

Description

A block is the highest level of keyword organization in Dakota. There are currently 6 blocks in the Dakota input spec:

Related Topics

- block_identifier
- block_pointer
Related Keywords

- **environment**: Top-level settings for Dakota execution
- **interface**: Specifies how function evaluations will be performed in order to map the variables into the responses.
- **method**: Begins Dakota method selection and behavioral settings.
- **model**: Specifies how variables are mapped into a set of responses
- **responses**: Description of the model output data returned to Dakota upon evaluation of an interface.
- **variables**: Specifies the parameter set to be iterated by a particular method.

**block_identifier**

**Description**

empty

**Related Topics**

**Related Keywords**

- **id_interface**: Name the interface block; helpful when there are multiple
- **id_method**: Name the method block; helpful when there are multiple
- **id_model**: Give the model block an identifying name, in case of multiple model blocks
- **id_responses**: Name the responses block; helpful when there are multiple
- **id_variables**: Name the variables block; helpful when there are multiple

**block_pointer**

**Description**

See **block_pointer** for details about pointers.

**Related Topics**

**Related Keywords**

- **top_method_pointer**: Identify which method leads the Dakota study
- **model_pointer**: Identifier for model block to be used by a method
- **model_pointer**: Identifier for model block to be used by a method
- **model_pointer**: Identifier for model block to be used by a method
- **model_pointer**: Identifier for model block to be used by a method
- **method_pointer**: Pointer to sub-method to apply to a surrogate or branch-and-bound sub-problem
• **model_pointer** : Identifier for model block to be used by a method
• **model_pointer** : Identifier for model block to be used by a method
• **model_pointer** : Identifier for model block to be used by a method
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• **model_pointer** : Identifier for model block to be used by a method
• **model_pointer** : Identifier for model block to be used by a method
• **model_pointer_list** : Associate models with method names
• **method_pointer_list** : Pointers to methods to execute sequentially or collaboratively
• **global_model_pointer** : Pointer to model used by global method
• **global_method_pointer**: Pointer to global method
• **local_model_pointer**: Pointer to model used by local method
• **local_method_pointer**: Pointer to local method
• **model_pointer_list**: Associate models with method names
• **method_pointer_list**: Pointers to methods to execute sequentially or collaboratively
• **model_pointer**: Identifier for model block to be used by a method
• **method_pointer**: Pointer to sub-method to run from each starting point
5.3. DAKOTA_CONCEPTS

- method_pointer : Pointer to optimization or least-squares sub-method
- model_pointer : Identifier for model block to be used by a method
- model_pointer : Identifier for model block to be used by a method
- model_pointer : Identifier for model block to be used by a method
- model_pointer : Identifier for model block to be used by a method
- model_pointer : Identifier for model block to be used by a method
- method_pointer : Pointer to sub-method to apply to a surrogate or branch-and-bound sub-problem
- model_pointer : Identifier for model block to be used by a method
- method_pointer : Pointer to sub-method to apply to a surrogate or branch-and-bound sub-problem
- model_pointer : Identifier for model block to be used by a method
- model_pointer : Identifier for model block to be used by a method
- actual_model_pointer : Pointer to specify a full-space model, from which to construct a lower dimensional surrogate
- actual_model_pointer : Pointer to specify a "truth" model, from which to construct a surrogate
- optional_interface_pointer : Pointer to interface that provides non-nested responses
- optional_interface_responses_pointer : Pointer to responses block that defines non-nested responses
- sub_method_pointer : The sub_method_pointer specifies the method block for the sub-iterator
- responses_pointer : Specify which responses block will be used by this model block
- interface_pointer : Interface block pointer for the single model type
- dace_method_pointer : Specify a method to gather training data
- actual_model_pointer : Pointer to specify a "truth" model, from which to construct a surrogate
- actual_model_pointer : Pointer to specify a "truth" model, from which to construct a surrogate
- variables_pointer : Specify which variables block will be included with this model block

5.3.3 strategies

Description

empty
Related Topics

- advanced_strategies

Related Keywords

5.3.4 advanced_strategies

Description

empty

Related Topics

Related Keywords

5.3.5 command_line_options

Description

empty

Related Topics

Related Keywords

- check : Invoke Dakota in input check mode
- error_file : Base filename for error redirection
- output_file : Base filename for output redirection
- post_run : Invoke Dakota with post-run mode active
- pre_run : Invoke Dakota with pre-run mode active
- read_restart : Base filename for restart file read
- run : Invoke Dakota with run mode active
- write_restart : Base filename for restart file write

5.3.6 restarts

Description

empty
5.3. **DAKOTA_CONCEPTS**

**Related Topics**

**Related Keywords**

5.3.7 **pointers**

**Description**

For all pointer specifications, if a pointer string is specified and no corresponding id string is available, Dakota will exit with an error message.

If the pointer is optional and no pointer string is specified, then the last specification parsed will be used.

It is appropriate to omit optional cross-referencing whenever the relationships are unambiguous due to the presence of only one specification.

**Related Topics**

- block_pointer
- objective_function_pointer

**Related Keywords**

5.3.8 **block_pointer**

**Description**

See block_pointer for details about pointers.

**Related Topics**

**Related Keywords**

- top_method_pointer : Identify which method leads the Dakota study
- model_pointer : Identifier for model block to be used by a method
- model_pointer : Identifier for model block to be used by a method
- model_pointer : Identifier for model block to be used by a method
- model_pointer : Identifier for model block to be used by a method
- method_pointer : Pointer to sub-method to apply to a surrogate or branch-and-bound sub-problem
- model_pointer : Identifier for model block to be used by a method
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• **model_pointer**: Identifier for model block to be used by a method
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• **model_pointer_list**: Associate models with method names
• **method_pointer_list**: Pointers to methods to execute sequentially or collaboratively
• **model_pointer**: Identifier for model block to be used by a method
5.3. DAKOTA_CONCEPTS

- model_pointer : Identifier for model block to be used by a method
- model_pointer : Identifier for model block to be used by a method
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- method_pointer : Pointer to sub-method to run from each starting point
- model_pointer : Identifier for model block to be used by a method
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- model_pointer : Identifier for model block to be used by a method
- model_pointer : Identifier for model block to be used by a method
- model_pointer : Identifier for model block to be used by a method
- model_pointer : Identifier for model block to be used by a method
- method_pointer : Pointer to optimization or least-squares sub-method
- model_pointer : Identifier for model block to be used by a method
- model_pointer : Identifier for model block to be used by a method
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- model_pointer : Identifier for model block to be used by a method
- model_pointer : Identifier for model block to be used by a method
- **model_pointer**: Identifier for model block to be used by a method
- **model_pointer**: Identifier for model block to be used by a method
- **model_pointer**: Identifier for model block to be used by a method
- **model_pointer**: Identifier for model block to be used by a method
- **method_pointer**: Pointer to sub-method to apply to a surrogate or branch-and-bound sub-problem
- **model_pointer**: Identifier for model block to be used by a method
- **model_pointer**: Pointer to sub-method to apply to a surrogate or branch-and-bound sub-problem
- **model_pointer**: Identifier for model block to be used by a method
- **model_pointer**: Identifier for model block to be used by a method
- **actual_model_pointer**: Pointer to specify a full-space model, from which to construct a lower dimensional surrogate
- **actual_model_pointer**: Pointer to specify a “truth” model, from which to construct a surrogate
- **optional_interface_pointer**: Pointer to interface that provides non-nested responses
- **optional_interface_responses_pointer**: Pointer to responses block that defines non-nested responses
- **sub_method_pointer**: The **sub_method_pointer** specifies the method block for the sub-iterator
- **responses_pointer**: Specify which responses block will be used by this model block
- **interface_pointer**: Interface block pointer for the single model type
- **dace_method_pointer**: Specify a method to gather training data
- **actual_model_pointer**: Pointer to specify a “truth” model, from which to construct a surrogate
- **actual_model_pointer**: Pointer to specify a “truth” model, from which to construct a surrogate
- **variables_pointer**: Specify which variables block will be included with this model block

### 5.3.9 objective_function_pointer

**Description**

See **block_pointer** for details about pointers.

**Related Topics**

**Related Keywords**

- **id_analytic_gradients**: Identify which analytical gradient corresponds to which response
- **id_numerical_gradients**: Identify which numerical gradient corresponds to which response
- **id_analytic_hessians**: Identify which analytical Hessian corresponds to which response
- **id_numerical_hessians**: Identify which numerical-Hessian corresponds to which response
- **id_quasi_hessians**: Identify which quasi-Hessian corresponds to which response
5.4 models

Description
Keywords and Concepts relating to the model block

Related Topics

- surrogate_models
- recast_models
- multifidelity_models
- reduced_order_models
- nested_models
- advanced_model_recursion

Related Keywords

5.4.1 surrogate_models

Description
empty

Related Topics

- surrogate_based_optimization_methods

Related Keywords

- auto_refinement: Experimental auto-refinement of surrogate model
- point_selection: Enable greedy selection of well-spaced build points
- export_model: Exports surrogate model in user-selected format
- filename_prefix: User-customizable portion of exported model filenames
- formats: Formats for surrogate model export
- algebraic_console: Export surrogate model in algebraic format to the console
- algebraic_file: Export surrogate model in algebraic format to a file
- binary_archive: Export surrogate model to a binary archive file
- text_archive: Export surrogate model to a plain-text archive file
- export_model: Exports surrogate model in user-selected format
- filename_prefix: User-customizable portion of exported model filenames
• **formats**: Formats for surrogate model export
  
  • **binary_archive**: Export surrogate model to a binary archive file
  
  • **text_archive**: Export surrogate model to a plain-text archive file
  
  • **metrics**: Compute surrogate quality metrics
  
  • **cross_validation**: Perform k-fold cross validation
  
  • **export_model**: Exports surrogate model in user-selected format
  
  • **filename_prefix**: User-customizable portion of exported model filenames
  
  • **formats**: Formats for surrogate model export
  
  • **binary_archive**: Export surrogate model to a binary archive file
  
  • **text_archive**: Export surrogate model to a plain-text archive file
  
  • **export_model**: Exports surrogate model in user-selected format
  
  • **filename_prefix**: User-customizable portion of exported model filenames
  
  • **formats**: Formats for surrogate model export
  
  • **algebraic_console**: Export surrogate model in algebraic format to the console
  
  • **algebraic_file**: Export surrogate model in algebraic format to a file
  
  • **binary_archive**: Export surrogate model to a binary archive file
  
  • **text_archive**: Export surrogate model to a plain-text archive file
  
  • **max_nodes**: Maximum number of hidden layer nodes
  
  • **random_weight**: (Inactive) Random weight control
  
  • **range**: Range for neural network random weights
  
  • **export_model**: Exports surrogate model in user-selected format
  
  • **filename_prefix**: User-customizable portion of exported model filenames
  
  • **formats**: Formats for surrogate model export
  
  • **algebraic_console**: Export surrogate model in algebraic format to the console
  
  • **algebraic_file**: Export surrogate model in algebraic format to a file
  
  • **binary_archive**: Export surrogate model to a binary archive file
  
  • **text_archive**: Export surrogate model to a plain-text archive file
  
  • **bases**: Initial number of radial basis functions
  
  • **export_model**: Exports surrogate model in user-selected format
  
  • **filename_prefix**: User-customizable portion of exported model filenames
5.4. MODELS

- **formats**: Formats for surrogate model export
- **algebraic_console**: Export surrogate model in algebraic format to the console
- **algebraic_file**: Export surrogate model in algebraic format to a file
- **binary_archive**: Export surrogate model to a binary archive file
- **text_archive**: Export surrogate model to a plain-text archive file
- **max_pts**: Maximum number of RBF CVT points
- **max_subsets**: Number of trial RBF subsets
- **min_partition**: (Inactive) Minimum RBF partition
- **reuse_points**: Surrogate model training data reuse control

5.4.2 surrogate_based_optimization_methods

**Description**
empty

**Related Topics**

**Related Keywords**
- **efficient_global**: Global Surrogate Based Optimization, a.k.a. EGO
- **surrogate_based_global**: Global Surrogate Based Optimization
- **surrogate_based_local**: Local Surrogate Based Optimization

5.4.3 recast_models

**Description**
empty

**Related Topics**

**Related Keywords**

5.4.4 multifidelity_models

**Description**
empty
5.4.5 reduced_order_models
Description
empty

5.4.6 nested_models
Description
empty

5.4.7 advanced_model_recursion
Description
empty

- hybrid_and_recursions_logic

5.5 variables
Description
Keywords and concepts relating to the variables block
5.5. VARIABLES

Related Topics
- variable_domain
- linear_constraints
- variable_type

Related Keywords
5.5.1 variable_domain

Description
Dakota variables can be grouped by their valid domains.

1. Mixed: continuous and discrete variables are treated separately
2. Relaxed: noncategorical discrete variables are relaxed and treated as continuous variables (categorical variables are non-relaxable and remain discrete)

Refer to mixed and relaxed for additional information.

Related Topics
- continuous_variables
- discrete_variables

Related Keywords
5.5.2 continuous_variables

Description
This page collects information related to the topic of continuous design, uncertain, and state variables.

Related Topics
Related Keywords
- beta_uncertain : Aleatory uncertain variable - beta
- continuous_design : Design variable - continuous
- continuous_interval_uncertain : Epistemic uncertain variable - values from one or more continuous intervals
- continuous_state : State variable - continuous
- exponential_uncertain : Aleatory uncertain variable - exponential
- frechet_uncertain : Aleatory uncertain variable - Frechet
- gamma_uncertain : Aleatory uncertain variable - gamma
- gumbel_uncertain : Aleatory uncertain variable - gumbel
• **histogram_bin_uncertain**: Aleatory uncertain variable - continuous histogram
• **lognormal_uncertain**: Aleatory uncertain variable - lognormal
• **loguniform_uncertain**: Aleatory uncertain variable - loguniform
• **normal_uncertain**: Aleatory uncertain variable - normal (Gaussian)
• **triangular_uncertain**: Aleatory uncertain variable - triangular
• **uniform_uncertain**: Aleatory uncertain variable - uniform
• **weibull_uncertain**: Aleatory uncertain variable - Weibull

### 5.5.3 discrete_variables

**Description**

This page discusses discrete design, uncertain, and state variables (which have *discrete* in their keyword name) as they have similar specifications. These include:

1. Integer ranges
2. Sets of integers
3. Sets of reals
4. Sets of strings and each is described below.

In addition, some aleatory uncertain variables, e.g., **binomial_uncertain**, are discrete integer-valued random variables specified using parameters. These are described on their individual keyword pages.

**Sets**

Sets of integers, reals, and strings have similar specifications, though different value types. The variables are specified using three keywords:

- **Variable declaration keyword** - specifies the number of variables being defined
- **elements_per_variable** - a list of positive integers specifying how many set members each variable admits
  - Length = # of variables
- **elements** - a list of the permissible integer values in ALL sets, concatenated together.
  - Length = sum of elements_per_variable, or an integer multiple of number of variables
  - The order is very important here.
  - The list is partitioned according to the values of elements_per_variable, and each partition is assigned to a variable.
- **The ordering of elements_per_variable, and the partitions of elements must match the strings from descriptors**

For string variables, each string element value must be quoted and may contain alphanumeric, dash, underscore, and colon. White space, quote characters, and backslash/metacharacters are not permitted.

Examples are given on the pages:
5.5. VARIABLES

- discrete design set integer
- discrete design set real
- discrete design set string
- discrete uncertain set integer
- discrete uncertain set real
- discrete uncertain set string

**Range**

For discrete variables defined by range(s), the lower bounds and upper bounds restrict the permissible values. For design variables, this constrains the feasible design space and is frequently used to prevent nonphysical designs. This is a discrete interval variable that may take any integer value within bounds (e.g., [1, 4], allowing values of 1, 2, 3, or 4). For some variable types, each variable is can be defined by multiple ranges.

Examples are given on the pages:

- discrete_interval_uncertain

**Related Topics**

**Related Keywords**

- binomial_uncertain: Aleatory uncertain discrete variable - binomial
- discrete_design_range: Design variable - discrete range-valued
- discrete_design_set: Design variable - discrete set-valued
- integer: Integer-valued discrete design variables
- real: Real-valued discrete design variables
- string: String-valued discrete design set variables
- discrete_interval_uncertain: Epistemic uncertain variable - values from one or more discrete intervals
- discrete_state_range: State variables - discrete range-valued
- discrete_state_set: State variable - discrete set-valued
- integer: Discrete state variables, each defined by a set of permissible integers
- real: Discrete state variables, each defined by a set of permissible real numbers
- string: String-valued discrete state set variables
- discrete_uncertain_set: Epistemic uncertain variable - discrete set-valued
- integer: Discrete, epistemic uncertain variable - integers within a set
- real: Discrete, epistemic uncertain variable - real numbers within a set
- string: Discrete, epistemic uncertain variable - strings within a set
- geometric_uncertain: Aleatory uncertain discrete variable - geometric
• histogram_point_uncertain: Aleatory uncertain variable - discrete histogram
• hypergeometric_uncertain: Aleatory uncertain discrete variable - hypergeometric
• negative_binomial_uncertain: Aleatory uncertain discrete variable - negative binomial
• poisson_uncertain: Aleatory uncertain discrete variable - Poisson

5.5.4 linear_constraints

Description
Many methods can make use of linear equality or inequality constraints.

As the name implies, linear constraints are constraints that are linear functions of the variables. Constraints that are nonlinear functions of variables are specified using the nonlinear_constraints family of keywords. From a Dakota usage point of view, the most important difference between linear and nonlinear constraints is that the former are specified entirely within the Dakota input file and calculated by Dakota itself, while the latter must be calculated by the user’s simulation and returned as responses to Dakota.

The Optimization chapter of the User’s Manual[4] states which methods support linear constraints. Of those methods, a subset strictly obey linear constraints; that is, no candidate points are generated by the optimizer that violate the constraints. These include asynch_pattern_search, the optpp_* family of optimizers (with the exception of optpp_fd_newton), and npsol_sqp. The other methods seek feasible solutions (i.e. solutions that satisfy the linear constraints), but may violate the constraints as they run. Linear constraints may also be violated, even when using an optimizer that itself strictly respects them, if numerical_gradients are used. In this case, Dakota may request evaluations that lie outside of the feasible region when computing a gradient near the boundary.

One final limitation that bears mentioning is that linear constraints are compatible only with continuous variables. No discrete types are permitted when using linear constraints.

Related Topics

Related Keywords
• linear.equality.constraint_matrix: Define coefficients of the linear equalities
• linear.equality.scale_types: Specify how each linear equality constraint is scaled
• linear.equality.scales: Define the characteristic values to scale linear equalities
• linear.equality.targets: Define target values for the linear equality constraints
• linear.inequality.constraint_matrix: Define coefficients of the linear inequality constraints
• linear.inequality.lower_bounds: Define lower bounds for the linear inequality constraint
• linear.inequality.scale_types: Specify how each linear inequality constraint is scaled
• linear.inequality.scales: Define the characteristic values to scale linear inequalities
• linear.inequality.upper_bounds: Define upper bounds for the linear inequality constraint
5.5. VARIABLEs

5.5.5 variable_type

Description
Dakota variables can be grouped by their type, including all, design, uncertain, aleatory, epistemic, or state. There are certain situations where the user may want to explicitly control the subset of variables that is considered active for a certain Dakota method, and override the default alignments between methods and variable types. Refer to active for additional information.

Related Topics
- design_variables
- aleatory_uncertain_variables
- epistemic_uncertain_variables
- state_variables

Related Keywords

5.5.6 design_variables

Description
Design variables are those variables which are modified for the purposes of computing an optimal design. The most common type of design variables encountered in engineering applications are of the continuous type. These variables may assume any real value within their bounds. All but a handful of the optimization algorithms in Dakota support continuous design variables exclusively.

Related Topics

Related Keywords

5.5.7 aleatory_uncertain_variables

Description
Aleatory uncertainty is also known as inherent variability, irreducible uncertainty, or randomness. Aleatory uncertainty is predominantly characterized using probability theory. This is the only option implemented in Dakota.
Related Topics

Related Keywords

- **beta_uncertain** : Aleatory uncertain variable - beta
- **binomial_uncertain** : Aleatory uncertain discrete variable - binomial
- **exponential_uncertain** : Aleatory uncertain variable - exponential
- **frechet_uncertain** : Aleatory uncertain variable - Frechet
- **gamma_uncertain** : Aleatory uncertain variable - gamma
- **geometric_uncertain** : Aleatory uncertain discrete variable - geometric
- **gumbel_uncertain** : Aleatory uncertain variable - gumbel
- **histogram_bin_uncertain** : Aleatory uncertain variable - continuous histogram
- **histogram_point_uncertain** : Aleatory uncertain variable - discrete histogram
- **hypergeometric_uncertain** : Aleatory uncertain discrete variable - hypergeometric
- **lognormal_uncertain** : Aleatory uncertain variable - lognormal
- **loguniform_uncertain** : Aleatory uncertain variable - loguniform
- **negative_binomial_uncertain** : Aleatory uncertain discrete variable - negative binomial
- **normal_uncertain** : Aleatory uncertain variable - normal (Gaussian)
- **poisson_uncertain** : Aleatory uncertain discrete variable - Poisson
- **triangular_uncertain** : Aleatory uncertain variable - triangular
- **uniform_uncertain** : Aleatory uncertain variable - uniform
- **weibull_uncertain** : Aleatory uncertain variable - Weibull

5.5.8 **epistemic_uncertain_variables**

Description

Epistemic uncertainty is uncertainty due to lack of knowledge.

In Dakota, epistemic uncertainty is characterized by interval analysis or the Dempster-Shafer theory of evidence.

Note that epistemic uncertainty can also be modeled with probability density functions - similarly to aleatory uncertainty Dakota does not support this capability.
5.6. RESPONSES

Related Topics

Related Keywords

- `continuous_interval_uncertain` : Epistemic uncertain variable - values from one or more continuous intervals
- `discrete_interval_uncertain` : Epistemic uncertain variable - values from one or more discrete intervals
- `discrete_uncertain_set` : Epistemic uncertain variable - discrete set-valued
- `integer` : Discrete, epistemic uncertain variable - integers within a set
- `real` : Discrete, epistemic uncertain variable - real numbers within a set
- `string` : Discrete, epistemic uncertain variable - strings within a set

5.5.9 state_variables

Description

State variables provide a convenient mechanism for managing additional model parameterizations such as mesh density, simulation convergence tolerances, and time step controls.

Only parameter studies and design of experiments methods will iterate on state variables.

The `initial_state` is used as the only value for the state variable for all other methods, unless `active state` is invoked.

If a method iterates on a state variable, the variable is treated as a design variable with the given bounds, or as a uniform uncertain variable with the given bounds.

If the state variable is defined only by its bounds, and the method does NOT iterate on state variables, then the `initial_state` must be inferred.

Related Topics

Related Keywords

- `continuous_state` : State variable - continuous
- `discrete_state_range` : State variables - discrete range-valued
- `discrete_state_set` : State variable - discrete set-valued
- `integer` : Discrete state variables, each defined by a set of permissible integers
- `real` : Discrete state variables, each defined by a set of permissible real numbers
- `string` : String-valued discrete state set variables

5.6 responses

Description

Keywords and concepts relating to the `responses` block
Related Topics
- response_types
- nonlinear_constraints

Related Keywords

5.6.1 response_types

Description
The specification must be one of three types:

1. objective and constraint functions
2. calibration (least squares) terms and constraint functions
3. a generic response functions specification.

These correspond to (a) optimization, (b) deterministic (least squares) or stochastic (Bayesian) inversion, and (c) general-purpose analyzer methods such as parameter studies, DACE, and UQ methods, respectively. Refer to responses for additional details and examples.

Related Topics

5.6.2 nonlinear_constraints

Description
Nonlinear constraints are supported by many of Dakota’s optimizers. For a discussion of the difference between nonlinear and linear constraints, see the linear constraints topic page. The Constraint Considerations section of the optimization and calibration page may also be of interest.

Related Topics

5.7 interface

Description
Keywords and Concepts relating to the interface block, which is used to connect Dakota to external analysis codes (simulations, etc.)
5.7. INTERFACE

Related Topics
- simulation_file_management
- workflow_management
- advanced_simulation_interfaces

Related Keywords
5.7.1 simulation_file_management
Description
empty

Related Topics
Related Keywords
5.7.2 workflow_management
Description
empty

Related Topics
Related Keywords
5.7.3 advanced_simulation_interfaces
Description
empty

Related Topics
- simulation_failure
  - concurrency_and_parallelism

Related Keywords
simulation_failure
Description
empty
Related Topics

Related Keywords

concurrency_and_parallelism

Description

empty

Related Topics

Related Keywords

- processors_per_analysis: Specify the number of processors per analysis when Dakota is run in parallel
- analysis_scheduling: Specify the scheduling of concurrent analyses when Dakota is run in parallel
- master: Specify a dedicated master partition for parallel analysis scheduling
- peer: Specify a peer partition for parallel analysis scheduling
- analysis_servers: Specify the number of analysis servers when Dakota is run in parallel
- asynchronous: Specify local evaluation or analysis concurrency
- analysis_concurrency: Limit the number of analysis drivers within an evaluation that Dakota will schedule
- evaluation_concurrency: Determine how many concurrent evaluations Dakota will schedule
- local_evaluation_scheduling: Control how local asynchronous jobs are scheduled
- master: Specify a dedicated master partition for parallel evaluation scheduling
- peer: Specify a peer partition for parallel evaluation scheduling
- dynamic: Specify dynamic scheduling in a peer partition when Dakota is run in parallel.
- static: Specify static scheduling in a peer partition when Dakota is run in parallel.
- evaluation_servers: Specify the number of evaluation servers when Dakota is run in parallel
- processors_per_evaluation: Specify the number of processors per evaluation server when Dakota is run in parallel
- iterator_scheduling: Specify the scheduling of concurrent iterators when Dakota is run in parallel
- master: Specify a dedicated master partition for parallel iterator scheduling
- peer: Specify a peer partition for parallel iterator scheduling
- iterator_servers: Specify the number of iterator servers when Dakota is run in parallel
- processors_per_iterator: Specify the number of processors per iterator server when Dakota is run in parallel
- iterator_scheduling: Specify the scheduling of concurrent iterators when Dakota is run in parallel
- master: Specify a dedicated master partition for parallel iterator scheduling
5.8 METHODS

- **peer**: Specify a peer partition for parallel iterator scheduling
- **iterator_servers**: Specify the number of iterator servers when Dakota is run in parallel
- **processors_per_iterator**: Specify the number of processors per iterator server when Dakota is run in parallel
- **iterator_scheduling**: Specify the scheduling of concurrent iterators when Dakota is run in parallel
- **master**: Specify a dedicated master partition for parallel iterator scheduling
- **peer**: Specify a peer partition for parallel iterator scheduling
- **iterator_servers**: Specify the number of iterator servers when Dakota is run in parallel
- **processors_per_iterator**: Specify the number of processors per iterator server when Dakota is run in parallel
- **iterator_scheduling**: Specify the scheduling of concurrent iterators when Dakota is run in parallel
- **master**: Specify a dedicated master partition for parallel iterator scheduling
- **peer**: Specify a peer partition for parallel iterator scheduling
- **iterator_servers**: Specify the number of iterator servers when Dakota is run in parallel
- **processors_per_iterator**: Specify the number of processors per iterator server when Dakota is run in parallel

5.8 methods

Description

Keywords and Concepts relating to the method block, including discussion of the different methods and algorithms available in Dakota

Related Topics

- **parameter_studies**
- **sensitivity_analysis_and_design_of_experiments**
- **uncertainty_quantification**
- **optimization_and_calibration**

Related Keywords

5.8.1 parameter_studies

Description

Parameter studies employ deterministic designs to explore the effect of parametric changes within simulation models, yielding one form of sensitivity analysis. They can help assess simulation characteristics such as smoothness, multi-modality, robustness, and nonlinearity, which affect the choice of algorithms and controls in follow-on optimization and UQ studies.
Dakota’s parameter study methods compute response data sets at a selection of points in the parameter space. These points may be specified as a vector, a list, a set of centered vectors, or a multi-dimensional grid. Capability overviews and examples of the different types of parameter studies are provided in the Users Manual [4].

With the exception of output verbosity (a setting of silent will suppress some parameter study diagnostic output), Dakota’s parameter study methods do not make use of the method independent controls. Therefore, the parameter study documentation which follows is limited to the method dependent controls for the vector, list, centered, and multidimensional parameter study methods.

**Related Topics**

**Related Keywords**

- centered\_parameter\_study : Samples variables along points moving out from a center point
- list\_parameter\_study : Samples variables as a specified values
- multidim\_parameter\_study : Samples variables on full factorial grid of study points
- partitions : Samples variables on full factorial grid of study points
- vector\_parameter\_study : Samples variables along a user-defined vector

### 5.8.2 sensitivity\_analysis\_and\_design\_of\_experiments

**Description**

empty

**Related Topics**

- design\_and\_analysis\_of\_computer\_experiments
- sampling

**Related Keywords**

### 5.8.3 design\_and\_analysis\_of\_computer\_experiments

**Description**

Design and Analysis of Computer Experiments (DACE) methods compute response data sets at a selection of points in the parameter space. Three libraries are provided for performing these studies: DDACE, FSUDace, and PSUADE. The design of experiments methods do not currently make use of any of the method independent controls.

**Related Topics**

**Related Keywords**

- dace : Design and Analysis of Computer Experiments
- fsu\_cvt : Design of Computer Experiments - Centroidal Voronoi Tessellation
- fsu\_quasi\_mc : Design of Computer Experiments - Quasi-Monte Carlo sampling
5.8. METHODS

- **hammersley**: Use Hammersley sequences
- **psuade_moat**: Morris One-at-a-Time

### 5.8.4 sampling

**Description**

Sampling techniques are selected using the `sampling` method selection. This method generates sets of samples according to the probability distributions of the uncertain variables and maps them into corresponding sets of response functions, where the number of samples is specified by the `samples` integer specification. Means, standard deviations, coefficients of variation (COVs), and 95% confidence intervals are computed for the response functions. Probabilities and reliabilities may be computed for `response_levels` specifications, and response levels may be computed for either `probability_levels` or `reliability_levels` specifications (refer to the Method Commands chapter in the Dakota Reference Manual\[5\] for additional information).

Currently, traditional Monte Carlo (MC) and Latin hypercube sampling (LHS) are supported by Dakota and are chosen by specifying `sample_type` as `random` or `lhs`. In Monte Carlo sampling, the samples are selected randomly according to the user-specified probability distributions. Latin hypercube sampling is a stratified sampling technique for which the range of each uncertain variable is divided into $N_s$ segments of equal probability, where $N_s$ is the number of samples requested. The relative lengths of the segments are determined by the nature of the specified probability distribution (e.g., uniform has segments of equal width, normal has small segments near the mean and larger segments in the tails). For each of the uncertain variables, a sample is selected randomly from each of these equal probability segments. These $N_s$ values for each of the individual parameters are then combined in a shuffling operation to create a set of $N_s$ parameter vectors with a specified correlation structure. A feature of the resulting sample set is that every row and column in the hypercube of partitions has exactly one sample. Since the total number of samples is exactly equal to the number of partitions used for each uncertain variable, an arbitrary number of desired samples is easily accommodated (as compared to less flexible approaches in which the total number of samples is a product or exponential function of the number of intervals for each variable, i.e., many classical design of experiments methods).

Advantages of sampling-based methods include their relatively simple implementation and their independence from the scientific disciplines involved in the analysis. The main drawback of these techniques is the large number of function evaluations needed to generate converged statistics, which can render such an analysis computationally very expensive, if not intractable, for real-world engineering applications. LHS techniques, in general, require fewer samples than traditional Monte Carlo for the same accuracy in statistics, but they still can be prohibitively expensive. For further information on the method and its relationship to other sampling techniques, one is referred to the works by McKay, et al.[59], Iman and Shortencarier[53], and Helton and Davis[46]. Note that under certain separability conditions associated with the function to be sampled, Latin hypercube sampling provides a more accurate estimate of the mean value than does random sampling. That is, given an equal number of samples, the LHS estimate of the mean will have less variance than the mean value obtained through random sampling.

**Related Topics**

**Related Keywords**

- **importance_sampling**: Importance sampling
- **sampling**: Randomly samples variables according to their distributions
CHAPTER 5. TOPICS AREA

5.8.5 uncertainty quantification

Description

Dakota provides a variety of methods for propagating both aleatory and epistemic uncertainty.

At a high level, uncertainty quantification (UQ) or nondeterministic analysis is the process of characterizing input uncertainties, forward propagating these uncertainties through a computational model, and performing statistical or interval assessments on the resulting responses. This process determines the effect of uncertainties and assumptions on model outputs or results. In Dakota, uncertainty quantification methods specifically focus on the forward propagation part of the process, where probabilistic or interval information on parametric inputs are mapped through the computational model to assess statistics or intervals on outputs. For an overview of these approaches for engineering applications, consult[42].

UQ is related to sensitivity analysis in that the common goal is to gain an understanding of how variations in the parameters affect the response functions of the engineering design problem. However, for UQ, some or all of the components of the parameter vector are considered to be uncertain as specified by particular probability distributions (e.g., normal, exponential, extreme value), or other uncertainty structures. By assigning specific distributional structure to the inputs, distributional structure for the outputs (i.e., response statistics) can be inferred. This migrates from an analysis that is more \{qualitative\} in nature, in the case of sensitivity analysis, to an analysis that is more rigorously \{quantitative\}.

UQ methods are often distinguished by their ability to propagate aleatory or epistemic input uncertainty characterizations, where aleatory uncertainties are irreducible variabilities inherent in nature and epistemic uncertainties are reducible uncertainties resulting from a lack of knowledge. Since sufficient data is generally available for aleatory uncertainties, probabilistic methods are commonly used for computing response distribution statistics based on input probability distribution specifications. Conversely, for epistemic uncertainties, any use of probability distributions is based on subjective knowledge rather than objective data, and we may alternatively explore nonprobabilistic methods based on interval specifications.

Dakota contains capabilities for performing nondeterministic analysis with both types of input uncertainty. These UQ methods have been developed by Sandia Labs, in conjunction with collaborators in academia[31],[32],[21],[79].

The aleatory UQ methods in Dakota include various sampling-based approaches (e.g., Monte Carlo and Latin Hypercube sampling), local and global reliability methods, and stochastic expansion (polynomial chaos expansions and stochastic collocation) approaches. The epistemic UQ methods include local and global interval analysis and Dempster-Shafer evidence theory. These are summarized below and then described in more depth in subsequent sections of this chapter. Dakota additionally supports mixed aleatory/epistemic UQ via interval-valued probability, second-order probability, and Dempster-Shafer theory of evidence. These involve advanced model recursions and are described in Section.

The choice of uncertainty quantification method depends on how the input uncertainty is characterized, the computational budget, and the desired output accuracy. The recommendations for UQ methods are summarized in Tablea and are discussed in the remainder of the section.

TODO: Put table in Doxygen if still needed
5.8. METHODS

Related Topics
- aleatory_uncertainty_quantification_methods
- epistemic_uncertainty_quantification_methods
- variable_support

Related Keywords
- adaptive_sampling : (Experimental) Adaptively refine a Gaussian process surrogate
- global_interval_est : Interval analysis using global optimization methods
- global_reliability : Global reliability methods
- gpais : Gaussian Process Adaptive Importance Sampling
- importance_sampling : Importance sampling
- local_interval_est : Interval analysis using local optimization
- local_reliability : Local reliability method
- mpp_search : Specify which MPP search option to use
- pof_darts : Probability-of-Failure (POF) darts is a novel method for estimating the probability of failure based on random sphere-packing.
- rkd_darts : Recursive k-d (RKD) Darts: Recursive Hyperplane Sampling for Numerical Integration of High-Dimensional Functions.
- sampling : Randomly samples variables according to their distributions

5.8.6 aleatory_uncertainty_quantification_methods

Description
Aleatory uncertainty is also known as inherent variability, irreducible uncertainty, or randomness. Aleatory uncertainty is typically characterized using probability theory.

Related Topics
- sampling
- reliability_methods
- stochastic_expansion_methods

Related Keywords
- importance_sampling : Importance sampling
CHAPTER 5. TOPICS AREA

**Sampling**

**Description**

Sampling techniques are selected using the `sampling` method selection. This method generates sets of samples according to the probability distributions of the uncertain variables and maps them into corresponding sets of response functions, where the number of samples is specified by the `samples` integer specification. Means, standard deviations, coefficients of variation (COVs), and 95% confidence intervals are computed for the response functions. Probabilities and reliabilities may be computed for `response_levels` specifications, and response levels may be computed for either `probability_levels` or `reliability_levels` specifications (refer to the Method Commands chapter in the Dakota Reference Manual [5] for additional information).

Currently, traditional Monte Carlo (MC) and Latin hypercube sampling (LHS) are supported by Dakota and are chosen by specifying `sample_type` as `random` or `lhs`. In Monte Carlo sampling, the samples are selected randomly according to the user-specified probability distributions. Latin hypercube sampling is a stratified sampling technique for which the range of each uncertain variable is divided into $N_s$ segments of equal probability, where $N_s$ is the number of samples requested. The relative lengths of the segments are determined by the nature of the specified probability distribution (e.g., uniform has segments of equal width, normal has small segments near the mean and larger segments in the tails). For each of the uncertain variables, a sample is selected randomly from each of these equal probability segments. These $N_s$ values for each of the individual parameters are then combined in a shuffling operation to create a set of $N_s$ parameter vectors with a specified correlation structure. A feature of the resulting sample set is that *every row and column in the hypercube of partitions has exactly one sample*. Since the total number of samples is exactly equal to the number of partitions used for each uncertain variable, an arbitrary number of desired samples is easily accommodated (as compared to less flexible approaches in which the total number of samples is a product or exponential function of the number of intervals for each variable, i.e., many classical design of experiments methods).

Advantages of sampling-based methods include their relatively simple implementation and their independence from the scientific disciplines involved in the analysis. The main drawback of these techniques is the large number of function evaluations needed to generate converged statistics, which can render such an analysis computationally very expensive, if not intractable, for real-world engineering applications. LHS techniques, in general, require fewer samples than traditional Monte Carlo for the same accuracy in statistics, but they still can be prohibitively expensive. For further information on the method and its relationship to other sampling techniques, one is referred to the works by McKay, et al.[59], Iman and Shortencarier[53], and Helton and Davis[46]. Note that under certain separability conditions associated with the function to be sampled, Latin hypercube sampling provides a more accurate estimate of the mean value than does random sampling. That is, given an equal number of samples, the LHS estimate of the mean will have less variance than the mean value obtained through random sampling.

**Related Topics**

**Related Keywords**

- importance_sampling : Importance sampling
- sampling : Randomly samples variables according to their distributions

reliability_methods

**Description**

Reliability methods provide an alternative approach to uncertainty quantification which can be less computationally demanding than sampling techniques. Reliability methods for uncertainty quantification are based on
probabilistic approaches that compute approximate response function distribution statistics based on specified uncertain variable distributions. These response statistics include response mean, response standard deviation, and cumulative or complementary cumulative distribution functions (CDF/CCDF). These methods are often more efficient at computing statistics in the tails of the response distributions (events with low probability) than sampling based approaches since the number of samples required to resolve a low probability can be prohibitive.

The methods all answer the fundamental question: “Given a set of uncertain input variables, $X$, and a scalar response function, $g$, what is the probability that the response function is below or above a certain level, $\bar{z}$?” The former can be written as $P[g(X) \leq \bar{z}] = F_g(\bar{z})$ where $F_g(\bar{z})$ is the cumulative distribution function (CDF) of the uncertain response $g(X)$ over a set of response levels. The latter can be written as $P[g(X) > \bar{z}]$ and defines the complementary cumulative distribution function (CCDF).

This probability calculation involves a multi-dimensional integral over an irregularly shaped domain of interest, $D$, where $g(X) < z$ as displayed in Figure figUQ05 for the case of two variables. The reliability methods all involve the transformation of the user-specified uncertain variables, $X$, with probability density function, $p(x_1, x_2)$, which can be non-normal and correlated, to a space of independent Gaussian random variables, $u$, possessing a mean value of zero and unit variance (i.e., standard normal variables). The region of interest, $D$, is also mapped to the transformed space to yield, $D_u$, where $g(U) < z$ as shown in Figure figUQ06. The Nataf transformation[17], which is identical to the Rosenblatt transformation[72] in the case of independent random variables, is used in Dakota to accomplish this mapping. This transformation is performed to make the probability calculation more tractable. In the transformed space, probability contours are circular in nature as shown in Figure figUQ06 unlike in the original uncertain variable space, Figure figUQ05. Also, the multi-dimensional integrals can be approximated by simple functions of a single parameter, $\beta$, called the reliability index. $\beta$ is the minimum Euclidean distance from the origin in the transformed space to the response surface. This point is also known as the most probable point (MPP) of failure. Note, however, the methodology is equally applicable for generic functions, not simply those corresponding to failure criteria; this nomenclature is due to the origin of these methods within the disciplines of structural safety and reliability. Note that there are local and global reliability methods. The majority of the methods available are local, meaning that a local optimization formulation is used to locate one MPP. In contrast, global methods can find multiple MPPs if they exist.

Related Topics

Related Keywords

- **global_reliability**: Global reliability methods
- **u_gaussian_process**: Create GP surrogate in u-space
- **x_gaussian_process**: Create GP surrogate in x-space
- **local_reliability**: Local reliability method
- **mpp_search**: Specify which MPP search option to use
- **integration**: Integration approach
- **first_order**: First-order integration scheme
- **probability_refinement**: Allow refinement of probability and generalized reliability results using importance sampling
- **second_order**: Second-order integration scheme
- **no_approx**: Perform MPP search on original response functions (use no approximation)
- **u_taylor_mean**: Form Taylor series approximation in ”u-space” at variable means
• **u_taylor_mpp** : U-space Taylor series approximation with iterative updates

• **u_two_point** : Predict MPP using Two-point Adaptive Nonlinear Approximation in “u-space”

• **x_taylor_mean** : Form Taylor series approximation in ”x-space” at variable means

• **x_taylor_mpp** : X-space Taylor series approximation with iterative updates

• **x_two_point** : Predict MPP using Two-point Adaptive Nonlinear Approximation in ”x-space”

• **probability_refinement** : Allow refinement of probability and generalized reliability results using importance sampling

• **probability_refinement** : Allow refinement of probability and generalized reliability results using importance sampling

**stochastic_expansion_methods**

**Description**

The development of these techniques mirrors that of deterministic finite element analysis utilizing the notions of projection, orthogonality, and weak convergence[31],[32]. Rather than estimating point probabilities, they form an approximation to the functional relationship between response functions and their random inputs, which provides a more complete uncertainty representation for use in multi-code simulations. Expansion methods include polynomial chaos expansions (PCE), which employ multivariate orthogonal polynomials that are tailored to representing particular input probability distributions, and stochastic collocation (SC), which employs multivariate interpolation polynomials. For PCE, expansion coefficients may be evaluated using a spectral projection approach (based on sampling, tensor-product quadrature, Smolyak sparse grid, or cubature methods for numerical integration) or a regression approach (least squares or compressive sensing). For SC, interpolants are formed over tensor-product or sparse grids and may be local or global, value-based or gradient-enhanced, and nodal or hierarchical. In global value-based cases (Lagrange polynomials), the barycentric formulation is used[10],[56],[49] to improve numerical efficiency and stability. Both sets of methods provide analytic response moments and variance-based metrics; however, CDF/CCDF probabilities are evaluated numerically by sampling on the expansion.

**Related Topics**

**Related Keywords**

5.8.7 **epistemic_uncertainty_quantification_methods**

**Description**

Epistemic uncertainty is uncertainty due to lack of knowledge.

In Dakota, epistemic uncertainty analysis is performed using interval analysis or Dempster-Shafer theory of evidence.

Note that epistemic uncertainty can also be modeled probabilistically. It would be more accurate to call this class of method, non-probabilistic uncertainty quantification, but the name persists for historical reasons.

**Related Topics**

• **interval_estimation**

• **evidence_theory**
5.8. METHODS

Related Keywords

- `global_evidence`: Evidence theory with evidence measures computed with global optimization methods
- `global_interval_est`: Interval analysis using global optimization methods
- `local_evidence`: Evidence theory with evidence measures computed with local optimization methods
- `local_interval_est`: Interval analysis using local optimization

**interval_estimation**

**Description**

In interval analysis, one assumes that nothing is known about an epistemic uncertain variable except that its value lies somewhere within an interval. In this situation, it is NOT assumed that the value has a uniform probability of occurring within the interval. Instead, the interpretation is that any value within the interval is a possible value or a potential realization of that variable. In interval analysis, the uncertainty quantification problem is one of determining the resulting bounds on the output (defining the output interval) given interval bounds on the inputs. Again, any output response that falls within the output interval is a possible output with no frequency information assigned to it.

We have the capability to perform interval analysis using either `global_interval_est` or `local_interval_est`. In the global approach, one uses either a global optimization method or a sampling method to assess the bounds. `global_interval_est` allows the user to specify either `lhs`, which performs Latin Hypercube Sampling and takes the minimum and maximum of the samples as the bounds (no optimization is performed) or `ego`. In the case of `ego`, the efficient global optimization method is used to calculate bounds. The `ego` method is described in Section

If the problem is amenable to local optimization methods (e.g., can provide derivatives or use finite difference method to calculate derivatives), then one can use local methods to calculate these bounds. `local_interval_est` allows the user to specify either `sqp` which is sequential quadratic programming, or `nip` which is a nonlinear interior point method.

Note that when performing interval analysis, it is necessary to define interval uncertain variables as described in Section . For interval analysis, one must define only one interval per input variable, in contrast with Dempster-Shafer evidence theory, where an input can have several possible intervals. Interval analysis can be considered a special case of Dempster-Shafer evidence theory where each input is defined by one input interval with a basic probability assignment of one. In Dakota, however, the methods are separate and semantic differences exist in the output presentation. If you are performing a pure interval analysis, we recommend using either `global_interval_est` or `local_interval_est` instead of `global_evidence` or `local_evidence`, for reasons of simplicity. An example of interval estimation is found in the Dakota/examples/users/cantilever_uq_global_interval.in, and also in Section

Note that we have kept separate implementations of interval analysis and Dempster-Shafer evidence theory because our users often want to couple interval analysis on an outer loop’’ with an aleatory, probabilistic analysis on an inner loop” for nested, second-order probability calculations. See Section for additional details on these nested approaches. These interval methods can also be used as the outer loop within an interval-valued probability analysis for propagating mixed aleatory and epistemic uncertainty – refer to Section for additional details.

Interval analysis is often used to model epistemic uncertainty. In interval analysis, the uncertainty quantification problem is one of determining the resulting bounds on the output (defining the output interval) given interval bounds on the inputs.

We can do interval analysis using either `global_interval_est` or `local_interval_est`. In the global approach, one uses either a global optimization method or a sampling method to assess the bounds, whereas the local method uses gradient information in a derivative-based optimization approach.
An example of interval estimation is shown in Figure, with example results in Figure. This example is a demonstration of calculating interval bounds for three outputs of the cantilever beam problem. The cantilever beam problem is described in detail in Section. Given input intervals of [1,10] on beam width and beam thickness, we can see that the interval estimate of beam weight is approximately [1,100].

Min and Max estimated values for each response function:

- **weight**: Min = 1.0000169352e+00 Max = 9.9999491948e+01
- **stress**: Min = -9.7749994284e-01 Max = 2.1499428450e+01
- **displ**: Min = -9.9315672724e-01 Max = 6.7429714485e+01

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### Related Topics

#### Related Keywords
- **global_interval_est**: Interval analysis using global optimization methods
- **local_interval_est**: Interval analysis using local optimization

#### evidence_theory

### Description

This section discusses Dempster-Shafer evidence theory. In this approach, one does not assign a probability distribution to each uncertain input variable. Rather, one divides each uncertain input variable into one or more intervals. The input parameters are only known to occur within intervals: nothing more is assumed.

Each interval is defined by its upper and lower bounds, and a Basic Probability Assignment (BPA) associated with that interval. The BPA represents a probability of that uncertain variable being located within that interval.

The intervals and BPAs are used to construct uncertainty measures on the outputs called "belief" and "plausibility." Belief represents the smallest possible probability that is consistent with the evidence, while plausibility represents the largest possible probability that is consistent with the evidence. For more information about the Dempster-Shafer theory of evidence, see [66] and [47].

Similar to the interval approaches, one may use global or local methods to determine plausibility and belief measures for the outputs.

#### Usage Notes

Note that to calculate the plausibility and belief cumulative distribution functions, one has to look at all combinations of intervals for the uncertain variables. Within each interval cell combination, the minimum and maximum value of the objective function determine the belief and plausibility, respectively. In terms of implementation, global methods use LHS sampling or global optimization to calculate the minimum and maximum values of the objective function within each interval cell, while local methods use gradient-based optimization methods to calculate these minima and maxima.

Finally, note that many non-deterministic keywords apply to the evidence methods, but one needs to be careful about the interpretation and translate probabilistic measures to epistemic ones. For example, if the user specifies distribution of type complementary, a complementary plausibility and belief function will be generated for the evidence methods (as opposed to a complementary distribution function in the sampling case). If the user specifies a set of responses levels, both the belief and plausibility will be calculated for each response level. Likewise, if the user specifies a probability level, the probability level will be interpreted both as a belief and plausibility, and response levels corresponding to the belief and plausibility levels will be calculated. Finally, if generalized reliability levels are specified, either as inputs (gen_reliability_levels) or outputs (response_levels with compute gen_reliabilities), then these are directly converted to/from probability levels and the same probability-based mappings described above are performed.
5.8. METHODS

5.8.8 variable_support

Description

Different nondeterministic methods have differing support for uncertain variable distributions. Tables 5.37, 5.38, and 5.39 summarize the uncertain variables that are available for use by the different methods, where a "-" indicates that the distribution is not supported by the method, a "U" means the uncertain input variables of this type must be uncorrelated, a "C" denotes that correlations are supported involving uncertain input variables of this type, and an "A" means the appropriate variables must be specified as active in the variables specification block. For example, if one wants to support sampling or a stochastic expansion method over both continuous uncertain and continuous state variables, the specification active all must be listed in the variables specification block. Additional notes include:

- we have four variants for stochastic expansions (SE), listed as Wiener, Askey, Extended, and Piecewise which draw from different sets of basis polynomials. The term stochastic expansion indicates polynomial chaos and stochastic collocation collectively, although the Piecewise option is only currently supported for stochastic collocation. Refer to polynomial_chaos and stoch_collocation for additional information on these three options.

- methods supporting the epistemic interval distributions have differing approaches: sampling and the lhs option of global_interval_est model the interval basic probability assignments (BPAs) as continuous histogram bin distributions for purposes of generating samples; local_interval_est and the ego option of global_interval_est ignore the BPA details and models these variables as simple bounded regions defined by the cell extremes; and local_evidence and global_evidence model the interval specifications as true BPAs.

Related Topics

Related Keywords

5.8.9 optimization_and_calibration

Description

Optimization algorithms work to minimize (or maximize) an objective function, typically calculated by the user simulation code, subject to constraints on design variables and responses. Available approaches in Dakota include well-tested, proven gradient-based, derivative-free local, and global methods for use in science and engineering design applications. Dakota also offers more advanced algorithms, e.g., to manage multi-objective optimization or perform surrogate-based minimization. This chapter summarizes optimization problem formulation, standard algorithms available in Dakota (mostly through included third-party libraries, see Section 6.5 of[4]), some advanced capabilities, and offers usage guidelines.
Optimization Formulations

This section provides a basic introduction to the mathematical formulation of optimization problems. The primary goal of this section is to introduce terms relating to these topics, and is not intended to be a description of theory or numerical algorithms. For further details, consult [8], [34], [41], [65], and [84].

A general optimization problem is formulated as follows:

\[
\begin{align*}
\text{minimize:} & \quad f(x) \\
\text{subject to:} & \quad g_L(x) \leq g(x) \leq g_U \\
& \quad h(x) = h_t \\
& \quad a_L \leq A_i x \leq a_U \\
& \quad x_L \leq x \leq x_U
\end{align*}
\]  

(5.1)

where vector and matrix terms are marked in bold typeface. In this formulation, \(x = [x_1, x_2, \ldots, x_n]\) is an \(n\)-dimensional vector of real-valued design variables or design parameters. The \(n\)-dimensional vectors, \(x_L\) and \(x_U\), are the lower and upper bounds, respectively, on the design parameters. These bounds define the allowable values for the elements of \(x\), and the set of all allowable values is termed the design space or the parameter space. A design point or a sample point is a particular set of values within the parameter space.

The optimization goal is to minimize the objective function, \(f(x)\), while satisfying the constraints. Constraints can be categorized as either linear or nonlinear and as either inequality or equality. The nonlinear inequality constraints, \(g(x)\), are “2-sided,” in that they have both lower and upper bounds, \(g_L\) and \(g_U\), respectively. The nonlinear equality constraints, \(h(x)\), have target values specified by \(h_t\). The linear inequality constraints create a linear system \(A_i x\), where \(A_i\) is the coefficient matrix for the linear system. These constraints are also 2-sided as they have lower and upper bounds, \(a_L\) and \(a_U\), respectively. The linear equality constraints create a linear system \(A_c x\), where \(A_c\) is the coefficient matrix for the linear system and \(a_t\) are the target values. The constraints partition the parameter space into feasible and infeasible regions. A design point is said to be feasible if and only if it satisfies all of the constraints. Correspondingly, a design point is said to be infeasible if it violates one or more of the constraints.

Many different methods exist to solve the optimization problem given in Section 6.1 of [4], all of which iterate on \(x\) in some manner. That is, an initial value for each parameter in \(x\) is chosen, the response quantities, \(f(x), g(x), h(x)\), are computed, often by running a simulation, and some algorithm is applied to generate a new \(x\) that will either reduce the objective function, reduce the amount of infeasibility, or both. To facilitate a general presentation of these methods, three criteria will be used in the following discussion to differentiate them: optimization problem type, search goal, and search method.

The optimization problem type can be characterized both by the types of constraints present in the problem and by the linearity or nonlinearity of the objective and constraint functions. For constraint categorization, a hierarchy of complexity exists for optimization algorithms, ranging from simple bound constraints, through linear constraints, to full nonlinear constraints. By the nature of this increasing complexity, optimization problem categorizations are inclusive of all constraint types up to a particular level of complexity. That is, an unconstrained problem has no constraints, a bound-constrained problem has only lower and upper bounds on the design parameters, a linearly-constrained problem has both linear and bound constraints, and a nonlinearly-constrained problem may contain the full range of nonlinear, linear, and bound constraints. If all of the linear and nonlinear constraints are equality constraints, then this is referred to as an equality-constrained problem, and if all of the linear and nonlinear constraints are inequality constraints, then this is referred to as an inequality-constrained problem. Further categorizations can be made based on the linearity of the objective and constraint functions. A problem where the objective function and all constraints are linear is called a linear programming (LP) problem.
5.8. METHODS

These types of problems commonly arise in scheduling, logistics, and resource allocation applications. Likewise, a problem where at least some of the objective and constraint functions are nonlinear is called a nonlinear programming (NLP) problem. These NLP problems predominate in engineering applications and are the primary focus of Dakota.

The search goal refers to the ultimate objective of the optimization algorithm, i.e., either global or local optimization. In global optimization, the goal is to find the design point that gives the lowest feasible objective function value over the entire parameter space. In contrast, in local optimization, the goal is to find a design point that is lowest relative to a “nearby” region of the parameter space. In almost all cases, global optimization will be more computationally expensive than local optimization. Thus, the user must choose an optimization algorithm with an appropriate search scope that best suits the problem goals and the computational budget.

The search method refers to the approach taken in the optimization algorithm to locate a new design point that has a lower objective function or is more feasible than the current design point. The search method can be classified as either gradient-based or nongradient-based. In a gradient-based algorithm, gradients of the response functions are computed to find the direction of improvement. Gradient-based optimization is the search method that underlies many efficient local optimization methods. However, a drawback to this approach is that gradients can be computationally expensive, inaccurate, or even nonexistent. In such situations, nongradient-based search methods may be useful. There are numerous approaches to nongradient-based optimization. Some of the more well known of these include pattern search methods (nongradient-based local techniques) and genetic algorithms (nongradient-based global techniques).

Because of the computational cost of running simulation models, surrogate-based optimization (SBO) methods are often used to reduce the number of actual simulation runs. In SBO, a surrogate or approximate model is constructed based on a limited number of simulation runs. The optimization is then performed on the surrogate model. Dakota has an extensive framework for managing a variety of local, multipoint, global, and hierarchical surrogates for use in optimization. Finally, sometimes there are multiple objectives that one may want to optimize simultaneously instead of a single scalar objective. In this case, one may employ multi-objective methods that are described in Section 6.3.1 of[4].

This overview of optimization approaches underscores that no single optimization method or algorithm works best for all types of optimization problems. Section 6.4 of[4] offers guidelines for choosing a Dakota optimization algorithm best matched to your specific optimization problem.

Constraint Considerations Dakota’s input commands permit the user to specify two-sided nonlinear inequality constraints of the form \( g_L \leq g_i(x) \leq g_U \), as well as nonlinear equality constraints of the form \( h_j(x) = h_{j_0} \).

Some optimizers (e.g., npsol, optpp, soga, and moga methods) can handle these constraint forms directly, whereas other optimizers (e.g., asynch_pattern_search, dot_, and conmin_, mesh_adaptive_search) require Dakota to perform an internal conversion of all constraints to one-sided inequality constraints of the form \( g_L(x) \leq 0 \). In the latter case, the two-sided inequality constraints are treated as \( g_L(x) - g_U \leq 0 \) and \( g_L(x) - g_U(x) \leq 0 \) and the equality constraints are treated as \( h_j(x) - h_{j_0} \leq 0 \) and \( h_{j_0} - h_j(x) \leq 0 \). The situation is similar for linear constraints: asynch_pattern_search, npsol_, optpp_, soga, and moga methods support them directly, whereas dot_ and conmin_ methods do not. For linear inequalities of the form \( a_{L_j} \leq a^T_j x \leq a_{U_j} \) and linear equalities of the form \( a^T_j x = a_{j_0} \), the nonlinear constraint arrays in dot_ and conmin_ methods are augmented to include \( a^T_j x - a_{U_j} \leq 0 \) and \( a_{L_j} - a^T_j x \leq 0 \) in the inequality case and \( a^T_j x - a_{j_0} \leq 0 \) and \( a_{L_j} - a^T_j x \leq 0 \) in the equality case. Awareness of these constraint augmentation procedures can be important for understanding the diagnostic data returned from the dot_ and conmin_ methods. Other optimizers fall somewhere in between. nlpql_ methods support nonlinear equality constraints \( h_j(x) = 0 \) and nonlinear one-sided inequalities \( g_i(x) \geq 0 \), but does not natively support linear constraints. Constraint mappings are used with NLPQL for both linear and nonlinear cases. Most coliny_ methods now support two-sided nonlinear inequality constraints and nonlinear constraints with targets, but do not natively support linear constraints.

When gradient and Hessian information is used in the optimization, derivative components are most com-
monly computed with respect to the active continuous variables, which in this case are the *continuous design variables*. This differs from parameter study methods (for which all continuous variables are active) and from nondeterministic analysis methods (for which the uncertain variables are active). Refer to Chapter 11 of [4] for additional information on derivative components and active continuous variables.

**Optimizing with Dakota: Choosing a Method**

This section summarizes the optimization methods available in Dakota. We group them according to search method and search goal and establish their relevance to types of problems. For a summary of this discussion, see Section 6.4 of [4].

**Gradient-Based Local Methods**  
Gradient-based optimizers are best suited for efficient navigation to a local minimum in the vicinity of the initial point. They are not intended to find global optima in nonconvex design spaces. For global optimization methods, see Section 6.2.3 of [4]. Gradient-based optimization methods are highly efficient, with the best convergence rates of all of the local optimization methods, and are the methods of choice when the problem is smooth, unimodal, and well-behaved. However, these methods can be among the least robust when a problem exhibits nonsmooth, discontinuous, or multimodal behavior. The derivative-free methods described in Section 6.2.2 of [4] are more appropriate for problems with these characteristics.

Gradient accuracy is a critical factor for gradient-based optimizers, as inaccurate derivatives will often lead to failures in the search or pre-mature termination of the method. Analytic gradients and Hessians are ideal but often unavailable. If analytic gradient and Hessian information can be provided by an application code, a full Newton method will achieve quadratic convergence rates near the solution. If only gradient information is available and the Hessian information is approximated from an accumulation of gradient data, the superlinear convergence rates can be obtained. It is most often the case for engineering applications, however, that a finite difference method will be used by the optimization algorithm to estimate gradient values. Dakota allows the user to select the step size for these calculations, as well as choose between forward-difference and central-difference algorithms. The finite difference step size should be selected as small as possible, to allow for local accuracy and convergence, but not so small that the steps are “in the noise.” This requires an assessment of the local smoothness of the response functions using, for example, a parameter study method. Central differencing will generally produce more reliable gradients than forward differencing but at roughly twice the expense.

Gradient-based methods for nonlinear optimization problems can be described as iterative processes in which a sequence of subproblems, usually which involve an approximation to the full nonlinear problem, are solved until the solution converges to a local optimum of the full problem. The optimization methods available in Dakota fall into several categories, each of which is characterized by the nature of the subproblems solved at each iteration.

**Related Topics**

- local_optimization_methods
- global_optimization_methods
- bayesian_calibration
- nonlinear_least_squares
- advanced_optimization

**Related Keywords**

- dl_solver : (Experimental) Dynamically-loaded solver
5.8. METHODS

5.8.10 local_optimization_methods

Description
empty

Related Topics

- unconstrained
- constrained
- sequential_quadratic_programming

Related Keywords

- coliny_cobyla : Constrained Optimization BY Linear Approximations (COBYLA)
- nlql_sqp : Sequential Quadratic Program
- nonlinear_cg : (Experimental) nonlinear conjugate gradient optimization
- npsol_sqp : Sequential Quadratic Program
- optpp_cg : A conjugate gradient optimization method
- optpp_fd_newton : Finite Difference Newton optimization method
- optpp_g_newton : Newton method based least-squares calibration
- optpp_newton : Newton method based optimization
- optpp_q_newton : Quasi-Newton optimization method

unconstrained

Description
empty

Related Topics

Related Keywords

constrained

Description
empty

Related Topics

Related Keywords

- coliny_cobyla : Constrained Optimization BY Linear Approximations (COBYLA)
sequential_quadratic_programming

Description

Sequential Quadratic Programming (SQP) algorithms are a class of mathematical programming problems used to solve nonlinear optimization problems with nonlinear constraints. These methods are a generalization of Newton’s method: each iteration involves minimizing a quadratic model of the problem. These subproblems are formulated as minimizing a quadratic approximation of the Lagrangian subject to linearized constraints. Only gradient information is required; Hessians are approximated by low-rank updates defined by the step taken at each iteration. It is important to note that while the solution found by an SQP method will respect the constraints, the intermediate iterates may not. SQP methods available in Dakota are dot_sqp, nlpql_sqp, nlssol_sqp, and npsol_sqp. The particular implementation in nlpql_sqp uses a variant with distributed and non-monotone line search. Thus, this variant is designed to be more robust in the presence of inaccurate or noisy gradients common in many engineering applications.

Related Topics

Related Keywords

- nlpql_sqp : Sequential Quadratic Program
- nlssol_sqp : Sequential Quadratic Program for nonlinear least squares
- npsol_sqp : Sequential Quadratic Program

5.8.11 global_optimization_methods

Description

empty

Related Topics

Related Keywords

- asynch_pattern_search : Pattern search, derivative free optimization method
- coliny_direct : Dlviding RECTangles method
- coliny_ea : Evolutionary Algorithm
- coliny_pattern_search : Pattern search, derivative free optimization method
- efficient_global : Global Surrogate Based Optimization, a.k.a. EGO
- ncsu_direct : Dlviding RECTangles method
- soga : Single-objective Genetic Algorithm (a.k.a Evolutionary Algorithm)

5.8.12 bayesian_calibration

Description

See the discussion of Bayesian Calibration in the Dakota User’s Manual [4].
5.8. METHODS

Related Topics

Related Keywords

- **bayes.calibration**: Bayesian calibration
- **dream**: DREAM (DiffeRential Evolution Adaptive Metropolis)
- **chains**: Number of chains in DREAM
- **crossover.chain.pairs**: Number of chains used in crossover.
- **gr.threshold**: Convergence tolerance for the Gelman-Rubin statistic
- **jump.step**: Number of generations a long jump step is taken
- **num.cr**: Number of candidate points for each crossover.
- **gpmsa**: (Experimental) Gaussian Process Models for Simulation Analysis (GPMSA) Bayesian calibration
- **adaptive.metropolis**: Use the Adaptive Metropolis MCMC algorithm
- **delayed.rejection**: Use the Delayed Rejection MCMC algorithm
- **dram**: Use the DRAM MCMC algorithm
- **metropolis.hastings**: Use the Metropolis-Hastings MCMC algorithm
- **proposal.covariance**: Defines the technique used to generate the MCMC proposal covariance.
- **derivatives**: Use derivatives to inform the MCMC proposal covariance.
- **prior**: Uses the covariance of the prior distributions to define the MCMC proposal covariance.
- **queso**: Markov Chain Monte Carlo algorithms from the QUESO package
- **adaptive.metropolis**: Use the Adaptive Metropolis MCMC algorithm
- **delayed.rejection**: Use the Delayed Rejection MCMC algorithm
- **dram**: Use the DRAM MCMC algorithm
- **metropolis.hastings**: Use the Metropolis-Hastings MCMC algorithm
- **multilevel**: Use the multilevel MCMC algorithm.
- **proposal.covariance**: Defines the technique used to generate the MCMC proposal covariance.
- **derivatives**: Use derivatives to inform the MCMC proposal covariance.
- **prior**: Uses the covariance of the prior distributions to define the MCMC proposal covariance.
5.8.13 nonlinear_least_squares

Description
Dakota’s least squares branch currently contains three methods for solving nonlinear least squares problems:

- NL2SOL, a trust-region method that adaptively chooses between two Hessian approximations (Gauss--Newton and Gauss-Newton plus a quasi-Newton approximation to the rest of the Hessian)
- NLSSOL, a sequential quadratic programming (SQP) approach that is from the same algorithm family as NPSOL
- Gauss-Newton, which supplies the Gauss-Newton Hessian approximation to the full-Newton optimizers from OPT++.

The important difference of these algorithms from general-purpose optimization methods is that the response set is defined by calibration terms (e.g. separate terms for each residual), rather than an objective function. Thus, a finer granularity of data is used by least squares solvers as compared to that used by optimizers. This allows the exploitation of the special structure provided by a sum of squares objective function.

Related Topics

Related Keywords
- nl2sol : Trust-region method for nonlinear least squares
- nlssol_sqp : Sequential Quadratic Program for nonlinear least squares

5.8.14 advanced_optimization

Description
empty

Related Topics
- scaling
  - multiobjective_methods
  - surrogate_based_optimization_methods

Related Keywords
- scaling

Description
empty
5.9. ADVANCED TOPICS

Related Topics

Related Keywords
multiobjective methods

Description
empty

Related Topics

Related Keywords
surrogate_based_optimization_methods

Description
empty

Related Topics

Related Keywords
• efficient_global : Global Surrogate Based Optimization, a.k.a. EGO
• surrogate_based_global : Global Surrogate Based Optimization
• surrogate_based_local : Local Surrogate Based Optimization

5.9 advanced_topics

Description
Advanced Dakota capabilities

Related Topics
• advanced_strategies
• advanced_model_recursion
• advanced_simulation_interfaces
• advanced_optimization

Related Keywords

5.9.1 advanced_strategies

Description
empty
5.9.2 advanced_model_recursion

Description
empty

Related Topics

- hybrid_and_recursions_logic

Related Keywords
hybrid_and_recursions_logic

5.9.3 advanced_simulation_interfaces

Description
empty

Related Topics

- simulation_failure
  - concurrency_and_parallelism

Related Keywords
simulation_failure

Description
empty

Related Topics
5.9. ADVANCED TOPICS

Related Topics

Related Keywords

- **processors_per_analysis**: Specify the number of processors per analysis when Dakota is run in parallel
- **analysis_scheduling**: Specify the scheduling of concurrent analyses when Dakota is run in parallel
- **master**: Specify a dedicated master partition for parallel analysis scheduling
- **peer**: Specify a peer partition for parallel analysis scheduling
- **analysis_servers**: Specify the number of analysis servers when Dakota is run in parallel
- **asynchronous**: Specify local evaluation or analysis concurrency
- **analysis_concurrency**: Limit the number of analysis drivers within an evaluation that Dakota will schedule
- **evaluation_concurrency**: Determine how many concurrent evaluations Dakota will schedule
- **local_evaluation_scheduling**: Control how local asynchronous jobs are scheduled
- **master**: Specify a dedicated master partition for parallel evaluation scheduling
- **peer**: Specify a peer partition for parallel evaluation scheduling
- **dynamic**: Specify dynamic scheduling in a peer partition when Dakota is run in parallel.
- **static**: Specify static scheduling in a peer partition when Dakota is run in parallel.
- **evaluation_servers**: Specify the number of evaluation servers when Dakota is run in parallel
- **processors_per_evaluation**: Specify the number of processors per evaluation server when Dakota is run in parallel
- **iterator_scheduling**: Specify the scheduling of concurrent iterators when Dakota is run in parallel
- **master**: Specify a dedicated master partition for parallel iterator scheduling
- **peer**: Specify a peer partition for parallel iterator scheduling
- **iterator_servers**: Specify the number of iterator servers when Dakota is run in parallel
- **processors_per_iterator**: Specify the number of processors per iterator server when Dakota is run in parallel
- **iterator_scheduling**: Specify the scheduling of concurrent iterators when Dakota is run in parallel
- **master**: Specify a dedicated master partition for parallel iterator scheduling
- **peer**: Specify a peer partition for parallel iterator scheduling
- **iterator_servers**: Specify the number of iterator servers when Dakota is run in parallel
- **processors_per_iterator**: Specify the number of processors per iterator server when Dakota is run in parallel
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• **iterator_scheduling**: Specify the scheduling of concurrent iterators when Dakota is run in parallel
• **master**: Specify a dedicated master partition for parallel iterator scheduling
• **peer**: Specify a peer partition for parallel iterator scheduling
• **iterator_servers**: Specify the number of iterator servers when Dakota is run in parallel
• **processors_per_iterator**: Specify the number of processors per iterator server when Dakota is run in parallel

### 5.9.4 advanced_optimization

**Description**

empty

**Related Topics**

• **scaling**

• **multiobjective_methods**

• **surrogate_based_optimization_methods**

**Related Keywords**

**scaling**

**Description**

empty

**Related Topics**

**Related Keywords**

**multiobjective_methods**

**Description**

empty

**Related Topics**

**Related Keywords**

**surrogate_based_optimization_methods**

**Description**

empty
5.10. PACKAGES

Related Topics

Related Keywords
- efficient_global : Global Surrogate Based Optimization, a.k.a. EGO
- surrogate_based_global : Global Surrogate Based Optimization
- surrogate_based_local : Local Surrogate Based Optimization

5.10 packages

Description
This topic organizes information about the different software packages (libraries) that are integrated into Dakota

Related Topics
- package_coliny
- package_conmin
- package_ddace
- package_dot
- package_fsudace
- package_hopspack
- package_jega
- package_nlpql
- package_npsol
- package_optpp
- package_psuade
- package_queso
- package_scolib

Related Keywords

5.10.1 package_coliny

Description
SCOLIB (formerly known as COLINY) is a collection of nongradient-based optimizers that support the Common Optimization Library INterface (COLIN). SCOLIB optimizers currently include coliny_cobyla, coliny_direct, coliny_ea, coliny_pattern_search and coliny_solis_wets. (Yes, the input spec still has "coliny" prepended to the method name.) Additional SCOLIB information is available from https://software-sandia.gov/trac/acro.
SCOLIB solvers now support bound constraints and general nonlinear constraints. Supported nonlinear constraints include both equality and two-sided inequality constraints. SCOLIB solvers do not yet support linear constraints. Most SCOLIB optimizers treat constraints with a simple penalty scheme that adds \( \text{constraint\_penalty} \times \text{the sum of squares of the constraint violations} \) to the objective function. Specific exceptions to this method for handling constraint violations are noted below. (The default value of \( \text{constraint\_penalty} \) is 1000.0, except for methods that dynamically adapt their constraint penalty, for which the default value is 1.0.)

The method independent controls for \text{max\_iterations} and \text{max\_function\_evaluations} limit the number of major iterations and the number of function evaluations that can be performed during a SCOLIB optimization, respectively. The \text{convergence\_tolerance} control defines the threshold value on relative change in the objective function that indicates convergence. The \text{output\_verbosity} specification controls the amount of information generated by SCOLIB: the \text{silent}, \text{quiet}, and \text{normal} settings correspond to minimal reporting from SCOLIB, whereas the \text{verbose} setting corresponds to a higher level of information, and \text{debug} outputs method initialization and a variety of internal SCOLIB diagnostics. The majority of SCOLIB’s methods perform independent function evaluations that can directly take advantage of Dakota’s parallel capabilities. Only \text{coliny\_solis\_wets}, \text{coliny\_cobyla}, and certain configurations of \text{coliny\_pattern\_search} are inherently serial. The parallel methods automatically utilize parallel logic when the Dakota configuration supports parallelism. Lastly, neither \text{speculative\_gradients} nor linear constraints are currently supported with SCOLIB.

Some SCOLIB methods exploit parallelism through the use of Dakota’s concurrent function evaluations. The nature of the algorithms, however, limits the amount of concurrency that can be exploited. The maximum amount of evaluation concurrency that can be leveraged by the various methods is as follows:

- COBYLA: one
- DIRECT: twice the number of variables
- Evolutionary Algorithms: size of the population
- Pattern Search: size of the search pattern
- Solis-Wets: one

All SCOLIB methods support the \text{show\_misc\_options} optional specification which results in a dump of all the allowable method inputs. Note that the information provided by this command refers to optimizer parameters that are internal to SCOLIB, and which may differ from corresponding parameters used by the Dakota interface. The \text{misc\_options} optional specification provides a means for inputting additional settings supported by the SCOLIB methods but which are not currently mapped through the Dakota input specification. Care must be taken in using this specification; they should only be employed by users familiar with the full range of parameter specifications available directly from SCOLIB and understand any differences that exist between those specifications and the ones available through Dakota.

Each of the SCOLIB methods supports the \text{solution\_target} control, which defines a convergence criterion in which the optimizer will terminate if it finds an objective function value lower than the specified target.

Related Topics

Related Keywords

- \text{coliny\_beta}: (Experimental) Coliny beta solver
- \text{coliny\_cobyla}: Constrained Optimization BY Linear Approximations (COBYLA)
- \text{coliny\_direct}: DIviding RECTangles method
5.10. PACKAGES

- **coliny_ea**: Evolutionary Algorithm
- **coliny_pattern_search**: Pattern search, derivative free optimization method
- **coliny_solis_wets**: Simple greedy local search method

5.10.2 **package_conmin**

**Description**

The CONMIN library\[83\] is a public domain library of nonlinear programming optimizers, specifically the Fletcher-Reeves conjugate gradient (Dakota’s `conmin.frcg` method) method for unconstrained optimization, and the method of feasible directions (Dakota’s `conmin.mfd` method) for constrained optimization. As CONMIN was a predecessor to the DOT commercial library, the algorithm controls are very similar.

**Related Topics**

**Related Keywords**

- **conmin**: Access to methods in the CONMIN library
- **frcg**: A conjugate gradient optimization method
- **mfd**: Method of feasible directions

5.10.3 **package_ddace**

**Description**

The Distributed Design and Analysis of Computer Experiments (DDACE) library provides the following DA-CE techniques: grid sampling (`grid`), pure random sampling (`random`), orthogonal array sampling (`oas`), latin hypercube sampling (`lhs`), orthogonal array latin hypercube sampling (`oa_lhs`), Box-Behnken (`box_behnken`), and central composite design (`central_composite`).

It is worth noting that there is some overlap in sampling techniques with those available from the non-deterministic branch. The current distinction is that the nondeterministic branch methods are designed to sample within a variety of probability distributions for uncertain variables, whereas the design of experiments methods treat all variables as having uniform distributions. As such, the design of experiments methods are well-suited for performing parametric studies and for generating data sets used in building global approximations, but are not currently suited for assessing the effect of uncertainties characterized with probability distribution. If a design of experiments over both design/state variables (treated as uniform) and uncertain variables (with probability distributions) is desired, then `sampling` can support this with active all specified in the Variables specification block.

**Related Topics**

**Related Keywords**

- **dace**: Design and Analysis of Computer Experiments
5.10.4 package_DOT

Description

The DOT library [85] contains nonlinear programming optimizers, specifically the Broyden-Fletcher-Goldfarb-Shanno (Dakota’s dot_bfgs method) and Fletcher-Reeves conjugate gradient (Dakota’s dot_frcg method) methods for unconstrained optimization, and the modified method of feasible directions (Dakota’s dot_mmfd method), sequential linear programming (Dakota’s dot_slp method), and sequential quadratic programming (Dakota’s dot_sqp method) methods for constrained optimization.

Related Topics

Related Keywords

- dot: Access to methods in the DOT package
- bfgs: A conjugate gradient optimization method
- frcg: A conjugate gradient optimization method
- mmfd: Method of feasible directions
- slp: Sequential Linear Programming
- sqp: Sequential Quadratic Program

5.10.5 package_FSUDace

Description

The Florida State University Design and Analysis of Computer Experiments (FSUDace) library provides the following DACE techniques: quasi-Monte Carlo sampling (fsu_quasi_mc) based on the Halton sequence (halton) or the Hammersley sequence (hammersley), and Centroidal Voronoi Tessellation (fsu_cvt).

Related Topics

Related Keywords

- quality_metrics: Calculate metrics to assess the quality of quasi-Monte Carlo samples
- fsu_cvt: Design of Computer Experiments - Centroidal Voronoi Tessellation
- quality_metrics: Calculate metrics to assess the quality of quasi-Monte Carlo samples
- halton: Generate samples from a Halton sequence
- fsu_quasi_mc: Design of Computer Experiments - Quasi-Monte Carlo sampling
- halton: Generate samples from a Halton sequence
- hammersley: Use Hammersley sequences
- quality_metrics: Calculate metrics to assess the quality of quasi-Monte Carlo samples
5.10.6 package_hopspack

Description
The HOPSPACK software [69] contains the asynchronous parallel pattern search (APPS) algorithm [37]. It can handle unconstrained problems as well as those with bound constraints, linear constraints, and general nonlinear constraints.

HOPSPACK is available to the public under the GNU LGPL and the source code is included with Dakota. HOPSPACK-specific software documentation is available from https://software.sandia.gov/trac/hopspack.

Related Topics

Related Keywords
- asynch_pattern_search : Pattern search, derivative free optimization method

5.10.7 package_jega

Description
The JEGA library[19] contains two global optimization methods. The first is a Multi-objective Genetic Algorithm (MOGA) which performs Pareto optimization. The second is a Single-objective Genetic Algorithm (SOGA) which performs optimization on a single objective function. Both methods support general constraints and a mixture of real and discrete variables. The JEGA library was written by John Eddy, currently a member of the technical staff in the System Readiness and Sustainment Technologies department at Sandia National Laboratories in Albuquerque. These algorithms are accessed as moga and soga within Dakota.

Related Topics

Related Keywords
- moga : Multi-objective Genetic Algorithm (a.k.a Evolutionary Algorithm)
- soga : Single-objective Genetic Algorithm (a.k.a Evolutionary Algorithm)

5.10.8 package_nlpql

Description
The NLPQL library includes a sequential quadratic programming (SQP) optimizer, specified as Dakota’s nlpql-sqp method, for constrained optimization. The particular implementation used is NLPQLP[74], a variant with distributed and non-monotone line search. NLPQL is commercially licensed (available from the author) and not distributed with public versions of Dakota.

Related Topics

Related Keywords
- nlpql_sqp : Sequential Quadratic Program
5.10.9 package npsol

Description

The NPSOL library[33] contains a sequential quadratic programming (SQP) implementation (the npsol_sqp method). SQP is a nonlinear programming optimizer for constrained minimization.

Related Topics

Related Keywords

- npsol_sqp: Sequential Quadratic Program

5.10.10 package optpp

Description

The OPT++ library[60] contains primarily gradient-based nonlinear programming optimizers for unconstrained, bound-constrained, and nonlinearly constrained minimization: Polak-Ribiere conjugate gradient (Dakota’s optpp_cg method), quasi-Newton (Dakota’s optpp_q_newton method), finite difference Newton (Dakota’s optpp_fd_newton method), and full Newton (Dakota’s optpp_newton method).

The conjugate gradient method is strictly unconstrained, and each of the Newton-based methods are automatically bound to the appropriate OPT++ algorithm based on the user constraint specification (unconstrained, bound-constrained, or generally-constrained). In the generally-constrained case, the Newton methods use a nonlinear interior-point approach to manage the constraints. The library also contains a direct search algorithm, PDS (parallel direct search, Dakota’s optpp_pds method), which supports bound constraints.

Controls

1. max_iterations
2. max_function_evaluations
3. convergence_tolerance
4. output
5. speculative

Concurrency

OPT++’s gradient-based methods are not parallel algorithms and cannot directly take advantage of concurrent function evaluations. However, if numerical_gradients with method_source dakota is specified, a parallel Dakota configuration can utilize concurrent evaluations for the finite difference gradient computations.

Constraints

Linear constraint specifications are supported by each of the Newton methods (optpp_newton, optpp_q_newton, optpp_fd_newton, and optpp_g_newton)

- optpp_cg must be unconstrained
- optpp_pds can be, at most, bound-constrained.

Related Topics

Related Keywords

- optpp_cg: A conjugate gradient optimization method
5.10. PACKAGES

- **optpp_fd_newton**: Finite Difference Newton optimization method
- **optpp_g_newton**: Newton method based least-squares calibration
- **optpp_newton**: Newton method based optimization
- **optpp_pds**: Simplex-based derivative free optimization method
- **optpp_q_newton**: Quasi-Newton optimization method

5.10.11 package_psuade

**Description**
The Problem Solving Environment for Uncertainty Analysis and Design Exploration (PSUADE) is a Lawrence Livermore National Laboratory tool for metamodeling, sensitivity analysis, uncertainty quantification, and optimization. Its features include non-intrusive and parallel function evaluations, sampling and analysis methods, an integrated design and analysis framework, global optimization, numerical integration, response surfaces (MARS and higher order regressions), graphical output with Ppplot or Matlab, and fault tolerance [81].

**Related Topics**

**Related Keywords**
- **psuade_moat**: Morris One-at-a-Time

5.10.12 package_queso

**Description**
QUESO stands for Quantification of Uncertainty for Estimation, Simulation, and Optimization. It supports Bayesian calibration methods. It is developed at The University of Texas at Austin.

**Related Topics**

**Related Keywords**
- **bayes_calibration**: Bayesian calibration
- **gpmsa**: (Experimental) Gaussian Process Models for Simulation Analysis (GPMSA) Bayesian calibration
- **queso**: Markov Chain Monte Carlo algorithms from the QUESO package

5.10.13 package_scolib

**Description**
SCOLIB (formerly known as COLINY) is a collection of nongradient-based optimizers that support the Common Optimization Library INterface (COLIN). SCOLIB optimizers currently include coliny_cobyla, coliny_direct, coliny_ea, coliny_pattern_search and coliny_solis_wets. (Yes, the input spec still has "coliny" prepended to the method name.) Additional SCOLIB information is available from https://software.sandia.gov/trac/acro.
SCOLIB solvers now support bound constraints and general nonlinear constraints. Supported nonlinear constraints include both equality and two-sided inequality constraints. SCOLIB solvers do not yet support linear constraints. Most SCOLIB optimizers treat constraints with a simple penalty scheme that adds constraint_penalty times the sum of squares of the constraint violations to the objective function. Specific exceptions to this method for handling constraint violations are noted below. (The default value of constraint_penalty is 1000.0, except for methods that dynamically adapt their constraint penalty, for which the default value is 1.0.)

The method independent controls for max_iterations and max_function_evaluations limit the number of major iterations and the number of function evaluations that can be performed during a SCOLIB optimization, respectively. The convergence_tolerance control defines the threshold value on relative change in the objective function that indicates convergence. The output verbosity specification controls the amount of information generated by SCOLIB: the silent, quiet, and normal settings correspond to minimal reporting from SCOLIB, whereas the verbose setting corresponds to a higher level of information, and debug outputs method initialization and a variety of internal SCOLIB diagnostics. The majority of SCOLIB’s methods perform independent function evaluations that can directly take advantage of Dakota’s parallel capabilities. Only coliny_solis_wets, coliny_cobyla, and certain configurations of coliny_pattern_search are inherently serial. The parallel methods automatically utilize parallel logic when the Dakota configuration supports parallelism. Lastly, neither speculative gradients nor linear constraints are currently supported with SCOLIB.

Some SCOLIB methods exploit parallelism through the use of Dakota’s concurrent function evaluations. The nature of the algorithms, however, limits the amount of concurrency that can be exploited. The maximum amount of evaluation concurrency that can be leveraged by the various methods is as follows:

- COBYLA: one
- DIRECT: twice the number of variables
- Evolutionary Algorithms: size of the population
- Pattern Search: size of the search pattern
- Solis-Wets: one

All SCOLIB methods support the show_m misc_options optional specification which results in a dump of all the allowable method inputs. Note that the information provided by this command refers to optimizer parameters that are internal to SCOLIB, and which may differ from corresponding parameters used by the Dakota interface. The misc_options optional specification provides a means for inputting additional settings supported by the SCOLIB methods but which are not currently mapped through the Dakota input specification. Care must be taken in using this specification; they should only be employed by users familiar with the full range of parameter specifications available directly from SCOLIB and understand any differences that exist between those specifications and the ones available through Dakota.

Each of the SCOLIB methods supports the solution_target control, which defines a convergence criterion in which the optimizer will terminate if it finds an objective function value lower than the specified target.

Related Topics

Related Keywords

- coliny_beta : (Experimental) Coliny beta solver
- coliny_cobyla : Constrained Optimization BY Linear Approximations (COBYLA)
- coliny_direct : DIviding RECTangles method
5.10. PACKAGES

- **coliny_ea**: Evolutionary Algorithm
- **coliny_pattern_search**: Pattern search, derivative free optimization method
- **coliny_solis_wets**: Simple greedy local search method
<table>
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<tr>
<th>Distribution Type</th>
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<th>Global Reliability</th>
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Table 5.1: Summary of Distribution Types supported by Nondeterministic Methods, Part I (Continuous Aleatory Types)
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<th>Sampling</th>
<th>Local Reliability</th>
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</tr>
<tr>
<td>Binomial</td>
<td>C</td>
<td>-</td>
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<tr>
<td>Negative Binomial</td>
<td>C</td>
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<td>Geometric</td>
<td>C</td>
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<td>-</td>
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<td>-</td>
</tr>
<tr>
<td>Discrete Histogram Point</td>
<td>C</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 5.2: Summary of Distribution Types supported by Nondeterministic Methods, Part II (Discrete Aleatory Types)
<table>
<thead>
<tr>
<th>Distribution Type</th>
<th>Sampling</th>
<th>Local Reliability</th>
<th>Global Reliability</th>
<th>Wiener SE</th>
<th>Askey SE</th>
<th>Extended SE</th>
<th>Piecewise SE</th>
<th>Local Interval</th>
<th>Global Interval</th>
<th>Local Evidence</th>
<th>Global Evidence</th>
</tr>
</thead>
<tbody>
<tr>
<td>Interval</td>
<td>U</td>
<td>-</td>
<td>U,A</td>
<td>U,A</td>
<td>U,A</td>
<td>U,A</td>
<td>U, A</td>
<td>U</td>
<td>U</td>
<td>U</td>
<td>U</td>
</tr>
<tr>
<td>Continuous Design</td>
<td>U,A</td>
<td>-</td>
<td>U,A</td>
<td>U,A</td>
<td>U,A</td>
<td>U,A</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Discrete Design</td>
<td>U,A</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Continuous State</td>
<td>U,A</td>
<td>-</td>
<td>U,A</td>
<td>U,A</td>
<td>U,A</td>
<td>U,A</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Discrete State</td>
<td>U,A</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 5.3: Summary of Distribution Types supported by Nondeterministic Methods, Part III (Epistemic, Design, and State Types)
Chapter 6

Keywords Area

This page summarizes the overall input file structure, syntax, and the six types of blocks that may appear in Dakota input. Some are optional and some may appear multiple times:

- **environment** (optional; 0 or 1 may appear)
- **method** (required; 1 or more may appear)
- **model** (optional; 0 or more may appear)
- **variables** (required; 1 or more may appear)
- **interface** (required; 1 or more may appear)
- **responses** (required; 1 or more may appear)

**Introduction to Dakota Keywords**

In Dakota, the **environment** manages execution modes and I/O streams and defines the top-level iterator. Generally speaking, an iterator contains a model and a model contains a set of **variables**, an **interface**, and a set of **responses**. An iterator repeatedly operates on the model to map the variables into responses using the interface. Each of these six components (environment, method, model, variables, interface, and responses) are separate specifications in the user’s input file, and as a whole, determine the study to be performed during an execution of the Dakota software.

A Dakota execution is limited to a single environment, but may involve multiple methods and multiple models. In particular, advanced iterators (i.e., meta- and component-based iterators) and advanced models (i.e., nested and surrogate models) may specialize to include recursions with additional sub-iterators and sub-models. Since each model may contain its own variables, interface, and responses, there may be multiple specifications of the method, model, variables, interface, and responses sections.

**Keyword Pages**

Every Dakota keyword has its own page in this manual. The page describes:

- Whether the keyword takes **ARGUMENTS**, and the data type Additional notes about **ARGUMENTS** can be found here: Specifying Arguments.
- Whether it has an **ALIAS**
- Which additional keywords can be specified to change its behavior
- Which of these additional keywords are required or optional
- Additional information about how to use the keyword in an input file
6.1 environment

- Keywords Area
- environment

Top-level settings for Dakota execution

Topics

This keyword is related to the topics:

- block

Specification

Alias: none

Argument(s): none

Default: no environment

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>tabular_data</td>
<td></td>
<td>Write a tabular results file with variable and response history</td>
</tr>
<tr>
<td>Optional</td>
<td>output_file</td>
<td></td>
<td>Base filename for output redirection</td>
</tr>
<tr>
<td>Optional</td>
<td>error_file</td>
<td></td>
<td>Base filename for error redirection</td>
</tr>
<tr>
<td>Optional</td>
<td>read_restart</td>
<td></td>
<td>Base filename for restart file read</td>
</tr>
<tr>
<td>Optional</td>
<td>write_restart</td>
<td></td>
<td>Base filename for restart file write</td>
</tr>
<tr>
<td>Optional</td>
<td>output_precision</td>
<td></td>
<td>Control the output precision</td>
</tr>
<tr>
<td>Optional</td>
<td>results_output</td>
<td></td>
<td>(Experimental) Write a summary file containing the final results</td>
</tr>
</tbody>
</table>
6.1. ENVIRONMENT

<table>
<thead>
<tr>
<th>Optional</th>
<th>graphics</th>
<th>Display a 2D graphics window of variables and responses</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>check</td>
<td>Invoke Dakota in input check mode</td>
</tr>
<tr>
<td>Optional</td>
<td>pre_run</td>
<td>Invoke Dakota with pre-run mode active</td>
</tr>
<tr>
<td>Optional</td>
<td>run</td>
<td>Invoke Dakota with run mode active</td>
</tr>
<tr>
<td>Optional</td>
<td>post_run</td>
<td>Invoke Dakota with post-run mode active</td>
</tr>
<tr>
<td>Optional</td>
<td>top_method_pointer</td>
<td>Identify which method leads the Dakota study</td>
</tr>
</tbody>
</table>

**Description**

The environment section in a Dakota input file is optional. It specifies the top-level solution environment, optionally including run modes, output controls, and identification of the primary iterative method (`top_method_pointer`). The output-related keywords address graphics, generation of tabular and results data, and precision of numerical output.

**Run Mode Defaults**

Dakota run phases include `check`, `pre_run`, `run`, and `post_run`. The default behavior is to `pre_run`, `run`, and `post_run`, though any or all of these may be specified to select specific run phases. Specifying `check` will cause Dakota to exit before any selected run modes.

**6.1.1 tabular_data**

- **Keywords Area**
- **environment**
- **tabular_data**

Write a tabular results file with variable and response history

**Topics**

This keyword is related to the topics:

- **dakota_output**
 CHAPTER 6. KEYWORDS AREA

Specification

Alias: tabular_graphics_data

Argument(s): none

Default: no tabular data output

<p>| Required/- | Description of | Dakota Keyword | Dakota Keyword |</p>
<table>
<thead>
<tr>
<th>Optional</th>
<th>Group</th>
<th></th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>Tabular Data Format (Group 1)</td>
<td>tabular_data_file</td>
<td>annotated</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Selects annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>custom_annotated</td>
<td>Selects custom-annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>freeform</td>
<td>Selects freeform file format</td>
</tr>
</tbody>
</table>

Description

Specifying the `tabular_data` flag writes to a data file the same variable and response function history data plotted when using the `graphics` flag. Within the generated data file, the variables and response functions appear as columns and each function evaluation provides a new table row. This capability is most useful for post-processing of Dakota results with third-party graphics tools such as MatLab, Excel, Tecplot, etc.

There is no dependence between the `graphics` flag and the `tabular_data` flag; they may be used independently or concurrently.

Dakota exports tabular data in one of three formats:

- `annotated` (default)
- `custom_annotated`
- `freeform`

See Also

These keywords may also be of interest:

- `graphics`

`tabular_data_file`

- Keywords Area
- environment
- `tabular_data`
- `tabular_data_file`

File name for tabular data output
6.1. ENVIRONMENT

Topics
This keyword is related to the topics:

- dakota_output

Specification

Alias: tabular_graphics_file

Argument(s): STRING

Default: dakota_tabular.dat

Description

Specifies a name to use for the tabular data file, overriding the default dakota_tabular.dat.

annotated

- Keywords Area
- environment
- tabular_data
- annotated

Selects annotated tabular file format

Topics
This keyword is related to the topics:

- file_formats

Specification

Alias: none

Argument(s): none

Default: annotated format

Description

An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior

By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips

- To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify custom_annotated header eval_id
• Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

• When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

• Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
annotated
```

Resulting tabular file:

```plaintext
%eval_id interface x1 x2 obj_fn nln_ineq_con_1 nln_ineq_con_2
1 NO_ID 0.9 1.1 0.0002 0.26 0.76
2 NO_ID 0.90009 1.1 0.0001996404857 0.2601620081 0.759955
3 NO_ID 0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...
```

custom_annotated

• Keywords Area

• environment

• tabular_data

• custom_annotated

Selects custom-annotated tabular file format

Topics

This keyword is related to the topics:

• file_formats

Specification

Alias: none

Argument(s): none

Default: annotated format
### Description

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

#### Default Behavior

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

#### Usage Tips

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

#### Examples

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
custom_annotated header eval_id
```

Resulting tabular file:

```
%eval_id   x1    x2    obj_fn nln_ineq_con_1 nln_ineq_con_2
1   0.9    1.1    0.0002   0.26   0.76
2   0.90009 1.1  0.0001996404857 0.2601620081 0.759955
3   0.89991 1.1  0.0002003604863 0.2598380081 0.760045
...```
header

- Keywords Area
- environment
- tabular_data
- custom_annotated
- header

Enable header row in custom-annotated tabular file

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no header

**Description**

See description of parent `custom_annotated`

eval_id

- Keywords Area
- environment
- tabular_data
- custom_annotated
- eval_id

Enable evaluation ID column in custom-annotated tabular file

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no eval_id column

**Description**

See description of parent `custom_annotated`
interface_id

- **Keywords Area**
- **environment**
- **tabular_data**
- **custom_annotated**
- **interface_id**

Enable interface ID column in custom-annotated tabular file

**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** no interface_id column

**Description**

See description of parent `custom_annotated`

**freeform**

- **Keywords Area**
- **environment**
- **tabular_data**
- **freeform**

Selects freeform file format

**Topics**

This keyword is related to the topics:

- **file_formats**

**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** annotated format
CHAPTER 6. KEYWORDS AREA

Description

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior

The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips

- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```dakota
environment
tabular_data
  tabular_data_file = 'dakota_summary.dat'
freeform
```

Resulting tabular file:

```
  0.9  1.1  0.0002  0.26  0.76
 0.90009  1.1 0.0001996404857  0.2601620081  0.759955
 0.89991  1.1 0.0002003604863  0.2598380081  0.760045
...
```

6.1.2 output_file

- Keywords Area
- environment
- output_file

Base filename for output redirection

Topics

This keyword is related to the topics:

- dakota_IO
- command_line_options
6.1. **ENVIRONMENT**

**Specification**

**Alias:** none  
**Argument(s):** STRING  
**Default:** output to console, not file

**Description**

Specify a base filename to which Dakota output will be directed. Output will (necessarily) be redirected after the input file is parsed. This option is overridden by any command-line -output option.

**Default Behavior**

Output to console (screen).

### 6.1.3 error_file

- **Keywords Area**
- environment
- error_file

Base filename for error redirection

**Topics**

This keyword is related to the topics:

- dakota.IO  
- command_line_options

**Specification**

**Alias:** none  
**Argument(s):** STRING  
**Default:** errors to console, not file

**Description**

Specify a base filename to which Dakota errors will be directed. Errors will (necessarily) be redirected after the input file is parsed. This option is overridden by any command-line -error option.

**Default Behavior**

Errors to console (screen).

### 6.1.4 read_restart

- **Keywords Area**
- environment
- read_restart

Base filename for restart file read
CHAPTER 6. KEYWORDS AREA

Topics
This keyword is related to the topics:

- dakota_IO
- command_line_options

Specification
Alias: none
Argument(s): STRING
Default: no restart read

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>stop_restart</td>
<td>Default: no restart read</td>
<td></td>
</tr>
</tbody>
</table>

Description
Specify a base filename for the restart file Dakota should read. This option is overridden by any command-line -read_restart option.

Default Behavior
No restart file is read.

stop_restart
- Keywords Area
- environment
- read_restart
- stop_restart

Evaluation ID number at which to stop reading restart file

Topics
This keyword is related to the topics:

- dakota_IO

Specification
Alias: none
Argument(s): INTEGER
Default: read all records
6.1. ENVIRONMENT

Description
This option is overridden by any command-line -stop restart option.

6.1.5 write_restart

- Keywords Area
- environment
- write_restart

Base filename for restart file write

Topics
This keyword is related to the topics:
- dakota.IO
- command_line_options

Specification
Alias: none
Argument(s): STRING
Default: dakota.rst

Description
Specify a base filename for the restart file Dakota should write. This option is overridden by any command-line -write_restart option.

6.1.6 output_precision

- Keywords Area
- environment
- output_precision

Control the output precision

Topics
This keyword is related to the topics:
- dakota_output

Specification
Alias: none
Argument(s): INTEGER
Default: 10
CHAPTER 6. KEYWORDS AREA

Description
The precision of numeric output precision can be set with output_precision, with an upper limit of 16. When not specified, most Dakota output will default to a precision of 10, though filesystem interfaces and pre-run output use higher precision for accuracy and better results reproducibility.

6.1.7 results_output

- Keywords Area
- environment
- results_output

(Experimental) Write a summary file containing the final results

Topics
This keyword is related to the topics:

- dakota_output

Specification

Alias: none
Argument(s): none
Default: no results output

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>results_output_file</td>
<td>The base file name of the results file</td>
</tr>
</tbody>
</table>

Description
(Experimental) Final results from a Dakota study can be output to dakota_results.txt by specifying results_output (optionally specifying an alternate file name with results_output_filename). The current experimental text file format is hierarchical and a precursor to planned output to structured text formats such as XML or YAML, and binary formats such as HDF5. The contents, organization, and format of results files are all under active development and are subject to change.

results_output_file

- Keywords Area
- environment
- results_output
- results_output_file

The base file name of the results file
6.1. ENVIRONMENT

Topics
This keyword is related to the topics:

- dakota_output

Specification
Alias: none
Argument(s): STRING
Default: dakota_results.txt

Description
Default file name is dakota_results.txt

6.1.8 graphics

- Keywords Area
- environment
- graphics

Display a 2D graphics window of variables and responses

Topics
This keyword is related to the topics:

- dakota_output

Specification
Alias: none
Argument(s): none
Default: graphics off

Description
For most studies, the graphics flag activates a 2D graphics window containing history plots for the variables and response functions in the study. This window is updated in an event loop with approximately a 2 second cycle time. Some study types such as surrogate-based optimization or local reliability specialize the use of the graphics window.

There is no dependence between the graphics flag and the tabular_data flag; they may be used independently or concurrently.

See Also
These keywords may also be of interest:

- tabular_data
6.1.9 check

- Keywords Area
- environment
- check

Invoke Dakota in input check mode

Topics
This keyword is related to the topics:
- command_line_options

Specification
Alias: none
Argument(s): none
Default: no check; proceed to run

Description
When specified, Dakota input will be parsed and the problem instantiated. Dakota will exit reporting whether any errors were found.

6.1.10 pre_run

- Keywords Area
- environment
- pre_run

Invoke Dakota with pre-run mode active

Topics
This keyword is related to the topics:
- command_line_options

Specification
Alias: none
Argument(s): none
Default: pre-run, run, post-run all executed

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
6.1. ENVIRONMENT

<table>
<thead>
<tr>
<th>Optional</th>
<th>input</th>
<th>Base filename for pre-run mode data input</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>output</td>
<td>Base filename for pre-run mode data output</td>
</tr>
</tbody>
</table>

**Description**

When specified, Dakota execution will include the pre-run mode, which sets up methods and often generates parameter sets to evaluate. This mode is currently useful for parameter study, DACE, and Monte Carlo sampling methods.

**Default Behavior**

When no run modes are specified, Dakota will perform pre-run, run, and post-run phases.

**input**

- Keywords Area
- environment
- pre_run
- input

  Base filename for pre-run mode data input

**Topics**

This keyword is related to the topics:

- dakota.IO

**Specification**

Alias: none

Argument(s): STRING

Default: no pre-run specific input read

**Description**

(For future expansion; not currently used by any methods.) Specify a base filename from which Dakota will read any pre-run input data. This option is overridden by any command-line -pre_run arguments.

**output**

- Keywords Area
- environment
- pre_run
• output

Base filename for pre-run mode data output

Topics

This keyword is related to the topics:

• dakota_IO

Specification

Alias: none

Argument(s): STRING

Default: no pre-run specific output written

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional(Choose One)</td>
<td>Tabular Format (Group 1)</td>
<td>annotated</td>
<td>Selects annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>custom_annotated</td>
<td>Selects custom-annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>freeform</td>
<td>Selects freeform file format</td>
</tr>
</tbody>
</table>

Description

Specify a base filename to which Dakota will write any pre-run output data (typically parameter sets to be evaluated). This option is overridden by any command-line -pre_run arguments.

Usage Tips

Dakota exports tabular data in one of three formats:

• annotated (default)
• custom_annotated
• freeform

annotated

• Keywords Area
• environment
• pre_run
• output
• annotated

Selects annotated tabular file format
6.1. ENVIRONMENT

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none

Argument(s): none

Default: annotated format

Description

An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior

By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips

- To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify custom_annotated header eval_id

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
  tabular_data_file = 'dakota_summary.dat'
  annotated
```

Resulting tabular file:

```plaintext
%eval_id interface x1   x2  obj_fn nln_ineq_con_1 nln_ineq_con_2
1   NO_ID    0.9   1.1  0.0002  0.26  0.76
2   NO_ID    0.90009 1.1  0.0001996404857 0.2601620081 0.759955
3   NO_ID    0.89991 1.1  0.0002003604863 0.2598380081 0.760045
...```
custom_annotated

• Keywords Area
• environment
• pre_run
• output
• custom_annotated

Selects custom-annotated tabular file format

Topics

This keyword is related to the topics:

• file_formats

Specification

Alias: none

Argument(s): none

Default: annotated format

<table>
<thead>
<tr>
<th>Required-/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>header</td>
<td>Enable header row in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>eval_id</td>
<td>Enable evaluation ID column in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>interface_id</td>
<td>Enable interface ID column in custom-annotated tabular file</td>
</tr>
</tbody>
</table>

Description

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

Default Behavior

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

Usage Tips
Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:

evironment

    tabular_data
    tabular_data_file = 'dakota_summary.dat'
    custom_annotated header eval_id

Resulting tabular file:

<table>
<thead>
<tr>
<th>%eval_id</th>
<th>x1</th>
<th>x2</th>
<th>obj_fn</th>
<th>nln_ineq_con_1</th>
<th>nln_ineq_con_2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.9</td>
<td>1.1</td>
<td>0.0002</td>
<td>0.26</td>
<td>0.76</td>
</tr>
<tr>
<td>2</td>
<td>0.90009</td>
<td>1.1</td>
<td>0.0001996404857</td>
<td>0.2601620081</td>
<td>0.759955</td>
</tr>
<tr>
<td>3</td>
<td>0.89991</td>
<td>1.1</td>
<td>0.0002003604863</td>
<td>0.2598380081</td>
<td>0.760045</td>
</tr>
<tr>
<td>...</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

    header

    Keywords Area

    environment

    pre_run

    output

    custom_annotated

    header

Enable header row in custom-annotated tabular file

Specification

Alias: none
Argument(s): none
Default: no header

Description

See description of parent custom_annotated
eval_id

- Keywords Area
- environment
- pre_run
- output
- custom_annotated
- eval_id

Enable evaluation ID column in custom-annotated tabular file

**Specification**

Alias: none

- **Argument(s):** none
- **Default:** no eval_id column

**Description**

See description of parent custom_annotated

interface_id

- Keywords Area
- environment
- pre_run
- output
- custom_annotated
- interface_id

Enable interface ID column in custom-annotated tabular file

**Specification**

Alias: none

- **Argument(s):** none
- **Default:** no interface_id column

**Description**

See description of parent custom_annotated
freeform

- Keywords Area
- environment
- pre_run
- output
- freeform

Selects freeform file format

Topics
This keyword is related to the topics:

- file_formats

Specification

Alias: none
Argument(s): none
Default: annotated format

Description
A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior
The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips

- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.
Examples
Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```plaintext
environment
  tabular_data
  tabular_data_file = 'dakota_summary.dat'
freeform
```

Resulting tabular file:

```
   0.9  1.1   0.0002   0.26   0.76
0.90009  1.1  0.0001996404857  0.2601620081  0.759955
  0.89991  1.1  0.0002003604863  0.2598380081  0.760045
...```

6.1.11 run
- Keywords Area
- environment
- run

Invoke Dakota with run mode active

Topics
This keyword is related to the topics:
- command_line_options

Specification
Alias: none
Argument(s): none
Default: pre-run, run, post-run all executed

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>input</td>
<td>Base filename for run mode data input</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>output</td>
<td>Base filename for run mode data output</td>
</tr>
</tbody>
</table>

Description
When specified, Dakota execution will include the run mode, which invokes interfaces to map parameters to responses.

Default Behavior
When no run modes are specified, Dakota will perform pre-run, run, and post-run phases.
6.1. ENVIRONMENT

input

• Keywords Area
• environment
• run
• input

Base filename for run mode data input

Topics
This keyword is related to the topics:

• dakota_IO

Specification
Alias: none
Argument(s): STRING
Default: no run specific input read

Description
(For future expansion; not currently used by any methods.) Specify a base filename from which Dakota will read any run input data, such as parameter sets to evaluate. This option is overridden by any command-line -run arguments.

output

• Keywords Area
• environment
• run
• output

Base filename for run mode data output

Topics
This keyword is related to the topics:

• dakota_IO

Specification
Alias: none
Argument(s): STRING
Default: no run specific output written
**Description**

(For future expansion; not currently used by any methods.) Specify a base filename to which Dakota will write any run output data (typically parameter, response pairs). This option is overridden by any command-line -run arguments.

### 6.1.12 post_run

- **Keywords Area**
- **environment**
- **post_run**

Invoke Dakota with post-run mode active

**Topics**

This keyword is related to the topics:

- **command_line_options**

**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** pre-run, run, post-run all executed

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Description of Group</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>input</td>
<td>input</td>
<td>Base filename for post-run mode data input</td>
</tr>
<tr>
<td>output</td>
<td></td>
<td>output</td>
<td>Base filename for post-run mode data output</td>
</tr>
</tbody>
</table>

**Description**

When specified, Dakota execution will include the post-run mode, which analyzes parameter/response data sets and computes final results. This mode is currently useful for parameter study, DACE, and Monte Carlo sampling methods.

**Default Behavior**

When no run modes are specified, Dakota will perform pre-run, run, and post-run phases.

**input**

- **Keywords Area**
- **environment**
- **post_run**
6.1. ENVIRONMENT

- **input**

  Base filename for post-run mode data input

**Topics**

This keyword is related to the topics:

- **dakota.IO**

**Specification**

**Alias:** none  
**Argument(s):** STRING  
**Default:** no post-run specific input read

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>Tabular Format (Group 1)</td>
<td>annotated</td>
<td>Selects annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>custom_annotated</td>
<td>Selects custom-annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>freeform</td>
<td>Selects freeform file format</td>
</tr>
</tbody>
</table>

**Description**

Specify a base filename from which Dakota will read any post-run input data, such as parameter/response data on which to calculate final statistics. This option is overridden by any command-line -post_run arguments.

**Usage Tips**

Dakota imports tabular data in one of three formats:

- **annotated** (default)
- **custom_annotated**
- **freeform**

**annotated**

- **Keywords Area**
  - environment
  - post_run
  - input
  - annotated

  Selects annotated tabular file format
Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none

Argument(s): none

Default: annotated format

Description

An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior

By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips

- To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify custom_annotated header eval_id

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```
environment
tabular_data
  tabular_data_file = 'dakota_summary.dat'
  annotated
```

Resulting tabular file:

```
%eval_id interface  x1   x2   obj_fn  nln_ineq_con_1  nln_ineq_con_2
1    NO_ID     0.9   1.1   0.0002   0.26     0.76
2    NO_ID     0.90009 1.1  0.0001996404857 0.2601620081 0.759955
3    NO_ID     0.89991 1.1  0.0002003604863 0.2598380081 0.760045
...
```
6.1. ENVIRONMENT

custom_annotated

- Keywords Area
- environment
- post_run
- input
- custom_annotated

Selects custom-annotated tabular file format

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none
Argument(s): none
Default: annotated format

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>header</td>
<td></td>
<td>Enable header row in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td>eval_id</td>
<td></td>
<td>Enable evaluation ID column in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td>interface_id</td>
<td></td>
<td>Enable interface ID column in custom-annotated tabular file</td>
</tr>
</tbody>
</table>

Description

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

Default Behavior

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

Usage Tips
Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples
Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
custom_annotated header eval_id
```

Resulting tabular file:

```
%eval_id x1 x2 obj_fn nln_ineq_con_1 nln_ineq_con_2
1 0.9 1.1 0.0002 0.26 0.76
2 0.90009 1.1 0.0001996404857 0.2601620081 0.759955
3 0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...
```

header

- **Keywords Area**
- **environment**
- **post_run**
- **input**
- **custom_annotated**
- **header**

Enable header row in custom-annotated tabular file

Specification

**Alias:** none

**Argument(s):** none

**Default:** no header

Description

See description of parent custom_annotated
6.1. ENVIRONMENT

**eval_id**
- **Keywords Area**
- **environment**
- **post_run**
- **input**
- **custom_annotated**
- **eval_id**

Enable evaluation ID column in custom-annotated tabular file

**Specification**

**Alias:** none
- **Argument(s):** none
- **Default:** no eval_id column

**Description**

See description of parent *custom_annotated*

**interface_id**
- **Keywords Area**
- **environment**
- **post_run**
- **input**
- **custom_annotated**
- **interface_id**

Enable interface ID column in custom-annotated tabular file

**Specification**

**Alias:** none
- **Argument(s):** none
- **Default:** no interface_id column

**Description**

See description of parent *custom_annotated*
freeform

- Keywords Area
- environment
- post_run
- input
- freeform

Selects freeform file format

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none

Argument(s): none

Default: annotated format

Description

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

**Default Behavior**

The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

**Usage Tips**

- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.
6.1. ENVIRONMENT

Examples
Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
freeform
```

Resulting tabular file:

```
0.9  1.1  0.0002  0.26  0.76
0.90009  1.1  0.0001996404857  0.2601620081  0.759955
0.89991  1.1  0.0002003604863  0.2598380081  0.760045
```

output

- Keywords Area
- environment
- post_run
- output

Base filename for post-run mode data output

Topics
This keyword is related to the topics:

- dakota_IO

Specification

Alias: none

- Argument(s): STRING
- Default: no post-run specific output written

Description

(For future expansion; not currently used by any methods.) Specify a base filename to which Dakota will write any post-run output data. This option is overridden by any command-line -post_run arguments.

6.1.13 top_method_pointer

- Keywords Area
- environment
- top_method_pointer

Identify which method leads the Dakota study
CHAPTER 6. KEYWORDS AREA

Topics
This keyword is related to the topics:

- block_pointer

Specification
Alias: method_pointer
Argument(s): STRING
Default: see discussion

Description
An optional top_method_pointer specification may be used to point to a particular method specification that will lead the Dakota analysis. The associated string must be a method identifier specified via id_method. If top_method_pointer is not used, then it will be inferred as described below (no top_method_pointer within an environment specification is treated the same as no environment specification).

Default Behavior
The top_method_pointer keyword is typically used in Dakota studies consisting of more than one method block to clearly indicate which is the leading method. This method provides the starting point for the iteration. The corresponding method specification may recurse with additional sub-method pointers in the case of "meta-iteration" (see method) or may specify a single method without recursion. Either case will ultimately result in identification of one or more model specifications using model_pointer, which again may or may not involve further recursion (see nested and surrogate for recursion cases). Each of the model specifications identify the variables and responses specifications (using variables_pointer and responses_pointer) that are used to build the model, and depending on the type of model, may also identify an interface specification (for example, using interface_pointer). If one of these specifications does not provide an optional pointer, then that component will be constructed using the last specification parsed.

When the environment block is omitted, the top level method will be inferred as follows: When a single method is specified, there is no ambiguity and the sole method will be the top method. When multiple methods are specified, the top level method will be deduced from the hierarchical relationships implied by method pointers. If this inference is not well defined (e.g., there are multiple method specifications without any pointer relationship), then the default behavior is to employ the last method specification parsed.

Examples
Specify that the optimization method is the outermost method in an optimization under uncertainty study

```plaintext
environment
top_method_pointer 'OPTIMIZATION_METHOD'
method
  id_method 'UQ_METHOD'
...
method
  id_method 'OPTIMIZATION_METHOD'
...
```

See Also
These keywords may also be of interest:

- id_method
6.2 method

- Keywords Area
- method

Begins Dakota method selection and behavioral settings.

Topics

This keyword is related to the topics:
- block

Specification

Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>id_method</td>
<td>Name the method block; helpful when there are multiple</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>output</td>
<td>Control how much method information is written to the screen and output file</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>final_solutions</td>
<td>Number of designs returned as the best solutions</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>hybrid</td>
<td>Strategy in which a set of methods synergistically seek an optimal design</td>
</tr>
<tr>
<td></td>
<td></td>
<td>multi_start</td>
<td>Multi-Start Optimization Method</td>
</tr>
<tr>
<td></td>
<td></td>
<td>pareto_set</td>
<td>Pareto set optimization</td>
</tr>
</tbody>
</table>
### Chapter 6. Keywords Area

<table>
<thead>
<tr>
<th>Keyword</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>branch_and_bound</code></td>
<td>(Experimental Capability) Solves a mixed integer nonlinear optimization problem</td>
</tr>
<tr>
<td><code>surrogate_based_local</code></td>
<td>Local Surrogate Based Optimization</td>
</tr>
<tr>
<td><code>surrogate_based_global</code></td>
<td>Global Surrogate Based Optimization</td>
</tr>
<tr>
<td><code>dot_frcg</code></td>
<td>A conjugate gradient optimization method</td>
</tr>
<tr>
<td><code>dot_mmfd</code></td>
<td>Method of feasible directions</td>
</tr>
<tr>
<td><code>dot_bfgs</code></td>
<td>A conjugate gradient optimization method</td>
</tr>
<tr>
<td><code>dot_slp</code></td>
<td>Sequential Linear Programming</td>
</tr>
<tr>
<td><code>dot_sqp</code></td>
<td>Sequential Quadratic Program</td>
</tr>
<tr>
<td><code>dot</code></td>
<td>Access to methods in the DOT package</td>
</tr>
<tr>
<td><code>conmin_frcg</code></td>
<td>A conjugate gradient optimization method</td>
</tr>
<tr>
<td><code>conmin_mfd</code></td>
<td>Method of feasible directions</td>
</tr>
<tr>
<td><code>conmin</code></td>
<td>Access to methods in the CONMIN library</td>
</tr>
<tr>
<td><code>dl_solver</code></td>
<td>(Experimental) Dynamically-loaded solver</td>
</tr>
</tbody>
</table>
### 6.2. METHOD

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>npsol_sqp</strong></td>
<td>Sequential Quadratic Program</td>
</tr>
<tr>
<td><strong>nlssol_sqp</strong></td>
<td>Sequential Quadratic Program for nonlinear least squares</td>
</tr>
<tr>
<td><strong>stanford</strong></td>
<td>Select methods from the Stanford package</td>
</tr>
<tr>
<td><strong>nlpql_sqp</strong></td>
<td>Sequential Quadratic Program</td>
</tr>
<tr>
<td><strong>optpp_cg</strong></td>
<td>A conjugate gradient optimization method</td>
</tr>
<tr>
<td><strong>optpp_q_newton</strong></td>
<td>Quasi-Newton optimization method</td>
</tr>
<tr>
<td><strong>optpp_fd_newton</strong></td>
<td>Finite Difference Newton optimization method</td>
</tr>
<tr>
<td><strong>optpp_g_newton</strong></td>
<td>Newton method based least-squares calibration</td>
</tr>
<tr>
<td><strong>optpp_newton</strong></td>
<td>Newton method based optimization</td>
</tr>
<tr>
<td><strong>optpp_pds</strong></td>
<td>Simplex-based derivative free optimization method</td>
</tr>
<tr>
<td><strong>asynch_pattern_search</strong></td>
<td>Pattern search, derivative free optimization method</td>
</tr>
<tr>
<td><strong>mesh_adaptive_search</strong></td>
<td>Finds optimal variable values using adaptive mesh-based search</td>
</tr>
<tr>
<td>Keyword</td>
<td>Description</td>
</tr>
<tr>
<td>-----------</td>
<td>-------------</td>
</tr>
<tr>
<td>nowpac</td>
<td>Gradient-free inequality-constrained optimization using Nonlinear Optimization With Path Augmented Constraints (NOWPAC).</td>
</tr>
<tr>
<td>snowpac</td>
<td>Stochastic version of NOWPAC that incorporates error estimates and noise mitigation.</td>
</tr>
<tr>
<td>moga</td>
<td>Multi-objective Genetic Algorithm (a.k.a Evolutionary Algorithm)</td>
</tr>
<tr>
<td>soga</td>
<td>Single-objective Genetic Algorithm (a.k.a Evolutionary Algorithm)</td>
</tr>
<tr>
<td>coliny_pattern_search</td>
<td>Pattern search, derivative free optimization method</td>
</tr>
<tr>
<td>coliny_solis_wets</td>
<td>Simple greedy local search method</td>
</tr>
<tr>
<td>coliny_cobyla</td>
<td>Constrained Optimization BY Linear Approximations (COBYLA)</td>
</tr>
<tr>
<td>coliny_direct</td>
<td>DIViding RECTangles method</td>
</tr>
<tr>
<td>coliny_ea</td>
<td>Evolutionary Algorithm</td>
</tr>
<tr>
<td>coliny_beta</td>
<td>(Experimental) Coliny beta solver</td>
</tr>
</tbody>
</table>
### 6.2. METHOD

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>nl2sol</td>
<td>Trust-region method for nonlinear least squares</td>
</tr>
<tr>
<td>nonlinear_cg</td>
<td>(Experimental) nonlinear conjugate gradient optimization</td>
</tr>
<tr>
<td>ncsu_direct</td>
<td>DIviding RECTangles method</td>
</tr>
<tr>
<td>genie_opt_darts</td>
<td>Voronoi-based high-dimensional global Lipschitzian optimization</td>
</tr>
<tr>
<td>genie_direct</td>
<td>Classical high-dimensional global Lipschitzian optimization</td>
</tr>
<tr>
<td>efficient_global</td>
<td>Global Surrogate Based Optimization, a.k.a. EGO</td>
</tr>
<tr>
<td>polynomial_chaos</td>
<td>Uncertainty quantification using polynomial chaos expansions</td>
</tr>
<tr>
<td>stoch_collocation</td>
<td>Uncertainty quantification with stochastic collocation</td>
</tr>
<tr>
<td><strong>sampling</strong></td>
<td>Randomly samples variables according to their distributions</td>
</tr>
<tr>
<td><strong>multilevel_sampling</strong></td>
<td>Multilevel methods for sampling-based UQ</td>
</tr>
<tr>
<td><strong>importance_sampling</strong></td>
<td>Importance sampling</td>
</tr>
<tr>
<td><strong>gpais</strong></td>
<td>Gaussian Process Adaptive Importance Sampling (Experimental)</td>
</tr>
<tr>
<td><strong>adaptive_sampling</strong></td>
<td>Adaptively refine a Gaussian process surrogate</td>
</tr>
<tr>
<td><strong>pof_darts</strong></td>
<td>Probability-of-Failure (POF) darts is a novel method for estimating the probability of failure based on random sphere-packing.</td>
</tr>
<tr>
<td><strong>rkd_darts</strong></td>
<td>Recursive k-d (RKD) Darts: Recursive Hyperplane Sampling for Numerical Integration of High-Dimensional Functions.</td>
</tr>
<tr>
<td>Method</td>
<td>Description</td>
</tr>
<tr>
<td>----------------------------</td>
<td>-----------------------------------------------------------------------------</td>
</tr>
<tr>
<td>global_evidence</td>
<td>Evidence theory with evidence measures computed with global optimization methods</td>
</tr>
<tr>
<td>global_interval_est</td>
<td>Interval analysis using global optimization methods</td>
</tr>
<tr>
<td>bayes_calibration</td>
<td>Bayesian calibration</td>
</tr>
<tr>
<td>dace</td>
<td>Design and Analysis of Computer Experiments</td>
</tr>
<tr>
<td>fsu_cvt</td>
<td>Design of Computer Experiments - Centroidal Voronoi Tessellation</td>
</tr>
<tr>
<td>psuade_moat</td>
<td>Morris One-at-a-Time</td>
</tr>
<tr>
<td>local_evidence</td>
<td>Evidence theory with evidence measures computed with local optimization methods</td>
</tr>
<tr>
<td>local_interval_est</td>
<td>Interval analysis using local optimization methods</td>
</tr>
<tr>
<td>local_reliability</td>
<td>Local reliability method</td>
</tr>
<tr>
<td>global_reliability</td>
<td>Global reliability methods</td>
</tr>
<tr>
<td>fsu_quasi_mc</td>
<td>Design of Computer Experiments - Quasi-Monte Carlo sampling</td>
</tr>
</tbody>
</table>
### Description

The `method` keyword signifies the start of a block in the Dakota input file. A method block contains the various keywords necessary to select a method and to control its behavior.

#### Method Block Requirements

At least one `method` block must appear in the Dakota input file. Multiple `method` blocks may be needed to fully define advanced analysis approaches.

Each `method` block must specify one method and, optionally, any associated keywords that govern the behavior of the method.

#### The Methods

Each `method` block must select one method.

Starting with Dakota v6.0, the methods are grouped into two types: standard methods and multi-component methods.

The standard methods are stand-alone and self-contained in the sense that they only require a model to perform a study. They do not call other methods. While methods such as `polynomial_chaos` and `efficient_global` internally utilize multiple iterator and surrogate model components, these components are generally hidden from user control due to restrictions on modularity; thus, these methods are stand-alone.

The multi-component group of methods provides a higher level “meta-algorithm” that points to other methods and models that support sub-iteration. For example, in a sequential hybrid method, the `hybrid` method specification must identify a list of subordinate methods, and the “meta-algorithm” executes these methods in sequence and transfers information between them. Surrogate-based minimizers provide another example in that they point both to other methods (e.g. what optimization method is used to solve the approximate subproblem) as well as to models (e.g. what type of surrogate model is employed). Multi-component methods generally provide some level of “plug and play” modularity, through their flexible support of a variety of method and model selections.

#### Component-Based Iterator Commands

Component-based iterator specifications include hybrid, multi-start, pareto set, surrogate-based local, surrogate-based global, and branch and bound methods. Whereas a standard iterator specification only needs an optional model pointer string (specified with `model_pointer`), component-based iterator specifications can include

<table>
<thead>
<tr>
<th>Keyword</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>vector_parameter_study</code></td>
<td>Samples variables along a user-defined vector</td>
</tr>
<tr>
<td><code>list_parameter_study</code></td>
<td>Samples variables as a specified values</td>
</tr>
<tr>
<td><code>centered_parameter_study</code></td>
<td>Samples variables along points moving out from a center point</td>
</tr>
<tr>
<td><code>multidim_parameter_study</code></td>
<td>Samples variables on full factorial grid of study points</td>
</tr>
<tr>
<td><code>richardson_extrap</code></td>
<td>Estimate order of convergence of a response as model fidelity increases</td>
</tr>
</tbody>
</table>
6.2. **METHOD**

method pointer, method name, and model pointer specifications in order to define the components employed in the "meta-iteration." In particular, these specifications identify one or more methods (by pointer or by name) to specify the subordinate iterators that will be used in the top-level algorithm. Identifying a sub-iterator by name instead of by pointer is a lightweight option that relaxes the need for a separate method specification for the sub-iterator; however, a model pointer may be required in this case to provide the specification connectivity normally supported by the method pointer. Refer to these individual method descriptions for specific requirements for these advanced methods.

**Method Independent Controls**

In addition to the method, there are 10 optional keywords, which are referred to as method independent controls. These controls are valid for enough methods that it was reasonable to pull them out of the method dependent blocks and consolidate the specifications, however, they are NOT universally respected by all methods.

**Examples**

Several examples follow. The first example shows a minimal specification for an optimization method.

```plaintext
method
dot_sqp
```

This example uses all of the defaults for this method.

A more sophisticated example would be

```plaintext
method,
id_method = 'NLP1'
dot_sqp
max_iterations = 50
convergence_tolerance = 1e-4
output verbose
model_pointer = 'M1'
```

This example demonstrates the use of identifiers and pointers as well as some method independent and method dependent controls for the sequential quadratic programming (SQP) algorithm from the DOT library. The `max_iterations`, `convergence_tolerance`, and `output` settings are method independent controls, in that they are defined for a variety of methods (see `dot` for usage of these controls).

The next example shows a specification for a least squares method.

```plaintext
method
optpp_g_newton
max_iterations = 10
convergence_tolerance = 1.e-8
search_method trust_region
gradient_tolerance = 1.e-6
```

Some of the same method independent controls are present along with several method dependent controls (`search_method` and `gradient_tolerance`) which are only meaningful for OPT++ methods (see `package_optpp`).

The next example shows a specification for a nondeterministic method with several method dependent controls (refer to `sampling`).

```plaintext
method
sampling
samples = 100
seed = 12345
sample_type lhs
response_levels = 1000. 500.
```

The last example shows a specification for a parameter study method where, again, each of the controls are method dependent (refer to `vector_parameter_study`).

```plaintext
method
vector_parameter_study
step_vector = 1. 1. 1.
um_steps = 10
```
6.2.1 id_method

- Keywords Area
- method
- id_method

Name the method block; helpful when there are multiple

Topics
This keyword is related to the topics:
- block_identifier
- method-independent_controls

Specification
Alias: none
Argument(s): STRING
Default: strategy use of last method parsed

Description
The method identifier string is supplied with id_method and is used to provide a unique identifier string for use with environment or meta-iterator specifications (refer to environment). It is appropriate to omit a method identifier string if only one method is included in the input file, since the single method to use is unambiguous in this case.

6.2.2 output

- Keywords Area
- method
- output

Control how much method information is written to the screen and output file

Topics
This keyword is related to the topics:
- dakota_output
- method-independent_controls

Specification
Alias: none
Argument(s): none
Default: normal
### Description

Choose from a total of five output levels during the course of a Dakota study. If there is no user specification for output verbosity, then the default setting is `normal`.

Specific mappings are as follows:

- **silent** (i.e., really quiet): silent iterators, silent model, silent interface, quiet approximation, quiet file operations
- **quiet**: quiet iterators, quiet model, quiet interface, quiet approximation, quiet file operations
- **normal**: normal iterators, normal model, normal interface, quiet approximation, quiet file operations
- **verbose**: verbose iterators, normal model, verbose interface, verbose approximation, verbose file operations
- **debug** (i.e., really verbose): debug iterators, normal model, debug interface, verbose approximation, verbose file operations

Note that iterators and interfaces utilize the full granularity in verbosity, whereas models, approximations, and file operations do not. With respect to iterator verbosity, different iterators implement this control in slightly different ways (as described below in the method independent controls descriptions for each iterator), however the meaning is consistent.

For models, interfaces, approximations, and file operations, `quiet` suppresses parameter and response set reporting and `silent` further suppresses function evaluation headers and scheduling output. Similarly, `verbose` adds file management, approximation evaluation, and global approximation coefficient details, and `debug` further adds diagnostics from nonblocking schedulers.

---

#### debug

- **Keywords Area**
  - method
  - output
  - debug

  Level 5 of 5 - maximum
CHAPTER 6. KEYWORDS AREA

Specification
Alias: none
Argument(s): none

Description
This is described on output

verbose
- Keywords Area
- method
- output
- verbose

Level 4 of 5 - more than normal

Specification
Alias: none
Argument(s): none

Description
This is described on output

normal
- Keywords Area
- method
- output
- normal

Level 3 of 5 - default

Specification
Alias: none
Argument(s): none

Description
This is described on output
6.2. METHOD

quiet

- Keywords Area
- method
- output
- quiet

Level 2 of 5 - less than normal

Specification

Alias: none
- Argument(s): none

Description

This is described on output

silent

- Keywords Area
- method
- output
- silent

Level 1 of 5 - minimum

Specification

Alias: none
- Argument(s): none

Description

This is described on output

6.2.3 final_solutions

- Keywords Area
- method
- final_solutions

Number of designs returned as the best solutions
Topics
This keyword is related to the topics:
  * method_independent_controls

Specification
Alias: none
  Argument(s): INTEGER
  Default: 1

Description
The final_solutions controls the number of final solutions returned by the iterator as the best solutions. For most optimizers, this is one, but some optimizers can produce multiple solutions (e.g. genetic algorithms). When using a hybrid strategy, the number of final solutions dictates how many solutions are passed from one method to another.

Examples
In the case of sampling methods, if one specifies 100 samples (for example) but also specifies final_solutions = 5, the five best solutions (in order of lowest response function value) are returned.

6.2.4 hybrid
  * Keywords Area
  * method
  * hybrid

Strategy in which a set of methods synergistically seek an optimal design

Specification
Alias: none
  Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required (Choose One)</td>
<td>Group 1</td>
<td>sequential</td>
<td>Methods are run one at a time, in sequence</td>
</tr>
<tr>
<td>embedded</td>
<td>A subordinate local method provides periodic refinements to a top-level global method</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
6.2. METHOD

| Optional | collaborative | Multiple methods run concurrently and share information |
| Optional | iterator_servers: | Specify the number of iterator servers when Dakota is run in parallel |
| Optional | iterator_scheduling: | Specify the scheduling of concurrent iterators when Dakota is run in parallel |
| Optional | processors_per_iter: | Specify the number of processors per iterator server when Dakota is run in parallel |

**Description**

In a hybrid minimization method (**hybrid**), a set of methods synergistically seek an optimal design. The relationships among the methods are categorized as:

- collaborative
- embedded
- sequential

The goal in each case is to exploit the strengths of different optimization and nonlinear least squares algorithms at different stages of the minimization process. Global + local hybrids (e.g., genetic algorithms combined with nonlinear programming) are a common example in which the desire for identification of a global optimum is balanced with the need for efficient navigation to a local optimum.

**sequential**

- **Keywords Area**
- method
- hybrid
- sequential

Methods are run one at a time, in sequence

**Specification**

**Alias:** uncoupled

**Argument(s):** none
CHAPTER 6. KEYWORDS AREA

<table>
<thead>
<tr>
<th>Required/-Optional Required (Choose One)</th>
<th>Description of Group 1</th>
<th>Dakota Keyword Description</th>
<th>Dakota Keyword</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Description of Group 1</td>
<td>method_name_list</td>
</tr>
<tr>
<td></td>
<td></td>
<td>List of Dakota methods to sequentially or collaboratively run</td>
<td>method_pointer_list</td>
</tr>
</tbody>
</table>

**Description**

In the **sequential** approach, methods are run one at a time, in sequence. The best solutions from one method are used to initialize the next method.

The sequence of methods (i.e. iterators) to run are specified using either a method_pointer_list or a method_name_list (with optional model_pointer_list). Any number of iterators may be specified.

Method switching is managed through the separate convergence controls of each method. The number of solutions transferred between methods is specified by the particular method through its final_solutions method control.

For example, if one sets up a two-level study with a first method that generates multiple solutions such as a genetic algorithm, followed by a second method that is initialized only at a single point such as a gradient-based algorithm, it is possible to take the multiple solutions generated by the first method and create several instances of the second method, each one with a different initial starting point.

The logic governing the transfer of multiple solutions between methods is as follows:

- if one solution is returned from method A, then one solution is transferred to method B.
- If multiple solutions are returned from method A, and method B can accept multiple solutions as input (for example, as a genetic algorithm population), then one instance of method B is initialized with multiple solutions.
- If multiple solutions are returned from method A but method B only can accept one initial starting point, then method B is run several times, each one with a separate starting point from the results of method A.

**method_name_list**

- Keywords Area
- method
- hybrid
- sequential
- method_name_list

List of Dakota methods to sequentially or collaboratively run

**Specification**

**Alias:** none

**Argument(s):** STRINGLIST
### Description

*method_name_list* specifies a list of Dakota methods (e.g. *soga, conmin_frcg*) that will be run by a hybrid sequential or hybrid collaborative method. The methods are executed with default options. The optional *model_pointer_list* may be used to associate a model with each method.

- **model_pointer_list**
  - Keywords Area
  - *method*
  - *hybrid*
  - *sequential*
  - *method_name_list*
  - *model_pointer_list*

Associate models with method names

### Topics

This keyword is related to the topics:

- *block_pointer*

### Specification

**Alias:** none

**Argument(s):** STRING

### Description

Using the optional keyword *model_pointer_list*, models can be assigned to methods specified in the *method_name_list*. Models are referred to by name (i.e. by their *id_model* labels). The length of the *model_pointer_list* must be either 1 or match the length of the *method_name_list*. If the former, the same model will be used for all methods, and if the latter, methods and models will be paired in the order that they appear in the two lists.
method_pointer_list

- Keywords Area
- method
- hybrid
- sequential
- method_pointer_list

Pointers to methods to execute sequentially or collaboratively

**Topics**
This keyword is related to the topics:
- block_pointer

**Specification**
Alias: none  
Argument(s): STRINGLIST

**Description**
method_pointer_list specifies by name the methods that are to be executed by a hybrid sequential or hybrid collaborative method. Its argument is a list of strings that refer to method blocks by name (i.e. to their id_method labels).

**embedded**

- Keywords Area
- method
- hybrid
- embedded

A subordinate local method provides periodic refinements to a top-level global method

**Specification**
Alias: coupled  
Argument(s): none
6.2. METHOD

### Required (One) Group 1

<table>
<thead>
<tr>
<th>Specification</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>global_method_name</td>
<td>Specify the global method by Dakota name</td>
</tr>
<tr>
<td>global_method_pointer</td>
<td>Pointer to global method</td>
</tr>
</tbody>
</table>

### Required (One) Group 2

<table>
<thead>
<tr>
<th>Specification</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>local_method_name</td>
<td>Specify the local method by Dakota name</td>
</tr>
<tr>
<td>local_method_pointer</td>
<td>Pointer to local method</td>
</tr>
</tbody>
</table>

### Optional

<table>
<thead>
<tr>
<th>Specification</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>local_search_probability</td>
<td>Probability of executing local searches</td>
</tr>
</tbody>
</table>

### Description

In the **embedded** approach, a tightly-coupled hybrid is employed in which a subordinate local method provides periodic refinements to a top-level global method.

Global and local method strings supplied with the `global_method_pointer` and `local_method_pointer` specifications identify the two methods to be used. Alternatively, Dakota method names (e.g. ‘soga’) can be supplied using the `global_method_name` and `local_method_name` keywords, which each have optional model pointer specifications. The `local_search_probability` setting is an optional specification for supplying the probability (between 0.0 and 1.0) of employing local search to improve estimates within the global search.

**global_method_name**

- Keywords Area
- method
- hybrid
- embedded
- global_method_name

Specify the global method by Dakota name

### Specification

**Alias:** none

**Argument(s):** STRING

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>global_model_pointer</td>
<td>Pointer to model used by global method</td>
<td></td>
</tr>
</tbody>
</table>
**Description**

`global_method_name` is used to specify the global method in a hybrid embedded optimization by Dakota name (e.g. 'soga'). The name of the method is provided as a string. The method is executed with default options.

**global_model_pointer**

- Keywords Area
- method
- hybrid
- embedded
- `global_method_name`
- `global_model_pointer`

Pointer to model used by global method

**Topics**

This keyword is related to the topics:

- `block_pointer`

**Specification**

Alias: none

Argument(s): STRING

**Description**

`global_model_pointer` can be used to specify a model for use with the Dakota method named by the `global_method_name` specification. The argument is a string that refers to the `id_model` label of the desired model.

**global_method_pointer**

- Keywords Area
- method
- hybrid
- embedded
- `global_method_pointer`

Pointer to global method
6.2. METHOD

Topics

This keyword is related to the topics:

- block_pointer

Specification

Alias: none

Argument(s): STRING

Description

The global_method_pointer identifies the method block to use as the global method in a hybrid embedded optimization using its id_method label.

local_method_name

- Keywords Area
- method
- hybrid
- embedded
- local_method_name

Specify the local method by Dakota name

Specification

Alias: none

Argument(s): STRING

| Required/- | Description of | Dakota Keyword | Dakota Keyword |
| Optional | Group | local_model_- | Description |
| Optional | pointer | Pointer to model | used by local |
| method | used by local method |

Description

local_method_name is used to specify the local method in a hybrid embedded optimization by Dakota name (e.g. 'conmin_mfd'). The name of the method is provided as a string. The method is executed with default options.

local_model_pointer

- Keywords Area
- method
- hybrid
• embedded
• local_method_name
• local_model_pointer

Pointer to model used by local method

Topics
This keyword is related to the topics:
• block_pointer

Specification
Alias: none
Argument(s): STRING

Description
local_model_pointer can be used to specify a model for use with the Dakota method named by the local_method_name specification. The argument is a string that refers to the id_model label of the desired model.

local_method_pointer
• Keywords Area
• method
• hybrid
• embedded
• local_method_pointer

Pointer to local method

Topics
This keyword is related to the topics:
• block_pointer

Specification
Alias: none
Argument(s): STRING

Description
The local_method_pointer identifies the method block to use as the local method in a hybrid embedded optimization using its id_method
6.2. METHOD

local_search_probability

- Keywords Area
- method
- hybrid
- embedded
- local_search_probability

Probability of executing local searches

Specification

Alias: none
Argument(s): REAL

Description

The local_search_probability setting is an optional specification for supplying the probability (between 0.0 and 1.0) of employing local search to improve estimates within the global search. Its default value is 0.1.

collaborative

- Keywords Area
- method
- hybrid
- collaborative

Multiple methods run concurrently and share information

Specification

Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional Required(Choose One)</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<tbody>
<tr>
<td>method_name_list</td>
<td>List of Dakota methods to sequentially or collaboratively run</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Description

In the collaborative approach, multiple methods work together and share solutions while executing concurrently. A list of method strings specifies the pool of iterators to be used. Any number of iterators may be specified. The method collaboration logic follows that of either the Agent-Based Optimization or HOPSPACK codes and is currently under development and not available at this time.

method_name_list

- Keywords Area
- method
- hybrid
- collaborative
- method_name_list

List of Dakota methods to sequentially or collaboratively run

Specification

Alias: none

Argument(s): STRINGLIST

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>model_pointer_list</td>
<td>Associate models with method names</td>
</tr>
</tbody>
</table>

Description

method_name_list specifies a list of Dakota methods (e.g. soga, conmin_frcg) that will be run by a hybrid sequential or hybrid collaborative method. The methods are executed with default options. The optional model_pointer_list may be used to associate a model with each method.

model_pointer_list

- Keywords Area
- method
- hybrid
- collaborative
- method_name_list
- model_pointer_list

Associate models with method names
6.2. METHOD

Topics
This keyword is related to the topics:

- block_pointer

Specification
Alias: none
Argument(s): STRING

Description
Using the optional keyword model_pointer_list, models can be assigned to methods specified in the method_name_list. Models are referred to by name (i.e. by their id_model labels). The length of the model_pointer_list must be either 1 or match the length of the method_name_list. If the former, the same model will be used for all methods, and if the latter, methods and models will be paired in the order that they appear in the two lists.

method_pointer_list

- Keywords Area
- method
- hybrid
- collaborative
- method_pointer_list

Pointers to methods to execute sequentially or collaboratively

Topics
This keyword is related to the topics:

- block_pointer

Specification
Alias: none
Argument(s): STRINGLIST

Description
method_pointer_list specifies by name the methods that are to be executed by a hybrid sequential or hybrid collaborative method. Its argument is a list of strings that refer to method blocks by name (i.e. to their id_method labels).
iterator_servers

- Keywords Area
- method
- hybrid
- iterator_servers

Specify the number of iterator servers when Dakota is run in parallel

Topics
This keyword is related to the topics:
- concurrency_and_parallelism

Specification
Alias: none
Argument(s): INTEGER

Description
An important feature for component-based iterators is that execution of sub-iterator runs may be performed concurrently. The optional iterator_servers specification supports user override of the automatic parallel configuration for the number of iterator servers. That is, if the automatic configuration is undesirable for some reason, the user can enforce a desired number of partitions at the iterator parallelism level. Currently, hybrid, multi_start, and pareto_set component-based iterators support concurrency in their sub-iterators. Refer to ParallelLibrary and the Parallel Computing chapter of the Users Manual [4] for additional information.

iterator_scheduling

- Keywords Area
- method
- hybrid
- iterator_scheduling

Specify the scheduling of concurrent iterators when Dakota is run in parallel

Topics
This keyword is related to the topics:
- concurrency_and_parallelism

Specification
Alias: none
Argument(s): none
### Description

An important feature for component-based iterators is that execution of sub-iterator runs may be performed concurrently. The optional `iterator_scheduling` specification supports user override of the automatic parallel configuration for the number of iterator servers. That is, if the automatic configuration is undesirable for some reason, the user can enforce a desired number of partitions at the iterator parallelism level. Currently, `hybrid`, `multi_start`, and `pareto_set` component-based iterators support concurrency in their sub-iterators. Refer to ParallelLibrary and the Parallel Computing chapter of the Users Manual [4] for additional information.

**master**

- **Keywords Area**
- **method**
- **hybrid**
- **iterator_scheduling**
- **master**

Specify a dedicated master partition for parallel iterator scheduling

### Topics

This keyword is related to the topics:

- `concurrency_and_parallelism`

### Specification

**Alias:** none

**Argument(s):** none

### Description

This option overrides the Dakota parallel automatic configuration, forcing the use of a dedicated master partition. In a dedicated master partition, one processor (the "master") dynamically schedules work on the iterator servers. This reduces the number of processors available to create servers by 1.
peer

- Keywords Area
- method
- hybrid
- iterator_scheduling
- peer

Specify a peer partition for parallel iterator scheduling

Topics
This keyword is related to the topics:
- concurrency_and_parallelism

Specification
Alias: none
Argument(s): none

Description
This option overrides the Dakota parallel automatic configuration, forcing the use of a peer partition. In a peer partition, all processors are available to be assigned to iterator servers. Note that unlike the case of evaluation_scheduling, it is not possible to specify static or dynamic.

processors_per_iterator

- Keywords Area
- method
- hybrid
- processors_per_iterator

Specify the number of processors per iterator server when Dakota is run in parallel

Topics
This keyword is related to the topics:
- concurrency_and_parallelism

Specification
Alias: none
Argument(s): INTEGER
6.2. METHOD

Description

An important feature for component-based iterators is that execution of sub-iterator runs may be performed concurrently. The optional `processors_per_iterator` specification supports user override of the automatic parallel configuration for the number of processors in each iterator server. That is, if the automatic configuration is undesirable for some reason, the user can enforce a desired server size at the iterator parallelism level. Currently, `hybrid`, `multi_start`, and `pareto_set` component-based iterators support concurrency in their sub-iterators. Refer to ParallelLibrary and the Parallel Computing chapter of the Users Manual[4] for additional information.

6.2.5 multi_start

- **Keywords Area**
  - method
  - multi_start

Multi-Start Optimization Method

**Specification**

Alias: none

Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
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<tr>
<td>Required (Choose One)</td>
<td>method_name</td>
<td>method_pointer</td>
<td>Pointer to sub-method to run from each starting point</td>
</tr>
<tr>
<td>Optional</td>
<td>random_starts</td>
<td></td>
<td>Number of random starting points</td>
</tr>
<tr>
<td>Optional</td>
<td>starting_points</td>
<td></td>
<td>List of user-specified starting points</td>
</tr>
<tr>
<td>Optional</td>
<td>iterator_servers</td>
<td></td>
<td>Specify the number of iterator servers when Dakota is run in parallel</td>
</tr>
</tbody>
</table>
CHAPTER 6. KEYWORDS AREA

### Description

In the multi-start iteration method (*multi_start*), a series of iteration runs are performed for different values of parameters in the model. A common use is for multi-start optimization (i.e., different local optimization runs from different starting points for the design variables), but the concept and the code are more general. Multi-start iteration is implemented within the MetaIterator branch of the Iterator hierarchy within the ConcurrentMetaIterator class. Additional information on the multi-start algorithm is available in the Users Manual[4].

The *multi_start* meta-iterator must specify a sub-iterator using either a *method_pointer* or a *method_name* plus optional *model_pointer*. This iterator is responsible for completing a series of iterative analyses from a set of different starting points. These starting points can be specified as follows: (1) using *random_starts*, for which the specified number of starting points are selected randomly within the variable bounds, (2) using *starting_points*, in which the starting values are provided in a list, or (3) using both *random_starts* and *starting_points*, for which the combined set of points will be used. In aggregate, at least one starting point must be specified. The most common example of a multi-start algorithm is multi-start optimization, in which a series of optimizations are performed from different starting values for the design variables. This can be an effective approach for problems with multiple minima.

**method_name**

- Keywords Area
- method
- *multi_start*
- *method_name*

Specify sub-method by name

### Specification

**Alias:** none

**Argument(s):** STRING

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
</table>

**iterator_scheduling**

Specify the scheduling of concurrent iterators when Dakota is run in parallel

**processors_per_-iterator**

Specify the number of processors per iterator server when Dakota is run in parallel
### Optional model_pointer

<table>
<thead>
<tr>
<th>Optional</th>
<th>model_pointer</th>
<th>Identifier for model block to be used by a method</th>
</tr>
</thead>
</table>

### Description

The `method_name` keyword is used to specify a sub-method by Dakota method name (e.g. `npsol_sqp`) rather than block pointer. The method will be executed using its default settings. The optional `model_pointer` specification can be used to associate a model block with the method.

### `model_pointer`

- **Keywords Area**
  - `method`
  - `multi_start`
  - `method_name`
  - `model_pointer`

  Identifier for model block to be used by a method

### Topics

This keyword is related to the topics:

- `block_pointer`

### Specification

**Alias:** none

**Argument(s):** STRING

**Default:** method use of last model parsed (or use of default model if none parsed)

### Description

The `model_pointer` is used to specify which `model` block will be used to perform the function evaluations needed by the Dakota method.

#### Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a `model` block in the Dakota input file that has a corresponding `id_model` with the same name.

#### Usage Tips

When doing advanced analyses that involve using multiple methods and multiple models, defining a `model_pointer` for each method is imperative.

See `block_pointer` for details about pointers.
Examples

environment
  tabular_graphics_data
  method_pointer = 'UQ'

method
  id_method = 'UQ'
  model_pointer = 'SURR'
  sampling,
    samples = 10
  seed = 98765 rng rnum2
  response_levels = 0.1 0.2 0.6
  0.1 0.2 0.6
  0.1 0.2 0.6
  sample_type lhs
distribution cumulative

model
  id_model = 'SURR'
  surrogate global,
  dace_method_pointer = 'DACE'
polynomial quadratic

method
  id_method = 'DACE'
  model_pointer = 'DACE_M'
  sampling sample_type lhs
  samples = 121 seed = 5034 rng rnum2

model
  id_model = 'DACE_M'
single
  interface_pointer = 'I1'

variables
  uniform_uncertain = 2
  lower_bounds = 0. 0.
  upper_bounds = 1. 1.
descriptors = 'x1' 'x2'

interface
  id_interface = 'I1'
  system asynch evaluation_concurrency = 5
  analysis_driver = 'text_book'

responses
  response_functions = 3
  no_gradients
  no_hessians

method_pointer

- Keywords Area
- method
- multi_start
- method_pointer

Pointer to sub-method to run from each starting point
6.2. METHOD

Topics
This keyword is related to the topics:
- block_pointer

Specification
Alias: none
Argument(s): STRING

Description
The method_pointer keyword is used to specify a pointer to the sub-method block that will be run from each starting point.

random_starts
- Keywords Area
- method
- multi_start
- random_starts

Number of random starting points

Specification
Alias: none
Argument(s): INTEGER

<table>
<thead>
<tr>
<th>Required/ Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>seed</td>
<td>seed</td>
<td>Seed of the random number generator</td>
<td></td>
</tr>
</tbody>
</table>

Description
The multi_start meta-iterator must specify a sub-iterator using either a method_pointer or a method_name plus optional model_pointer. This iterator is responsible for completing a series of iterative analyses from a set of different starting points. These starting points can be specified as follows: (1) using random_starts, for which the specified number of starting points are selected randomly within the variable bounds, (2) using starting_points, in which the starting values are provided in a list, or (3) using both random_starts and starting_points, for which the combined set of points will be used.
 CHAPTER 6. KEYWORDS AREA

seed

- Keywords Area
- method
- multi_start
- random_starts
- seed

Seed of the random number generator

Specification

Alias: none

Argument(s): INTEGER

Default: system-generated (non-repeatable)

Description

The random seed control provides a mechanism for making a stochastic method repeatable. That is, the use of the same random seed in identical studies will generate identical results.

Default Behavior

If not specified, the seed is randomly generated.

Expected Output

If seed is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

Usage Tips

If a stochastic study was run without seed specified, and the user later wishes to repeat the study using the same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen. That value can then be added to the Dakota input file.

Examples

method
  sampling
    sample_type lhs
    samples = 10
    seed = 15347

starting_points

- Keywords Area
- method
- multi_start
- starting_points

List of user-specified starting points
6.2. METHOD

Specification

Alias: none

Argument(s): REALLIST

Description

The multi_start meta-iterator must specify a sub-iterator using either a method_pointer or a method_name plus optional model_pointer. This iterator is responsible for completing a series of iterative analyses from a set of different starting points. These starting points can be specified as follows: (1) using random_starts, for which the specified number of starting points are selected randomly within the variable bounds, (2) using starting_points, in which the starting values are provided in a list, or (3) using both random_starts and starting_points, for which the combined set of points will be used.

iterator_servers

- Keywords Area
- method
- multi_start
- iterator_servers

Specify the number of iterator servers when Dakota is run in parallel.

Topics

This keyword is related to the topics:

- concurrency_and_parallelism

Specification

Alias: none

Argument(s): INTEGER

Description

An important feature for component-based iterators is that execution of sub-iterator runs may be performed concurrently. The optional iterator_servers specification supports user override of the automatic parallel configuration for the number of iterator servers. That is, if the automatic configuration is undesirable for some reason, the user can enforce a desired number of partitions at the iterator parallelism level. Currently, hybrid, multi_start, and pareto_set component-based iterators support concurrency in their sub-iterators. Refer to ParallelLibrary and the Parallel Computing chapter of the Users Manual [4] for additional information.

iterator_scheduling

- Keywords Area
- method
- multi_start
• iterator_scheduling

Specify the scheduling of concurrent iterators when Dakota is run in parallel

Topics
This keyword is related to the topics:
• concurrency_and_parallelism

Specification
Alias: none
Argument(s): none

<table>
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<th>Required-/Optional Required (Choose One)</th>
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<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<tbody>
<tr>
<td></td>
<td></td>
<td>master</td>
<td>Specify a dedicated master partition for parallel iterator scheduling</td>
</tr>
<tr>
<td></td>
<td></td>
<td>peer</td>
<td>Specify a peer partition for parallel iterator scheduling</td>
</tr>
</tbody>
</table>

Description
An important feature for component-based iterators is that execution of sub-iterator runs may be performed concurrently. The optional iterator_scheduling specification supports user override of the automatic parallel configuration for the number of iterator servers. That is, if the automatic configuration is undesirable for some reason, the user can enforce a desired number of partitions at the iterator parallelism level. Currently, hybrid, multi_start, and pareto_set component-based iterators support concurrency in their sub-iterators. Refer to ParallelLibrary and the Parallel Computing chapter of the Users Manual [4] for additional information.

master
• Keywords Area
• method
• multi_start
• iterator_scheduling
• master
  Specify a dedicated master partition for parallel iterator scheduling

Topics
This keyword is related to the topics:
• concurrency_and_parallelism
6.2. METHOD

Specification

Alias: none
Argument(s): none

Description

This option overrides the Dakota parallel automatic configuration, forcing the use of a dedicated master partition. In a dedicated master partition, one processor (the "master") dynamically schedules work on the iterator servers. This reduces the number of processors available to create servers by 1.

peer

- Keywords Area
- method
- multi_start
- iterator_scheduling
- peer

Specify a peer partition for parallel iterator scheduling

Topics

This keyword is related to the topics:

- concurrency_and_parallelism

Specification

Alias: none
Argument(s): none

Description

This option overrides the Dakota parallel automatic configuration, forcing the use of a peer partition. In a peer partition, all processors are available to be assigned to iterator servers. Note that unlike the case of evaluation_scheduling, it is not possible to specify static or dynamic.

processors_per_iterator

- Keywords Area
- method
- multi_start
- processors_per_iterator

Specify the number of processors per iterator server when Dakota is run in parallel.
CHAPTER 6. KEYWORDS AREA

Topics
This keyword is related to the topics:

- concurrency and parallelism

Specification
Alias: none
Argument(s): INTEGER

Description
An important feature for component-based iterators is that execution of sub-iterator runs may be performed concurrently. The optional `processors_per_iterator` specification supports user override of the automatic parallel configuration for the number of processors in each iterator server. That is, if the automatic configuration is undesirable for some reason, the user can enforce a desired server size at the iterator parallelism level. Currently, `hybrid`, `multi_start`, and `pareto_set` component-based iterators support concurrency in their sub-iterators. Refer to ParallelLibrary and the Parallel Computing chapter of the Users Manual[4] for additional information.

6.2.6 pareto_set

- Keywords Area
- method
- pareto_set

Pareto set optimization

Specification
Alias: none
Argument(s): none

<table>
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<th>Description of</th>
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<td>Description</td>
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<td></td>
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<td>least-squares</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>sub-method</td>
</tr>
</tbody>
</table>


### Description

In the pareto set minimization method (`pareto_set`), a series of optimization or least squares calibration runs are performed for different weightings applied to multiple objective functions. This set of optimal solutions defines a "Pareto set," which is useful for investigating design trade-offs between competing objectives. The code is similar enough to the `multi_start` technique that both algorithms are implemented in the same Concurrent-MetaIterator class.

The `pareto_set` specification must identify an optimization or least squares calibration method using either a `method_pointer` or a `method_name` plus optional `model_pointer`. This minimizer is responsible for computing a set of optimal solutions from a set of response weightings (multi-objective weights or least squares term weights). These weightings can be specified as follows: (1) using `random_weight_sets`, in which case weightings are selected randomly within [0,1] bounds, (2) using `weight_sets`, in which the weighting sets are specified in a list, or (3) using both `random_weight_sets` and `weight_sets`, for which the combined set of weights will be used. In aggregate, at least one set of weights must be specified. The set of optimal solutions is called the "pareto set," which can provide valuable design trade-off information when there are competing objectives.

**method_name**

- **Keywords Area**

- **method**

- **pareto_set**

- **method_name**

  Specify sub-method by name
CHAPTER 6. KEYWORDS AREA

**Specification**

**Alias:** opt_method_name

**Argument(s):** STRING

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>model_pointer</td>
<td>Identifier for model block to be used by a method</td>
</tr>
</tbody>
</table>

**Description**

The `method_name` keyword is used to specify a sub-method by Dakota method name (e.g. ‘npsol_sqp’) rather than block pointer. The method will be executed using its default settings. The optional `model_pointer` specification can be used to associate a model block with the method.

**model_pointer**

- Keywords Area
- method
- pareto_set
- method_name
- model_pointer

Identifier for model block to be used by a method

**Topics**

This keyword is related to the topics:

- block_pointer

**Specification**

**Alias:** opt_model_pointer

**Argument(s):** STRING

**Default:** method use of last model parsed (or use of default model if none parsed)

**Description**

The `model_pointer` is used to specify which `model` block will be used to perform the function evaluations needed by the Dakota method.

**Default Behavior**

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a `model` block in the Dakota input file that has a corresponding `id_model` with the same name.

**Usage Tips**

When doing advanced analyses that involve using multiple methods and multiple models, defining a `model-pointer` for each method is imperative.

See `block_pointer` for details about pointers.
6.2. METHOD

Examples

environment
tabular_graphics_data
method_pointer = 'UQ'

method
id_method = 'UQ'
model_pointer = 'SURT'
sampling,
samples = 10
seed = 98765 rng rnum2
response_levels = 0.1 0.2 0.6
                  0.1 0.2 0.6
                  0.1 0.2 0.6
sample_type lhs
distribution cumulative

model
id_model = 'SURT'
surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
id_method = 'DACE'
model_pointer = 'DACE_M'
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = 'DACE_M'
single
interface_pointer = 'I1'

variables
uniform_uncertain = 2
lower_bounds = 0. 0.
upper_bounds = 1. 1.
descriptors = 'x1' 'x2'

interface
id_interface = 'I1'
system asynch evaluation_concurrency = 5
analysis_driver = 'text_book'

responses
response_functions = 3
no_gradients
no_hessians

method_pointer

- Keywords Area
- method
- pareto_set
- method_pointer

Pointer to optimization or least-squares sub-method
CHAPTER 6. KEYWORDS AREA

Topics
This keyword is related to the topics:

- block_pointer

Specification
Alias: opt_method_pointer
Argument(s): STRING

Description
The method_pointer keyword is used to specify a pointer to an optimization or least-squares sub-method that is responsible for computing a set of optimal solutions for a set of response weightings.

random_weight_sets
- Keywords Area
- method
- pareto_set
- random_weight_sets

Number of random weighting sets

Specification
Alias: none
Argument(s): INTEGER

<table>
<thead>
<tr>
<th>Required/- Optional Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>seed</td>
<td>Seed of the random number generator</td>
</tr>
</tbody>
</table>

Description
The pareto_set specification must identify an optimization or least squares calibration method using either a method_pointer or a method_name plus optional model_pointer. This minimizer is responsible for computing a set of optimal solutions from a set of response weightings (multi-objective weights or least squares term weights). These weightings can be specified as follows: (1) using random_weight_sets, in which case weightings are selected randomly within [0,1] bounds, (2) using weight_sets, in which the weighting sets are specified in a list, or (3) using both random_weight_sets and weight_sets, for which the combined set of weights will be used. In aggregate, at least one set of weights must be specified. The set of optimal solutions is called the "pareto set," which can provide valuable design trade-off information when there are competing objectives.
6.2. METHOD

seed

- Keywords Area
- method
- pareto.set
- random_weight_sets
- seed

Seed of the random number generator

Specification

Alias: none

Argument(s): INTEGER
Default: system-generated (non-repeatable)

Description

The random seed control provides a mechanism for making a stochastic method repeatable. That is, the use of the same random seed in identical studies will generate identical results.

Default Behavior
If not specified, the seed is randomly generated.

Expected Output
If seed is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

Usage Tips
If a stochastic study was run without seed specified, and the user later wishes to repeat the study using the same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen. That value can then be added to the Dakota input file.

Examples

method sampling
  sample_type lhs
  samples = 10
  seed = 15347

weight_sets

- Keywords Area
- method
- pareto.set
- weight_sets

List of user-specified weighting sets
CHAPTER 6. KEYWORDS AREA

Specification

Alias: multi_objective_weight_sets
   Argument(s): REALIST

Description

The pareto_set specification must identify an optimization or least squares calibration method using either a method_pointer or a method_name plus optional model_pointer. This minimizer is responsible for computing a set of optimal solutions from a set of response weightings (multi-objective weights or least squares term weights). These weightings can be specified as follows: (1) using random_weight_sets, in which case weightings are selected randomly within [0,1] bounds, (2) using weight_sets, in which the weighting sets are specified in a list, or (3) using both random_weight_sets and weight_sets, for which the combined set of weights will be used. In aggregate, at least one set of weights must be specified. The set of optimal solutions is called the "pareto set," which can provide valuable design trade-off information when there are competing objectives.

iterator_servers

- Keywords Area
- method
- pareto_set
- iterator_servers

Specify the number of iterator servers when Dakota is run in parallel

Topics

This keyword is related to the topics:

- concurrency_and_parallelism

Specification

Alias: none
   Argument(s): INTEGER

Description

An important feature for component-based iterators is that execution of sub-iterator runs may be performed concurrently. The optional iterator_servers specification supports user override of the automatic parallel configuration for the number of iterator servers. That is, if the automatic configuration is undesirable for some reason, the user can enforce a desired number of partitions at the iterator parallelism level. Currently, hybrid, multi_start, and pareto_set component-based iterators support concurrency in their sub-iterators. Refer to ParallelLibrary and the Parallel Computing chapter of the Users Manual [4] for additional information.
6.2. METHOD

iterator_scheduling

- Keywords Area
- method
- pareto_set
- iterator_scheduling

Specify the scheduling of concurrent iterators when Dakota is run in parallel

Topics

This keyword is related to the topics:

- concurrency_and_parallelism

Specification

Alias: none

Argument(s): none

<table>
<thead>
<tr>
<th>Required/Optional Required (Choose One)</th>
<th>Description of Group Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>master</td>
<td>Specify a dedicated master partition for parallel iterator scheduling</td>
</tr>
<tr>
<td></td>
<td></td>
<td>peer</td>
<td>Specify a peer partition for parallel iterator scheduling</td>
</tr>
</tbody>
</table>

Description

An important feature for component-based iterators is that execution of sub-iterator runs may be performed concurrently. The optional iterator_scheduling specification supports user override of the automatic parallel configuration for the number of iterator servers. That is, if the automatic configuration is undesirable for some reason, the user can enforce a desired number of partitions at the iterator parallelism level. Currently, hybrid, multi_start, and pareto_set component-based iterators support concurrency in their sub-iterators. Refer to ParallelLibrary and the Parallel Computing chapter of the Users Manual [4] for additional information.

master

- Keywords Area
- method
- pareto_set
- iterator_scheduling
- master

Specify a dedicated master partition for parallel iterator scheduling
CHAPTER 6. KEYWORDS AREA

Topics
This keyword is related to the topics:

- concurrency_and_parallelism

Specification
Alias: none
Argument(s): none

Description
This option overrides the Dakota parallel automatic configuration, forcing the use of a dedicated master partition. In a dedicated master partition, one processor (the "master") dynamically schedules work on the iterator servers. This reduces the number of processors available to create servers by 1.

peer

- Keywords Area
- method
- pareto_set
- iterator_scheduling
- peer

Specify a peer partition for parallel iterator scheduling

Topics
This keyword is related to the topics:

- concurrency_and_parallelism

Specification
Alias: none
Argument(s): none

Description
This option overrides the Dakota parallel automatic configuration, forcing the use of a peer partition. In a peer partition, all processors are available to be assigned to iterator servers. Note that unlike the case of evaluation_scheduling, it is not possible to specify static or dynamic.
processors\_per\_iterator

- Keywords Area
- method
- pareto\_set
- processors\_per\_iterator

Specify the number of processors per iterator server when Dakota is run in parallel

Topics

This keyword is related to the topics:

- concurrency\_and\_parallelism

Specification

Alias: none

Argument(s): INTEGER

Description

An important feature for component-based iterators is that execution of sub-iterator runs may be performed concurrently. The optional processors\_per\_iterator specification supports user override of the automatic parallel configuration for the number of processors in each iterator server. That is, if the automatic configuration is undesirable for some reason, the user can enforce a desired server size at the iterator parallelism level. Currently, hybrid, multi\_start, and pareto\_set component-based iterators support concurrency in their sub-iterations. Refer to ParallelLibrary and the Parallel Computing chapter of the Users Manual\[4\] for additional information.

6.2.7 branch\_and\_bound

- Keywords Area
- method
- branch\_and\_bound

(Experimental Capability) Solves a mixed integer nonlinear optimization problem

Specification

Alias: none

Argument(s): none

<table>
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<th>Dakota Keyword</th>
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<td></td>
<td></td>
</tr>
</tbody>
</table>
CHAPTER 6. KEYWORDS AREA

### Required (Choose One)

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<thead>
<tr>
<th>Group 1</th>
<th>method_pointer</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Pointer to sub-method to apply to a surrogate or branch-and-bound sub-problem</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>method_name</th>
</tr>
</thead>
<tbody>
<tr>
<td>Specify sub-method by name</td>
</tr>
</tbody>
</table>

### Optional

<table>
<thead>
<tr>
<th>scaling</th>
</tr>
</thead>
<tbody>
<tr>
<td>Turn on scaling for variables, responses, and constraints</td>
</tr>
</tbody>
</table>

### Description

The branch-and-bound optimization methods solves mixed integer nonlinear optimization problems. It does so by partitioning the parameter space according to some criteria along the integer or discrete variables. It then relaxes (i.e., treats all variables as continuous) the sub-problems created by the partitions and solves each sub-problem with a continuous nonlinear optimization method. Results of the sub-problems are combined in such a way that yields the solution to the original optimization problem.

#### Default Behavior

Branch-and-bound expects all discrete variables to be relaxable. If your problem has categorical or otherwise non-relaxable discrete variables, then this is not the optimization method you are looking for.

#### Expected Output

The optimal solution and associated parameters will be printed to the screen output.

#### Usage Tips

The user must choose a nonlinear optimization method to solve the sub-problems. We recommend choosing a method that would be chosen to solve a continuous problem that has similar form to the mixed integer problem.

#### Examples

```python
environment
    method_pointer = 'BandB'

method
    id_method = 'BandB'
    branch_and_bound
        output verbose
            method_pointer = 'SubNLP'

method
    id_method = 'SubNLP'
    coliny_ea
        seed = 12345
        max_iterations = 100
        max_function_evaluations = 100

variables,
    continuous_design = 3
        initial_point = [-1.0, 1.5, 2.0]
        upper_bounds = [10.0, 10.0, 10.0]
        lower_bounds = [-10.0, -10.0, -10.0]
```
6.2. METHOD

descriptors 'x1' 'x2' 'x3'
discrete_design_range = 2
initial_point 2 2
lower_bounds  1  1
upper_bounds  4  9
descriptors 'y1' 'y2'

interface,
  fork
    analysis_driver = 'text_book'

responses,
  objective_functions = 1
  nonlinear_inequality_constraints = 2
  numerical_gradients
  no_hessians

method_pointer

  • Keywords Area
  • method
  • branch_and_bound
  • method_pointer

  Pointer to sub-method to apply to a surrogate or branch-and-bound sub-problem

Topics

This keyword is related to the topics:

  • block_pointer

Specification

Alias: none

  Argument(s): STRING

Description

The method_pointer keyword is used to specify a pointer to an optimization or least-squares sub-method to apply in the context of what could be described as hierarchical methods. In surrogate-based methods, the sub-method is applied to the surrogate model. In the branch-and-bound method, the sub-method is applied to the relaxed sub-problems.

Any model_pointer identified in the sub-method specification is ignored. Instead, the parent method is responsible for selecting the appropriate model to use as specified by its model_pointer. In surrogate-based methods, it is a surrogate model defined using its model_pointer. In branch-and-bound methods, it is the relaxed model that is constructed internally from the original model.
**method_name**

- Keywords Area
- method
- branch_and_bound
- method_name

Specify sub-method by name

**Specification**

**Alias:** none

**Argument(s):** STRING

<table>
<thead>
<tr>
<th>Required/ Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>model_pointer</td>
<td>Identifier for model block to be used by a method</td>
</tr>
</tbody>
</table>

**Description**

The `method_name` keyword is used to specify a sub-method by Dakota method name (e.g. ‘npsol_sqp’) rather than block pointer. The method will be executed using its default settings. The optional `model_pointer` specification can be used to associate a model block with the method.

**model_pointer**

- Keywords Area
- method
- branch_and_bound
- method_name
- model_pointer

Identifier for model block to be used by a method

**Topics**

This keyword is related to the topics:

- `block_pointer`

**Specification**

**Alias:** none

**Argument(s):** STRING

**Default:** method use of last model parsed (or use of default model if none parsed)
6.2. METHOD

Description

The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.

Usage Tips

When doing advanced analyses that involve using multiple methods and multiple models, defining a model_pointer for each method is imperative.

See block_pointer for details about pointers.

Examples

environment
  tabular_graphics_data
  method_pointer = 'UQ'

method
  id_method = 'UQ'
  model_pointer = 'SRR'
  sampling,
    samples = 10
    seed = 98765 rng rnum2
    response_levels = 0.1 0.2 0.6
    0.1 0.2 0.6
    0.1 0.2 0.6
  sample_type lhs
distribution cumulative

model
  id_model = 'SRR'
surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
  id_method = 'DACE'
  model_pointer = 'DACE_M'
sampling sample_type lhs
  samples = 121 seed = 5034 rng rnum2

model
  id_model = 'DACE_M'
single
  interface_pointer = 'I1'

variables
  uniform_uncertain = 2
  lower_bounds = 0. 0.
  upper_bounds = 1. 1.
descriptors = 'x1' 'x2'

interface
  id_interface = 'I1'
system asynch evaluation_concurrency = 5
  analysis_driver = 'text_book'

responses
Keywords Area

Method

Branch and Bound

Scaling

Turn on scaling for variables, responses, and constraints

Topics

This keyword is related to the topics:

- Method independent controls

Specification

Alias: none

Argument(s): none

Default: no scaling

Description

Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by providing the `scaling` keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the method, variables, and responses blocks. When the `scaling` keyword is omitted, all `_scale_types` and `*_scales` specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.

- A `*_scales` keyword, which gives characteristic values
- A `*_scale_type` keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

Scale Types

There are four scale types:

1. none (default) - no scaling, value of `*_scales` keyword is ignored
2. **value** - multiplicative scaling

3. **auto** - automatic scaling

   First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:

   - two-sided bounds scaled into the interval [0,1];
   - one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
   - no bounds or targets: no automatic scaling possible, therefore no scaling for this component

Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into [0,1].

4. **log** - logarithmic scaling

   First, any characteristic values from the optional *_scales* specification are applied. Then logarithm base 10 scaling is applied.

   Logarithmic scaling is not available for linear constraints.

   When continuous design variables are log scaled, linear constraints are not allowed.

**Scales**

The *scales* keywords are used to specify the characteristic values. These must be non-zero real numbers. The numbers are used according to the corresponding *scale_type*, as described above.

   Depending on the scale type, the characteristic values may be required or optional.

   - none, auto, log - optional
   - value - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than \(1.0\times10^{-16}\). User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.

**Examples**

The two examples below are equivalent:

```plaintext
responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value"
  primary_scales = 1 1 100

responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value" "value" "value"
  primary_scales = 1 1 100
```
6.2.8  **surrogate_based_local**

- **Keywords Area**
- **method**
- **surrogate_based_local**

Local Surrogate Based Optimization

**Topics**

This keyword is related to the topics:

- **surrogate_based_optimization_methods**

**Specification**

Alias: none  
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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</thead>
<tbody>
<tr>
<td>Required/(Choose One)</td>
<td>Group 1</td>
<td>method_pointer</td>
<td>Pointer to sub-method to apply to a surrogate or branch-and-bound sub-problem</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>method_name</td>
<td>Specify sub-method by name</td>
</tr>
<tr>
<td>Required</td>
<td></td>
<td>model_pointer</td>
<td>Identifier for model block to be used by a method</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>soft_convergence_limit</td>
<td>Limit number of iterations w/ little improvement</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>truth_surrogate_bypass</td>
<td>Bypass lower level surrogates when performing truth verifications on a top level surrogate</td>
</tr>
</tbody>
</table>
### Description

In surrogate-based optimization (SBO) and surrogate-based nonlinear least squares (SBNLS), minimization occurs using a set of one or more approximations, defined from a surrogate model, that are built and periodically updated using data from a “truth” model. The surrogate model can be a global data fit (e.g., regression or interpolation of data generated from a design of computer experiments), a multipoint approximation, a local Taylor Series expansion, or a model hierarchy approximation (e.g., a low-fidelity simulation model), whereas the truth model involves a high-fidelity simulation model. The goals of surrogate-based methods are to reduce the total number of truth model simulations and, in the case of global data fit surrogates, to smooth noisy data with an easily navigated analytic function.

In the surrogate-based local method, a trust region approach is used to manage the minimization process to maintain acceptable accuracy between the surrogate model and the truth model (by limiting the range over which the surrogate model is trusted). The process involves a sequence of minimizations performed on the surrogate model and bounded by the trust region. At the end of each approximate minimization, the candidate optimum point is validated using the truth model. If sufficient decrease has been obtained in the truth model, the trust region is re-centered around the candidate optimum point and the trust region will either shrink, expand, or remain the same size depending on the accuracy with which the surrogate model predicted the truth model decrease. If
sufficient decrease has not been attained, the trust region center is not updated and the entire trust region shrinks by a user-specified factor. The cycle then repeats with the construction of a new surrogate model, a minimization, and another test for sufficient decrease in the truth model. This cycle continues until convergence is attained.

**Theory**

For surrogate-based local problems with nonlinear constraints, a number of algorithm formulations exist as described in [23] and as summarized in the Advanced Examples section of the Models chapter of the Users Manual[4].

**See Also**

These keywords may also be of interest:

- `efficient_global`
- `surrogate_based_global`

**method_pointer**

- **Keywords Area**
- **method**
- **surrogate_based_local**
- **method_pointer**

Pointer to sub-method to apply to a surrogate or branch-and-bound sub-problem

**Topics**

This keyword is related to the topics:

- `block_pointer`

**Specification**

**Alias**: approx_method_pointer

**Argument(s)**: STRING

**Description**

The `method_pointer` keyword is used to specify a pointer to an optimization or least-squares sub-method to apply in the context of what could be described as hierarchical methods. In surrogate-based methods, the sub-method is applied to the surrogate model. In the branch-and-bound method, the sub-method is applied to the relaxed sub-problems.

Any `model_pointer` identified in the sub-method specification is ignored. Instead, the parent method is responsible for selecting the appropriate model to use as specified by its `model_pointer`. In surrogate-based methods, it is a surrogate model defined using its `model_pointer`. In branch-and-bound methods, it is the relaxed model that is constructed internally from the original model.
6.2. METHOD

method_name

• Keywords Area

• method

• surrogate_based_local

• method_name

Specify sub-method by name

Specification

Alias: approx_method_name

Argument(s): STRING

Description

The method_name keyword is used to specify a sub-method by Dakota method name (e.g. ‘npsol_sqp’) rather than block pointer. The method will be executed using its default settings. The optional model_pointer specification can be used to associate a model block with the method.

model_pointer

• Keywords Area

• method

• surrogate_based_local

• model_pointer

Identifier for model block to be used by a method

Topics

This keyword is related to the topics:

• block_pointer

Specification

Alias: approx_model_pointer

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)
CHAPTER 6. KEYWORDS AREA

Description

The `model_pointer` is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding `id_model` with the same name.

Usage Tips

When doing advanced analyses that involve using multiple methods and multiple models, defining a `model_pointer` for each method is imperative.

See `block_pointer` for details about pointers.

Examples

```plaintext
environment
tabular_graphics_data
method_pointer = 'UQ'

method
id_method = 'UQ'
model_pointer = 'SURR'
sampling,
samples = 10
seed = 98765 rng rnum2
response_levels = 0.1 0.2 0.6
0.1 0.2 0.6
0.1 0.2 0.6
sample_type lhs
distribution cumulative

model
id_model = 'SURR'
 surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
id_method = 'DACE'
model_pointer = 'DACE_M'
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = 'DACE_M'
single
interface_pointer = 'I1'

variables
uniform_uncertain = 2
lower_bounds = 0. 0.
upper_bounds = 1. 1.
descriptors = 'x1' 'x2'

interface
id_interface = 'I1'
system asynch evaluation_concurrency = 5
analysis_driver = 'text_book'

responses
```
6.2. METHOD

```plaintext
response_functions = 3
no_gradients
no_hessians
```

**soft_convergence_limit**

- **Keywords Area**
- **method**
- **surrogate_based_local**
- **soft_convergence_limit**

Limit number of iterations w/ little improvement

**Specification**

*Alias:* none

**Argument(s):** INTEGER

**Default:** 5

**Description**

**soft_convergence_limit** (a soft convergence control for the surrogate_based_local iterations which limits the number of consecutive iterations with improvement less than the convergence tolerance)

**truth_surrogate_bypass**

- **Keywords Area**
- **method**
- **surrogate_based_local**
- **truth_surrogate_bypass**

Bypass lower level surrogates when performing truth verifications on a top level surrogate

**Specification**

*Alias:* none

**Argument(s):** none

**Default:** no bypass

**Description**

**truth_surrogate_bypass** (a flag for bypassing all lower level surrogates when performing truth verifications on a top level surrogate).
approx_subproblem

- Keywords Area
- method
- surrogate_based_local
- approx_subproblem

Identify functions to be included in surrogate merit function

**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** original, primary, original_constraints

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
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<tr>
<td>Required(Choose One)</td>
<td>objective formulation (Group 1)</td>
<td>original_primary</td>
<td>Construct approximations of all primary functions</td>
</tr>
<tr>
<td></td>
<td></td>
<td>single_objective</td>
<td>Construct approximation a single objective functions only</td>
</tr>
<tr>
<td></td>
<td></td>
<td>augmented_lagrangian_objective</td>
<td>Augmented Lagrangian approximate subproblem formulation</td>
</tr>
<tr>
<td></td>
<td></td>
<td>lagrangian_objective</td>
<td>Lagrangian approximate subproblem formulation</td>
</tr>
<tr>
<td>Required(Choose One)</td>
<td>constraint formulation (Group 2)</td>
<td>original_constraints</td>
<td>Use the constraints directly</td>
</tr>
<tr>
<td></td>
<td></td>
<td>linearized_constraints</td>
<td>Use linearized approximations to the constraints</td>
</tr>
<tr>
<td></td>
<td></td>
<td>no_constraints</td>
<td>Don’t use constraints</td>
</tr>
</tbody>
</table>

**Description**

First, the "primary" functions (that is, the objective functions or calibration terms) in the approximate subproblem can be selected to be surrogates of the original primary functions (original, primary), a single objective function (single_objective) formed from the primary function surrogates, or either an augmented Lagrangian merit function (augmented_lagrangian_objective) or a Lagrangian merit function (lagrangian_objective) formed from the primary and secondary function surrogates. The former option may imply the
use of a nonlinear least squares method, a multiobjective optimization method, or a single objective optimization method to solve the approximate subproblem, depending on the definition of the primary functions. The latter three options all imply the use of a single objective optimization method regardless of primary function definition. Second, the surrogate constraints in the approximate subproblem can be selected to be surrogates of the original constraints (original_constraints) or linearized approximations to the surrogate constraints (linearized_constraints), or constraints can be omitted from the subproblem (no_constraints).

original_primary

- Keywords Area
- method
- surrogate_based_local
- approx_subproblem
- original_primary

Construct approximations of all primary functions

Specification

Alias: none
Argument(s): none

Description

For SBL problems with nonlinear constraints, a number of algorithm formulations exist as described in[23] and as summarized in the Advanced Examples section of the Models chapter of the Users Manual[4]. First, the "primary" functions (that is, the objective functions or calibration terms) in the approximate subproblem can be selected to be surrogates of the original primary functions (original_primary), a single objective function (single_objective) formed from the primary function surrogates, or either an augmented Lagrangian merit function (augmented_lagrangian.objective) or a Lagrangian merit function (lagrangian.-objective) formed from the primary and secondary function surrogates. The former option may imply the use of a nonlinear least squares method, a multiobjective optimization method, or a single objective optimization method to solve the approximate subproblem, depending on the definition of the primary functions. The latter three options all imply the use of a single objective optimization method regardless of primary function definition.

single_objective

- Keywords Area
- method
- surrogate_based_local
- approx_subproblem
- single_objective

Construct approximation a single objective functions only
CHAPTER 6. KEYWORDS AREA

Specification
Alias: none
  Argument(s): none

Description
For SBL problems with nonlinear constraints, a number of algorithm formulations exist as described in[23] and as summarized in the Advanced Examples section of the Models chapter of the Users Manual[4]. First, the "primary" functions (that is, the objective functions or calibration terms) in the approximate subproblem can be selected to be surrogates of the original primary functions (original_primary), a single objective function (single_objective) formed from the primary function surrogates, or either an augmented Lagrangian merit function (augmented_lagrangian_objective) or a Lagrangian merit function (lagrangian_objective) formed from the primary and secondary function surrogates. The former option may imply the use of a nonlinear least squares method, a multiobjective optimization method, or a single objective optimization method to solve the approximate subproblem, depending on the definition of the primary functions. The latter three options all imply the use of a single objective optimization method regardless of primary function definition.

**augmented_lagrangian_objective**
- Keywords Area
- method
- surrogate_based_local
- approx_subproblem
- augmented_lagrangian_objective

Augmented Lagrangian approximate subproblem formulation

Specification
Alias: none
  Argument(s): none

Description
For SBL problems with nonlinear constraints, a number of algorithm formulations exist as described in[23] and as summarized in the Advanced Examples section of the Models chapter of the Users Manual[4]. First, the "primary" functions (that is, the objective functions or calibration terms) in the approximate subproblem can be selected to be surrogates of the original primary functions (original_primary), a single objective function (single_objective) formed from the primary function surrogates, or either an augmented Lagrangian merit function (augmented_lagrangian_objective) or a Lagrangian merit function (lagrangian_objective) formed from the primary and secondary function surrogates. The former option may imply the use of a nonlinear least squares method, a multiobjective optimization method, or a single objective optimization method to solve the approximate subproblem, depending on the definition of the primary functions. The latter three options all imply the use of a single objective optimization method regardless of primary function definition.
6.2. METHOD

lagrangian_objective

- Keywords Area
- method
- surrogate_based_local
- approx_subproblem
- lagrangian_objective

Lagrangian approximate subproblem formulation

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

For SBL problems with nonlinear constraints, a number of algorithm formulations exist as described in [23] and as summarized in the Advanced Examples section of the Models chapter of the Users Manual [4]. First, the "primary" functions (that is, the objective functions or calibration terms) in the approximate subproblem can be selected to be surrogates of the original primary functions (original_primary), a single objective function (single_objective) formed from the primary function surrogates, or either an augmented Lagrangian merit function (augmented_lagrangian_objective) or a Lagrangian merit function (lagrangian_objective) formed from the primary and secondary function surrogates. The former option may imply the use of a nonlinear least squares method, a multiobjective optimization method, or a single objective optimization method to solve the approximate subproblem, depending on the definition of the primary functions. The latter three options all imply the use of a single objective optimization method regardless of primary function definition.

original_constraints

- Keywords Area
- method
- surrogate_based_local
- approx_subproblem
- original_constraints

Use the constraints directly

**Specification**

**Alias:** none

**Argument(s):** none
CHAPTER 6. KEYWORDS AREA

Description
The surrogate constraints in the approximate subproblem can be selected to be surrogates of the original constraints (original_constraints) or linearized approximations to the surrogate constraints (linearized_constraints), or constraints can be omitted from the subproblem (no_constraints).

linearized_constraints
- Keywords Area
- method
- surrogate_based_local
- approx_subproblem
- linearized_constraints

Use linearized approximations to the constraints

Specification
Alias: none
Argument(s): none

Description
The surrogate constraints in the approximate subproblem can be selected to be surrogates of the original constraints (original_constraints) or linearized approximations to the surrogate constraints (linearized_constraints), or constraints can be omitted from the subproblem (no_constraints).

no_constraints
- Keywords Area
- method
- surrogate_based_local
- approx_subproblem
- no_constraints

Don’t use constraints

Specification
Alias: none
Argument(s): none

Description
The surrogate constraints in the approximate subproblem can be selected to be surrogates of the original constraints (original_constraints) or linearized approximations to the surrogate constraints (linearized_constraints), or constraints can be omitted from the subproblem (no_constraints).
6.2. METHOD

merit_function

- Keywords Area
- method
- surrogate_based_local
- merit_function

Select type of penalty or merit function

Specification

Alias: none
Argument(s): none
Default: augmented_lagrangian_merit

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword</th>
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<tr>
<td>Required (Choose One)</td>
<td>merit function (Group 1)</td>
<td>penalty_merit</td>
<td>Use penalty merit function</td>
</tr>
<tr>
<td>adaptive_penalty_merit</td>
<td>Use adaptive penalty merit function</td>
<td></td>
<td></td>
</tr>
<tr>
<td>lagrangian_merit</td>
<td>Use first-order Lagrangian merit function</td>
<td></td>
<td></td>
</tr>
<tr>
<td>augmented_lagrangian_merit</td>
<td>Use combined penalty and zeroth-order Lagrangian merit function</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Description

Following optimization of the approximate subproblem, the candidate iterate is evaluated using a merit function, which can be selected to be a simple penalty function with penalty ramped by surrogate_based_local iteration number (penalty_merit), an adaptive penalty function where the penalty ramping may be accelerated in order to avoid rejecting good iterates which decrease the constraint violation (adaptive_penalty_merit), a Lagrangian merit function which employs first-order Lagrange multiplier updates (lagrangian_merit), or an augmented Lagrangian merit function which employs both a penalty parameter and zeroth-order Lagrange multiplier updates (augmented_lagrangian_merit). When an augmented Lagrangian is selected for either the subproblem objective or the merit function (or both), updating of penalties and multipliers follows the approach described in[16].

penalty_merit

- Keywords Area
- method
- surrogate_based_local
SECOND, THE SURROGATE CONSTRAINTS IN THE APPROXIMATE SUBPROBLEM CAN BE SELECTED TO BE SURROGATES OF THE ORIGINAL CONSTRAINTS (ORIGINAL_CONSTRAINTS) OR LINEARIZED APPROXIMATIONS TO THE SURROGATE CONSTRAINTS (LINEARIZED_CONSTRAINTS), OR CONSTRAINTS CAN BE OMITTED FROM THE SUBPROBLEM (NO_CONSTRAINTS). FOLLOWING OPTIMIZATION OF THE APPROXIMATE SUBPROBLEM, THE CANDIDATE ITERATE IS EVALUATED USING A MERIT FUNCTION, WHICH CAN BE SELECTED TO BE A SIMPLE PENALTY FUNCTION WITH PENALTY RAMPED BY SBL ITERATION NUMBER (PENALTY_MERIT), AN ADAPTIVE PENALTY FUNCTION WHERE THE PENALTY RAMPING MAY BE ACCELERATED IN ORDER TO AVOID REJECTING GOOD ITERATES WHICH DECREASE THE CONSTRAINT VIOLATION (ADAPTIVE_PENALTY_MERIT), A LAGRANGIAN MERIT FUNCTION WHICH EMPLOYS FIRST-ORDER LAGRANGE MULTIPLIER UPDATES (LAGRANGIAN_MERIT), OR AN AUGMENTED LAGRANGIAN MERIT FUNCTION WHICH EMPLOYS BOTH A PENALTY PARAMETER AND ZERO-ORDER LAGRANGE MULTIPLIER UPDATES (AUGMENTED_LAGRANGIAN_MERIT). WHEN AN AUGMENTED LAGRANGIAN IS SELECTED FOR EITHER THE SUBPROBLEM OBJECTIVE OR THE MERIT FUNCTION (OR BOTH), UPDATING OF PENALTIES AND MULTIPLIERS FOLLOWS THE APPROACH DESCRIBED IN [16].

### adaptive_penalty_merit
- **Keywords Area**
- **method**
- **surrogate_based_local**
- **merit_function**
- **adaptive_penalty_merit**

Use adaptive penalty merit function

### Specification
**Alias:** none  
**Argument(s):** none

### Description
Second, the surrogate constraints in the approximate subproblem can be selected to be surrogates of the original constraints (original_constraints) or linearized approximations to the surrogate constraints (linearized_constraints), or constraints can be omitted from the subproblem (no_constraints). Following optimization of the approximate subproblem, the candidate iterate is evaluated using a merit function, which can be selected to be a simple penalty function with penalty ramped by SBL iteration number (penalty_merit), an adaptive penalty function where the penalty ramping may be accelerated in order to avoid rejecting good iterates which decrease the constraint violation (adaptive_penalty_merit), a Lagrangian merit function which employs first-order Lagrange multiplier updates (lagrangian_merit), or an augmented Lagrangian merit function which employs both a penalty parameter and zeroth-order Lagrange multiplier updates (augmented_lagrangian_merit). When an augmented Lagrangian is selected for either the subproblem objective or the merit function (or both), updating of penalties and multipliers follows the approach described in [16].
employs first-order Lagrange multiplier updates (lagrangian_merit), or an augmented Lagrangian merit function which employs both a penalty parameter and zeroth-order Lagrange multiplier updates (augmented_lagrangian_merit). When an augmented Lagrangian is selected for either the subproblem objective or the merit function (or both), updating of penalties and multipliers follows the approach described in [16].

### lagrangian_merit

- **Keywords Area**
- **method**
- **surrogate_based_local**
- **merit_function**
- **lagrangian_merit**

Use first-order Lagrangian merit function

### Specification

**Alias:** none

**Argument(s):** none

### Description

Second, the surrogate constraints in the approximate subproblem can be selected to be surrogates of the original constraints (original_constraints) or linearized approximations to the surrogate constraints (linearized_constraints), or constraints can be omitted from the subproblem (no_constraints). Following optimization of the approximate subproblem, the candidate iterate is evaluated using a merit function, which can be selected to be a simple penalty function with penalty ramped by SBL iteration number (penalty_merit), an adaptive penalty function where the penalty ramping may be accelerated in order to avoid rejecting good iterates which decrease the constraint violation (adaptive_penalty_merit), a Lagrangian merit function which employs first-order Lagrange multiplier updates (lagrangian_merit), or an augmented Lagrangian merit function which employs both a penalty parameter and zeroth-order Lagrange multiplier updates (augmented_lagrangian_merit). When an augmented Lagrangian is selected for either the subproblem objective or the merit function (or both), updating of penalties and multipliers follows the approach described in [16].

### augmented_lagrangian_merit

- **Keywords Area**
- **method**
- **surrogate_based_local**
- **merit_function**
- **augmented_lagrangian_merit**

Use combined penalty and zeroth-order Lagrangian merit function
CHAPTER 6. KEYWORDS AREA

Specification
Alias: none
Argument(s): none

Description
Second, the surrogate constraints in the approximate subproblem can be selected to be surrogates of the original constraints (original_constraints) or linearized approximations to the surrogate constraints (linearized_constraints), or constraints can be omitted from the subproblem (no_constraints). Following optimization of the approximate subproblem, the candidate iterate is evaluated using a merit function, which can be selected to be a simple penalty function with penalty ramped by SBL iteration number (penaltyMerit), an adaptive penalty function where the penalty ramping may be accelerated in order to avoid rejecting good iterates which decrease the constraint violation (adaptive_penaltyMerit), a Lagrangian merit function which employs first-order Lagrange multiplier updates (lagrangian_merit), or an augmented Lagrangian merit function which employs both a penalty parameter and zeroth-order Lagrange multiplier updates (augmented_lagrangian_merit). When an augmented Lagrangian is selected for either the subproblem objective or the merit function (or both), updating of penalties and multipliers follows the approach described in[16].

Acceptance Logic

- Keywords Area
- method
- surrogate_based_local
- acceptance_logic

Set criteria for trusted surrogate

Specification
Alias: none
Argument(s): none
Default: filter

<table>
<thead>
<tr>
<th>Required/-Optional Required (Choose One)</th>
<th>Description of Group acceptance logic (Group 1)</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>tr_ratio</td>
<td>filter</td>
<td>filter</td>
<td>Surrogate-Based Local iterate acceptance logic</td>
</tr>
</tbody>
</table>

Description
Following calculation of the merit function for the new iterate, the iterate is accepted or rejected and the trust region size is adjusted for the next surrogate_based_local iteration. Iterate acceptance is governed either by a trust region ratio (tr_ratio) formed from the merit function values or by a filter method (filter); however, trust region resizing logic is currently based only on the trust region ratio. For infeasible iterates, constraint relaxation can be used for balancing constraint satisfaction and progress made toward an optimum.
6.2. METHOD

tr_ratio

- Keywords Area
- method
- surrogate_based_local
- acceptance_logic
- tr_ratio

Surrogate-Based Local iterate acceptance logic

Specification

Alias: none
Argument(s): none

Description

Following calculation of the merit function for the new iterate, the iterate is accepted or rejected and the trust region size is adjusted for the next SBL iteration. Iterate acceptance is governed either by a trust region ratio (tr_ratio) formed from the merit function values or by a filter method (filter); however, trust region resizing logic is currently based only on the trust region ratio. For infeasible iterates, constraint relaxation can be used for balancing constraint satisfaction and progress made toward an optimum. The command constraint_relax followed by a method name specifies the type of relaxation to be used. Currently, homotopy[68] is the only available method for constraint relaxation, and this method is dependent on the presence of the NPSOL library within the Dakota executable.

filter

- Keywords Area
- method
- surrogate_based_local
- acceptance_logic
- filter

Surrogate-Based Local iterate acceptance logic

Specification

Alias: none
Argument(s): none
CHAPTER 6. KEYWORDS AREA

Description

Following calculation of the merit function for the new iterate, the iterate is accepted or rejected and the trust region size is adjusted for the next SBL iteration. Iterate acceptance is governed either by a trust region ratio (tr_ratio) formed from the merit function values or by a filter method (filter); however, trust region resizing logic is currently based only on the trust region ratio. For infeasible iterates, constraint relaxation can be used for balancing constraint satisfaction and progress made toward an optimum. The command constraint_relax followed by a method name specifies the type of relaxation to be used. Currently, homotopy [68] is the only available method for constraint relaxation, and this method is dependent on the presence of the NPSOL library within the Dakota executable.

**constraint_relax**

- Keywords Area
- method
- surrogate_based_local
- constraint_relax

Enable constraint relaxation

**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** no relaxation

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
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<tbody>
<tr>
<td>Required</td>
<td></td>
<td>homotopy</td>
<td>Surrogate-Based local constraint relaxation method for infeasible iterates</td>
</tr>
</tbody>
</table>

**Description**

The command constraint_relax followed by a method name specifies the type of relaxation to be used. Currently, homotopy [68] is the only available method for constraint relaxation, and this method is dependent on the presence of the NPSOL library within the Dakota executable.

**homotopy**

- Keywords Area
- method
- surrogate_based_local
- constraint_relax
- homotopy

Surrogate-Based local constraint relaxation method for infeasible iterates
6.2. METHOD

Specification

Alias: none
  Argument(s): none

Description

Currently, homotopy [68] is the only available method for constraint relaxation, and this method is dependent on the presence of the NPSOL library within the Dakota executable.

trust_region

- Keywords Area
- method
- surrogate_based_local
- trust_region

Specification group for trust region model management

Specification

Alias: none
  Argument(s): none

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>initial_size</td>
<td>initial_size</td>
<td>Trust region initial size (relative to bounds)</td>
</tr>
<tr>
<td>Optional</td>
<td>minimum_size</td>
<td>minimum_size</td>
<td>Trust region minimum size</td>
</tr>
<tr>
<td>Optional</td>
<td>contract_threshold</td>
<td>contract_threshold</td>
<td>Shrink trust region if trust region ratio is below this value</td>
</tr>
<tr>
<td>Optional</td>
<td>expand_threshold</td>
<td>expand_threshold</td>
<td>Expand trust region if trust region ratio is above this value</td>
</tr>
<tr>
<td>Optional</td>
<td>contraction_factor</td>
<td>contraction_factor</td>
<td>Amount by which step length is rescaled</td>
</tr>
<tr>
<td>Optional</td>
<td>expansion_factor</td>
<td>expansion_factor</td>
<td>Trust region expansion factor</td>
</tr>
</tbody>
</table>

Description

The trust_region optional group specification can be used to specify the initial size of the trust region (using initial_size) relative to the total variable bounds, the minimum size of the trust region (using minimum_size), the contraction factor for the trust region size (using contraction_factor) used when the surrogate model is performing poorly, and the expansion factor for the trust region size (using expansion_factor) used
when the the surrogate model is performing well. Two additional commands are the trust region size contraction threshold (using contract_threshold) and the trust region size expansion threshold (using expand_threshold). These two commands are related to what is called the trust region ratio, which is the actual decrease in the truth model divided by the predicted decrease in the truth model in the current trust region. The command contract_threshold sets the minimum acceptable value for the trust region ratio, i.e., values below this threshold cause the trust region to shrink for the next surrogate_based_local iteration. The command expand_threshold determines the trust region value above which the trust region will expand for the next surrogate_based_local iteration.

Each of these specifications are REAL scalars, with the exception of initial_size, which is a REALLIST.

**initial_size**

- **Keywords Area**
- **method**
- **surrogate_based_local**
- **trust_region**
- **initial_size**

Trust region initial size (relative to bounds)

**Specification**

Alias: none

Argument(s): REALLIST

**Description**

The trust_region optional group specification can be used to specify the initial size of the trust region (using initial_size) relative to the total variable bounds, the minimum size of the trust region (using minimum_size), the contraction factor for the trust region size (using contraction_factor) used when the surrogate model is performing poorly, and the expansion factor for the trust region size (using expansion_factor) used when the the surrogate model is performing well. Two additional commands are the trust region size contraction threshold (using contract_threshold) and the trust region size expansion threshold (using expand_threshold). These two commands are related to what is called the trust region ratio, which is the actual decrease in the truth model divided by the predicted decrease in the truth model in the current trust region. The command contract_threshold sets the minimum acceptable value for the trust region ratio, i.e., values below this threshold cause the trust region to shrink for the next SBL iteration. The command expand_threshold determines the trust region value above which the trust region will expand for the next SBL iteration.

All of these specifications are REAL scalars, with the exception of the specification of initial_size, which is a REALLIST. This array corresponds to the case when there are more than 2 model forms or discretizations within a model hierarchy. The default initial_size involves a recursive halving of the global bounds for each trust region in the hierarchy: e.g., a scalar value of .5 for a single trust region managing two model forms/discretizations, or an array of (.125, .25, .5) for four model forms/discretizations (three trust regions ordered from the lowest to highest fidelity surrogate, with model four as truth).
6.2. METHOD

**minimum_size**

- Keywords Area
- method
- surrogate_based_local
- trust_region
- minimum_size

Trust region minimum size

**Specification**

**Alias:** none

**Argument(s):** REAL

**Default:** 1.e-6

**Description**

The trust_region optional group specification can be used to specify the initial size of the trust region (using initial_size) relative to the total variable bounds, the minimum size of the trust region (using minimum_size), the contraction factor for the trust region size (using contraction_factor) used when the surrogate model is performing poorly, and the expansion factor for the trust region size (using expansion_factor) used when the surrogate model is performing well. Two additional commands are the trust region size contraction threshold (using contract_threshold) and the trust region size expansion threshold (using expand_threshold). These two commands are related to what is called the trust region ratio, which is the actual decrease in the truth model divided by the predicted decrease in the truth model in the current trust region. The command contract_threshold sets the minimum acceptable value for the trust region ratio, i.e., values below this threshold cause the trust region to shrink for the next SBL iteration. The command expand_threshold determines the trust region value above which the trust region will expand for the next SBL iteration.

**contract_threshold**

- Keywords Area
- method
- surrogate_based_local
- trust_region
- contract_threshold

Shrink trust region if trust region ratio is below this value

**Specification**

**Alias:** none

**Argument(s):** REAL

**Default:** 0.25
Description

The trust_region optional group specification can be used to specify the initial size of the trust region (using initial_size) relative to the total variable bounds, the minimum size of the trust region (using minimum_size), the contraction factor for the trust region size (using contraction_factor) used when the surrogate model is performing poorly, and the expansion factor for the trust region size (using expansion_factor) used when the surrogate model is performing well. Two additional commands are the trust region size contraction threshold (using contract_threshold) and the trust region size expansion threshold (using expand_threshold). These two commands are related to what is called the trust region ratio, which is the actual decrease in the truth model divided by the predicted decrease in the truth model in the current trust region. The command contract_threshold sets the minimum acceptable value for the trust region ratio, i.e., values below this threshold cause the trust region to shrink for the next SBL iteration. The command expand_threshold determines the trust region value above which the trust region will expand for the next SBL iteration.

expand_threshold

- Keywords Area
- method
- surrogate_based_local
- trust_region
- expand_threshold

Expand trust region if trust region ratio is above this value

Specification

Alias: none

Argument(s): REAL
Default: 0.75

Description

The trust_region optional group specification can be used to specify the initial size of the trust region (using initial_size) relative to the total variable bounds, the minimum size of the trust region (using minimum_size), the contraction factor for the trust region size (using contraction_factor) used when the surrogate model is performing poorly, and the expansion factor for the trust region size (using expansion_factor) used when the surrogate model is performing well. Two additional commands are the trust region size contraction threshold (using contract_threshold) and the trust region size expansion threshold (using expand_threshold). These two commands are related to what is called the trust region ratio, which is the actual decrease in the truth model divided by the predicted decrease in the truth model in the current trust region. The command contract_threshold sets the minimum acceptable value for the trust region ratio, i.e., values below this threshold cause the trust region to shrink for the next SBL iteration. The command expand_threshold determines the trust region value above which the trust region will expand for the next SBL iteration.
6.2. METHOD

contraction_factor

- Keywords Area
- method
- surrogate_based_local
- trust_region
- contraction_factor

Amount by which step length is rescaled

Specification

Alias: none
Argument(s): REAL
Default: 0.25

Description

For pattern search methods, contraction_factor specifies the amount by which step length is rescaled after unsuccessful iterates, must be strictly between 0 and 1.

For methods that can expand the step length, the expansion is \( \frac{1}{\text{contraction_factor}} \)

expansion_factor

- Keywords Area
- method
- surrogate_based_local
- trust_region
- expansion_factor

Trust region expansion factor

Specification

Alias: none
Argument(s): REAL
Default: 2.0
CHAPTER 6. KEYWORDS AREA

Description

The `trust_region` optional group specification can be used to specify the initial size of the trust region (using `initial_size`) relative to the total variable bounds, the minimum size of the trust region (using `minimum_size`), the contraction factor for the trust region size (using `contraction_factor`) used when the surrogate model is performing poorly, and the expansion factor for the trust region size (using `expansion_factor`) used when the surrogate model is performing well. Two additional commands are the trust region size contraction threshold (using `contract_threshold`) and the trust region size expansion threshold (using `expand_threshold`). These two commands are related to what is called the trust region ratio, which is the actual decrease in the truth model divided by the predicted decrease in the truth model in the current trust region. The command `contract_threshold` sets the minimum acceptable value for the trust region ratio, i.e., values below this threshold cause the trust region to shrink for the next SBL iteration. The command `expand_threshold` determines the trust region value above which the trust region will expand for the next SBL iteration.

`max_iterations`

- Keywords Area
- method
- surrogate_based_local
- `max_iterations`

Number of iterations allowed for optimizers and adaptive UQ methods

Topics

This keyword is related to the topics:

- `method_independent_controls`

Specification

Alias: none

Argument(s): INTEGER

Default: 100 (exceptions: `fsu_cvt`, `local_reliability`: 25; `global_{reliability, interval_est, evidence}` / `efficient_global`: 25*n)

Description

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed `max_iterations` iterations. See also `max_function_evaluations`.

Default Behavior

Default value is 100.

`convergence_tolerance`

- Keywords Area
- method
6.2. METHOD

- surrogate_based_local
- convergence_tolerance

Stopping criterion based on convergence of the objective function or statistics

Topics

This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none

Argument(s): REAL

Default: 1.e-4

Description

The convergence_tolerance specification provides a real value for controlling the termination of iteration. For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by convergence_tolerance, then this convergence criterion is satisfied on the current iteration. Therefore, permissible values are between 0 and 1, non-inclusive.

Behavior Varies by Package/Library

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- DOT: must be satisfied for two consecutive iterations
- NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of convergence_tolerance approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., convergence_tolerance = 1.e-6 will result in approximately six digits of accuracy in the final objective function).
- NL2SOL: See nl2sol

constraint_tolerance

- Keywords Area
- method
- surrogate_based_local
- constraint_tolerance

The maximum allowable value of constraint violation still considered to be feasible
Topics
This keyword is related to the topics:

- method\_independent\_controls

Specification
Alias: none
Argument(s): REAL
Default: Library default

Description
The constraint\_tolerance specification determines the maximum allowable value of infeasibility that any constraint in an optimization problem may possess and still be considered to be satisfied. If a constraint function is greater than this value then it is considered to be violated by the optimization algorithm. This specification gives some control over how tightly the constraints will be satisfied at convergence of the algorithm. However, if the value is set too small the algorithm may terminate with one or more constraints being violated.

This specification is currently meaningful for the NPSOL, NLSSOL, DOT and CONMIN constrained optimizers.

Defaults
Defaults can vary depending on the method.

- DOT constrained optimizers: 0.003
- NPSOL: dependent upon the machine precision, typically on the order of 1.e-8 for double precision computations

6.2.9 surrogate\_based\_global

- Keywords Area
- method
- surrogate\_based\_global

Global Surrogate Based Optimization

Topics
This keyword is related to the topics:

- surrogate\_based\_optimization\_methods

Specification
Alias: none
Argument(s): none
## 6.2. METHOD

### Required/-Optional Group 1

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required (Choose One)</td>
<td>Method pointer</td>
<td>method_pointer</td>
<td>Pointer to sub-method to apply to a surrogate or branch-and-bound sub-problem</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>method_name</td>
<td>Specify sub-method by name</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>model_pointer</td>
<td>Identifier for model block to be used by a method</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>replace_points</td>
<td>(Recommended) Replace points in the surrogate training set, instead of appending</td>
</tr>
<tr>
<td></td>
<td></td>
<td>max_iterations</td>
<td>Number of iterations allowed for optimizers and adaptive UQ methods</td>
</tr>
</tbody>
</table>

### Description

The surrogate based global specification must identify:

- a sub-method, using either method_pointer or method_name
- model_pointer must be used to identify a surrogate model

**surrogate based global** works in an iterative scheme where optimization is performed on a global surrogate using the same bounds during each iteration.

- In one iteration, the optimal solutions of the surrogate model are found, and then a selected set of these optimal surrogate solutions are passed to the next iteration.

- At the next iteration, these surrogate points are evaluated with the "truth" model, and then these points are added back to the set of points upon which the next surrogate is constructed.

In this way, the optimization acts on a more accurate surrogate during each iteration, presumably driving to optimality quickly.

**Known Issue:** When using discrete variables, there have been sometimes significant differences in surrogate behavior observed across computing platforms in some cases. The cause has not yet been fully diagnosed and is currently under investigation. In addition, guidance on appropriate construction and use of surrogates with discrete variables is under development. In the meantime, users should therefore be aware that there is a risk of inaccurate results when using surrogates with discrete variables.

**Method Independent Controls**
max_iterations is used as a stopping criterion (see note below)

Notes
We have some cautionary notes before using the surrogate-based global method:

• **This approach has no guarantee of convergence.**

• One might first try a single minimization method coupled with a surrogate model prior to using the surrogate-based global method. This is essentially equivalent to setting max_iterations to 1 and will allow one to get a sense of what surrogate types are the most accurate to use for the problem.

• Also note that one can specify that surrogates be built for all primary functions and constraints or for only a subset of these functions and constraints. This allows one to use a "truth" model directly for some of the response functions, perhaps due to them being much less expensive than other functions.

• We initially recommend a small number of maximum iterations, such as 3-5, to get a sense of how the optimization is evolving as the surrogate gets updated. If it appears to be changing significantly, then a larger number (used in combination with restart) may be needed.

Theory
In surrogate-based optimization (SBO) and surrogate-based nonlinear least squares (SBNLS), minimization occurs using a set of one or more approximations, defined from a surrogate model, that are built and periodically updated using data from a "truth" model. The surrogate model can be a global data fit (e.g., regression or interpolation of data generated from a design of computer experiments), a multipoint approximation, a local Taylor Series expansion, or a model hierarchy approximation (e.g., a low-fidelity simulation model), whereas the truth model involves a high-fidelity simulation model. The goals of surrogate-based methods are to reduce the total number of truth model simulations and, in the case of global data fit surrogates, to smooth noisy data with an easily navigated analytic function.

It was originally designed for MOGA (a multi-objective genetic algorithm). Since genetic algorithms often need thousands or tens of thousands of points to produce optimal or near-optimal solutions, the use of surrogates can be helpful for reducing the truth model evaluations. Instead of creating one set of surrogates for the individual objectives and running the optimization algorithm on the surrogate once, the idea is to select points along the (surrogate) Pareto frontier, which can be used to supplement the existing points.

In this way, one does not need to use many points initially to get a very accurate surrogate. The surrogate becomes more accurate as the iterations progress.

See Also
These keywords may also be of interest:

• efficient_global

• surrogate_based_local

method_pointer

• Keywords Area

• method

• surrogate_based_global

• method_pointer

Pointer to sub-method to apply to a surrogate or branch-and-bound sub-problem
6.2. METHOD

Topics
This keyword is related to the topics:
- block_pointer

Specification
Alias: approx_method_pointer
Argument(s): STRING

Description
The *method_pointer* keyword is used to specify a pointer to an optimization or least-squares sub-method to apply in the context of what could be described as hierarchical methods. In surrogate-based methods, the sub-method is applied to the surrogate model. In the branch-and-bound method, the sub-method is applied to the relaxed sub-problems.

Any *model_pointer* identified in the sub-method specification is ignored. Instead, the parent method is responsible for selecting the appropriate model to use as specified by its *model_pointer*. In surrogate-based methods, it is a surrogate model defined using its *model_pointer*. In branch-and-bound methods, it is the relaxed model that is constructed internally from the original model.

*method_name*
- Keywords Area
- method
- surrogate_based_global
- *method_name*
  Specify sub-method by name

Specification
Alias: approx_method_name
Argument(s): STRING

Description
The *method_name* keyword is used to specify a sub-method by Dakota method name (e.g. `npsol_sqp`) rather than block pointer. The method will be executed using its default settings. The optional *model_pointer* specification can be used to associate a model block with the method.

*model_pointer*
- Keywords Area
- method
- surrogate_based_global
- *model_pointer*
  Identifier for model block to be used by a method
Topics

This keyword is related to the topics:

- `block_pointer`

Specification

Alias: `approx_model_pointer`

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)

Description

The `model_pointer` is used to specify which `model` block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a `model` block in the Dakota input file that has a corresponding `id_model` with the same name.

Usage Tips

When doing advanced analyses that involve using multiple methods and multiple models, defining a `model_pointer` for each method is imperative.

See `block_pointer` for details about pointers.

Examples

```plaintext
environment
tabular_graphics_data
method_pointer = 'UQ'

method
  id_method = 'UQ'
  model_pointer = 'Surr'
sampling,
    samples = 10
    seed = 98765 rng rnum2
    response_levels = 0.1 0.2 0.6
    0.1 0.2 0.6
    0.1 0.2 0.6
    sample_type lhs
    distribution cumulative

model
  id_model = 'Surr'
surrogate global,
  dace_method_pointer = 'DACE'
polynomial quadratic

method
  id_method = 'DACE'
  model_pointer = 'DACE_M'
sampling sample_type lhs
    samples = 121 seed = 5034 rng rnum2

model
  id_model = 'DACE_M'
single
```
6.2. METHOD

```python
interface_pointer = 'I1'

variables
uniform_uncertain = 2
lower_bounds = 0. 0.
upper_bounds = 1. 1.
descriptors = 'x1' 'x2'

interface
id_interface = 'I1'

system asynch evaluation_concurrency = 5
analysis_driver = 'text_book'

responses
response_functions = 3
no_gradients
no_hessians

replace_points

- Keywords Area
- method
- surrogate_based_global
- replace_points

(Recommended) Replace points in the surrogate training set, instead of appending

Specification

Alias: none
Argument(s): none
Default: Points appended, not replaced

Description

The user has the option of appending the optimal points from the surrogate model to the current set of truth points or using the optimal points from the surrogate model to replace the optimal set of points from the previous iteration. Although appending to the set is the default behavior, at this time we strongly recommend using the option replace_points because it appears to be more accurate and robust.

max_iterations

- Keywords Area
- method
- surrogate_based_global
- max_iterations

Number of iterations allowed for optimizers and adaptive UQ methods
CHAPTER 6. KEYWORDS AREA

Topics

This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none

Argument(s): INTEGER

Default: 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence} / efficient_global: 25*n)

Description

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed \texttt{max_iterations} iterations. See also \texttt{max_function_evaluations}.

Default Behavior

Default value is 100.

6.2.10 \texttt{dot_frcg}

- Keywords Area
- method
- \texttt{dot_frcg}

A conjugate gradient optimization method

Specification

Alias: none

Argument(s): none

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>\texttt{max_iterations}</td>
<td>Number of iterations allowed for optimizers and adaptive UQ methods</td>
</tr>
</tbody>
</table>
### 6.2. METHOD

<table>
<thead>
<tr>
<th>Optional</th>
<th>convergence_tolerance</th>
<th>Stopping criterion based on convergence of the objective function or statistics</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>constraint_tolerance</td>
<td>The maximum allowable value of constraint violation still considered to be feasible</td>
</tr>
<tr>
<td>Optional</td>
<td>speculative</td>
<td>Compute speculative gradients</td>
</tr>
<tr>
<td>Optional</td>
<td>max_function_evaluations</td>
<td>Number of function evaluations allowed for optimizers</td>
</tr>
<tr>
<td>Optional</td>
<td>scaling</td>
<td>Turn on scaling for variables, responses, and constraints</td>
</tr>
<tr>
<td>Optional</td>
<td>model_pointer</td>
<td>Identifier for model block to be used by a method</td>
</tr>
</tbody>
</table>

### Description

This is a duplicated keyword. Please use dot instead.

We here provide a caution regarding dot_frcg. In DOT Version 4.20, we have noticed inconsistent behavior of this algorithm across different versions of Linux. Our best assessment is that it is due to different treatments of uninitialized variables. As we do not know the intention of the code authors and maintaining DOT source code is outside of the Dakota project scope, we have not made nor are we recommending any code changes to address this. However, all users who use dot_frcg in DOT Version 4.20 should be aware that results may not be reliable.

### See Also

These keywords may also be of interest:

- frcg

**max_iterations**

- Keywords Area
- method
- dot_frcg
• max_iterations

Number of iterations allowed for optimizers and adaptive UQ methods

**Topics**

This keyword is related to the topics:

• method-independent_controls

**Specification**

Alias: none

**Argument(s):** INTEGER

**Default:** 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence} / efficient-global: 25*n)

**Description**

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed max_iterations iterations. See also max_function_evaluations.

**Default Behavior**

Default value is 100.

**convergence_tolerance**

- Keywords Area
- method
- dot_frcg
- convergence_tolerance

Stopping criterion based on convergence of the objective function or statistics

**Topics**

This keyword is related to the topics:

• method-independent_controls

**Specification**

Alias: none

**Argument(s):** REAL

**Default:** 1.e-4
6.2. METHOD

Description

The `convergence_tolerance` specification provides a real value for controlling the termination of iteration.

For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by `convergence_tolerance`, then this convergence criterion is satisfied on the current iteration.

Therefore, permissible values are between 0 and 1, non-inclusive.

Behavior Varies by Package/Library

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- **DOT**: must be satisfied for two consecutive iterations
- **NPSOL**: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of `convergence_tolerance` approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., `convergence_tolerance = 1.e-6` will result in approximately six digits of accuracy in the final objective function).
- **NL2SOL**: See `nl2sol`

**constraint_tolerance**

- **Keywords Area**
  - method
  - dot_frcg
  - `constraint_tolerance`

The maximum allowable value of constraint violation still considered to be feasible

Topics

This keyword is related to the topics:

- `method-independent_controls`

Specification

**Alias**: none

**Argument(s)**: REAL

**Default**: Library default
Description

The constraint_tolerance specification determines the maximum allowable value of infeasibility that any constraint in an optimization problem may possess and still be considered to be satisfied.

If a constraint function is greater than this value then it is considered to be violated by the optimization algorithm. This specification gives some control over how tightly the constraints will be satisfied at convergence of the algorithm. However, if the value is set too small the algorithm may terminate with one or more constraints being violated.

This specification is currently meaningful for the NPSOL, NLSSOL, DOT and CONMIN constrained optimizers.

Defaults

Defaults can vary depending on the method.

- DOT constrained optimizers: 0.003
- NPSOL: dependent upon the machine precision, typically on the order of $1 \cdot 10^{-8}$ for double precision computations

speculative

- Keywords Area
- method
- dot_frcg
- speculative

Compute speculative gradients

Topics

This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none

Argument(s): none

Default: no speculation

Description

When performing gradient-based optimization in parallel, speculative gradients can be selected to address the load imbalance that can occur between gradient evaluation and line search phases. In a typical gradient-based optimization, the line search phase consists primarily of evaluating the objective function and any constraints at a trial point, and then testing the trial point for a sufficient decrease in the objective function value and/or constraint violation. If a sufficient decrease is not observed, then one or more additional trial points may be attempted sequentially. However, if the trial point is accepted then the line search phase is complete and the gradient evaluation phase begins. By speculating that the gradient information associated with a given line search trial point will be used later, additional coarse grained parallelism can be introduced by computing the gradient information (either by finite difference or analytically) in parallel, at the same time as the line search phase trial-point function evaluation.
values. This balances the total amount of computation to be performed at each design point and allows for efficient utilization of multiple processors. While the total amount of work performed will generally increase (since some speculative gradients will not be used when a trial point is rejected in the line search phase), the run time will usually decrease (since gradient evaluations needed at the start of each new optimization cycle were already performed in parallel during the line search phase). Refer to [14] for additional details. The speculative specification is implemented for the gradient-based optimizers in the DOT, CONMIN, and OPT++ libraries, and it can be used with dakota numerical or analytic gradient selections in the responses specification (refer to responses gradient section for information on these specifications). It should not be selected with vendor numerical gradients since vendor internal finite difference algorithms have not been modified for this purpose. In full-Newton approaches, the Hessian is also computed speculatively. NPSOL and NLSSOL do not support speculative gradients, as their gradient-based line search in user-supplied gradient mode (dakota numerical or analytic gradients) is a superior approach for load-balanced parallel execution.

The speculative specification enables speculative computation of gradient and/or Hessian information, where applicable, for parallel optimization studies. By speculating that the derivative information at the current point will be used later, the complete data set (all available gradient/Hessian information) can be computed on every function evaluation. While some of these computations will be wasted, the positive effects are a consistent parallel load balance and usually shorter wall clock time. The speculative specification is applicable only when parallelism in the gradient calculations can be exploited by Dakota (it will be ignored for vendor numerical gradients).

max_function_evaluations

- **Keywords Area**
- method
- dot_frcg
- max_function_evaluations

Number of function evaluations allowed for optimizers

**Topics**

This keyword is related to the topics:

- method_independent_controls

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** 1000

**Description**

The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed max_function_evaluations evaluations. See also max_iterations.

**Default Behavior**

Default value is 1000.
Keywords Area

method

dot_frcg

scaling

Turn on scaling for variables, responses, and constraints

Topics

This keyword is related to the topics:

- method

- method_independent_controls

Specification

Alias: none

Argument(s): none

Default: no scaling

Description

Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by by providing the scaling keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the method, variables, and responses blocks. When the scaling keyword is omitted, all _scale_types and _scales specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.

- a _scales keyword, which gives characteristic values

- a _scale_type keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

Scale Types

There are four scale types:

1. none (default) - no scaling, value of _scales keyword is ignored

2. value - multiplicative scaling
3. auto - automatic scaling

First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:

- two-sided bounds scaled into the interval [0,1];
- one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
- no bounds or targets: no automatic scaling possible, therefore no scaling for this component

Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into [0,1].

4. log - logarithmic scaling

First, any characteristic values from the optional *scales specification are applied. Then logarithm base 10 scaling is applied.

Logarithmic scaling is not available for linear constraints.

When continuous design variables are log scaled, linear constraints are not allowed.

Scales

The *scales keywords are used to specify the characteristic values. These must be non-zero real numbers. The numbers are used according to the corresponding *scale_type, as described above.

Depending on the scale type, the characteristic values may be required or optional.

- none, auto, log - optional
- value - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than 1.0e10*DBL_MIN. User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.

Examples

The two examples below are equivalent:

```plaintext
responses
objective_functions 3
sense "maximize"
primary_scale_types = "value"
primary_scales = 1 1 100

responses
objective_functions 3
sense "maximize"
primary_scale_types = "value" "value" "value"
primary_scales = 1 1 100
```
model_pointer

- **Keywords Area**
- **method**
- **dot_frcg**
- **model_pointer**

Identifier for model block to be used by a method

**Topics**

This keyword is related to the topics:

- **block_pointer**

**Specification**

**Alias:** none

**Argument(s):** STRING

**Default:** method use of last model parsed (or use of default model if none parsed)

**Description**

The `model_pointer` is used to specify which `model` block will be used to perform the function evaluations needed by the Dakota method.

**Default Behavior**

- If not specified, a Dakota method will use the last model block parsed. If specified, there must be a `model` block in the Dakota input file that has a corresponding `id_model` with the same name.

**Usage Tips**

- When doing advanced analyses that involve using multiple methods and multiple models, defining a `model_pointer` for each method is imperative.

  See **block_pointer** for details about pointers.

**Examples**

```plaintext
environment
  tabular_graphics_data
  method_pointer = 'UQ'

method
  id_method = 'UQ'
  model_pointer = 'SURR'
  sampling,
  samples = 10
  seed = 98765 rng rnum2
  response_levels = 0.1 0.2 0.6
  0.1 0.2 0.6
  0.1 0.2 0.6
  sample_type lhs
  distribution cumulative

model
  id_model = 'SURR'
```
6.2. METHOD

```
surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
id_method = 'DACE'
model_pointer = 'DACE_M'
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = 'DACE_M'
single
interface_pointer = 'I1'

variables
uniform_uncertain = 2
lower_bounds = 0. 0.
upper_bounds = 1. 1.
descriptors = 'x1' 'x2'

interface
id_interface = 'I1'
system async evaluation_concurrency = 5
analysis_driver = 'text_book'

responses
response_functions = 3
no_gradients
no_hessians
```

6.2.11 dot_mmfd

- **Keywords Area**
- **method**
- **dot_mmfd**

Method of feasible directions

### Specification

**Alias:** none

**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>max_iterations</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Number of iterations allowed for optimizers and adaptive UQ methods
### Optional convergence_tolerance
Stopping criterion based on convergence of the objective function or statistics

### Optional constraint_tolerance
The maximum allowable value of constraint violation still considered to be feasible

### Optional speculative
Compute speculative gradients

### Optional max_function_evaluations
Number of function evaluations allowed for optimizers

### Optional scaling
Turn on scaling for variables, responses, and constraints

### Optional model_pointer
Identifier for model block to be used by a method

### Description
This is a duplicated keyword. Please use dot instead.

### See Also
These keywords may also be of interest:

- mmfd

**max_iterations**

- Keywords Area
- method
- dot.mmfd
- max_iterations

Number of iterations allowed for optimizers and adaptive UQ methods
6.2. **METHOD**

**Topics**
This keyword is related to the topics:

- `method_independent_controls`

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** 100 (exceptions: `fsu_cvt`, `local_reliability`: 25; `global`: `{reliability, interval_est, evidence}` / efficient- `global`: `25*n`)

**Description**

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed `max_iterations` iterations. See also `max_function_evaluations`.

**Default Behavior**

Default value is 100.

**convergence_tolerance**

- **Keywords Area**
- **method**
- **dot_mmfd**
- **convergence_tolerance**

Stopping criterion based on convergence of the objective function or statistics.

**Topics**
This keyword is related to the topics:

- `method_independent_controls`

**Specification**

**Alias:** none

**Argument(s):** REAL

**Default:** 1.e-4

**Description**

The `convergence_tolerance` specification provides a real value for controlling the termination of iteration.

For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by `convergence_tolerance`, then this convergence criterion is satisfied on the current iteration.
Therefore, permissible values are between 0 and 1, non-inclusive.

**Behavior Varies by Package/Library**

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- **DOT**: must be satisfied for two consecutive iterations
- **NPSOL**: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of convergence_tolerance approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., convergence_tolerance = 1.e-6 will result in approximately six digits of accuracy in the final objective function).
- **NL2SOL**: See nl2sol

**constraint_tolerance**

- **Keywords Area**
- **method**
- **dot_mmfd**
- **constraint_tolerance**

The maximum allowable value of constraint violation still considered to be feasible

**Topics**

This keyword is related to the topics:

- **method_independent_controls**

**Specification**

**Alias**: none

**Argument(s)**: REAL

**Default**: Library default

**Description**

The constraint_tolerance specification determines the maximum allowable value of infeasibility that any constraint in an optimization problem may possess and still be considered to be satisfied.

If a constraint function is greater than this value then it is considered to be violated by the optimization algorithm. This specification gives some control over how tightly the constraints will be satisfied at convergence of the algorithm. However, if the value is set too small the algorithm may terminate with one or more constraints being violated.
6.2. METHOD

This specification is currently meaningful for the NPSOL, NLSSOL, DOT and CONMIN constrained optimizers.

**Defaults**

Defaults can vary depending on the method.

- DOT constrained optimizers: 0.003
- NPSOL: dependent upon the machine precision, typically on the order of $1 \times 10^{-8}$ for double precision computations

**speculative**

- **Keywords Area**
  - method
  - dot_mmfd
  - speculative

  Compute speculative gradients

**Topics**

This keyword is related to the topics:

- method-independent controls

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no speculation

**Description**

When performing gradient-based optimization in parallel, speculative gradients can be selected to address the load imbalance that can occur between gradient evaluation and line search phases. In a typical gradient-based optimization, the line search phase consists primarily of evaluating the objective function and any constraints at a trial point, and then testing the trial point for a sufficient decrease in the objective function value and/or constraint violation. If a sufficient decrease is not observed, then one or more additional trial points may be attempted sequentially. However, if the trial point is accepted then the line search phase is complete and the gradient evaluation phase begins. By speculating that the gradient information associated with a given line search trial point will be used later, additional coarse grained parallelism can be introduced by computing the gradient information (either by finite difference or analytically) in parallel, at the same time as the line search phase trial-point function values. This balances the total amount of computation to be performed at each design point and allows for efficient utilization of multiple processors. While the total amount of work performed will generally increase (since some speculative gradients will not be used when a trial point is rejected in the line search phase), the run time will usually decrease (since gradient evaluations needed at the start of each new optimization cycle were already performed in parallel during the line search phase). Refer to [14] for additional details. The speculative specification is implemented for the gradient-based optimizers in the DOT, CONMIN, and OPT++ libraries, and it can be used with dakota numerical or analytic gradient selections in the responses specification.
to responses gradient section for information on these specifications). It should not be selected with vendor numerical gradients since vendor internal finite difference algorithms have not been modified for this purpose. In full-Newton approaches, the Hessian is also computed speculatively. NPSOL and NLSSOL do not support speculative gradients, as their gradient-based line search in user-supplied gradient mode (dakota numerical or analytic gradients) is a superior approach for load-balanced parallel execution.

The speculative specification enables speculative computation of gradient and/or Hessian information, where applicable, for parallel optimization studies. By speculating that the derivative information at the current point will be used later, the complete data set (all available gradient/Hessian information) can be computed on every function evaluation. While some of these computations will be wasted, the positive effects are a consistent parallel load balance and usually shorter wall clock time. The speculative specification is applicable only when parallelism in the gradient calculations can be exploited by Dakota (it will be ignored for vendor numerical gradients).

max_function_evaluations

- Keywords Area
- method
- dot_mmfd
- max_function_evaluations

Number of function evaluations allowed for optimizers

Topics

This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none

Argument(s): INTEGER

Default: 1000

Description

The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed max_function_evaluations evaluations. See also max_iterations.

Default Behavior

Default value is 1000.

scaling

- Keywords Area
- method
- dot_mmfd
6.2. METHOD

• scaling

Turn on scaling for variables, responses, and constraints

Topics

This keyword is related to the topics:

• method_independent_controls

Specification

Alias: none

Argument(s): none

Default: no scaling

Description

Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by providing the scaling keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the method, variables, and responses blocks. When the scaling keyword is omitted, all .scale_types and *.scales specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.

• a *scales keyword, which gives characteristic values

• a *scale_type keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

Scale Types

There are four scale types:

1. none (default) - no scaling, value of *scales keyword is ignored

2. value - multiplicative scaling

3. auto - automatic scaling

First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:

• two-sided bounds scaled into the interval [0,1];

• one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
• no bounds or targets: no automatic scaling possible, therefore no scaling for this component

Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into [0,1].

4. log - logarithmic scaling

First, any characteristic values from the optional *scales specification are applied. Then logarithm base 10 scaling is applied.

Logarithmic scaling is not available for linear constraints.

When continuous design variables are log scaled, linear constraints are not allowed.

Scales

The *scales keywords are used to specify the characteristic values. These must be non-zero real numbers. The numbers are used according to the corresponding *scale_type, as described above.

Depending on the scale type, the characteristic values may be required or optional.

• none, auto, log - optional

• value - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than 1.0e10*DBL_MIN. User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.

Examples

The two examples below are equivalent:

responses
objective_functions 3
sense "maximize"
primary_scale_types = "value"
primary_scales = 1 1 100

responses
objective_functions 3
sense "maximize"
primary_scale_types = "value" "value" "value"
primary_scales = 1 1 100

model_pointer

• Keywords Area

• method

• dot_mmfd

• model_pointer

Identifier for model block to be used by a method
6.2. METHOD

Topics

This keyword is related to the topics:

- block_pointer

Specification

Alias: none

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)

Description

The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.

Usage Tips

When doing advanced analyses that involve using multiple methods and multiple models, defining a model_pointer for each method is imperative.

See block_pointer for details about pointers.

Examples

```
environment
tabular_graphics_data
method_pointer = 'UQ'

method
id_method = 'UQ'
model_pointer = 'Surr'
sampling,
samples = 10
seed = 98765 rng rnum2
response_levels = 0.1 0.2 0.6
sample_type lhs
distribution cumulative

model
id_model = 'Surr'
surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
id_method = 'DACE'
model_pointer = 'DACE_M'
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = 'DACE_M'
single
```
interface_pointer = 'I1'

variables
    uniform_uncertain = 2
    lower_bounds = 0. 0.
    upper_bounds = 1. 1.
    descriptors = 'x1' 'x2'

interface
    id_interface = 'I1'
    system asynch evaluation_concurrency = 5
    analysis_driver = 'text_book'

responses
    response_functions = 3
    no_gradients
    no_hessians

6.2.12 dot_bfgs

- Keywords Area
- method
- dot_bfgs

A conjugate gradient optimization method

Specification

Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>max_iterations</td>
<td></td>
<td>Number of iterations allowed for optimizers and adaptive UQ methods</td>
</tr>
<tr>
<td></td>
<td>convergence_-tolerance</td>
<td></td>
<td>Stopping criterion based on convergence of the objective function or statistics</td>
</tr>
</tbody>
</table>
### Optional

<table>
<thead>
<tr>
<th>Keyword</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>constraint_tolerance</code></td>
<td>The maximum allowable value of constraint violation still considered to be feasible. Compute speculative gradients.</td>
</tr>
<tr>
<td><code>speculative</code></td>
<td>Number of function evaluations allowed for optimizers.</td>
</tr>
<tr>
<td><code>max_function_evaluations</code></td>
<td>Number of function evaluations allowed for optimizers.</td>
</tr>
<tr>
<td><code>scaling</code></td>
<td>Turn on scaling for variables, responses, and constraints. Model block to be used by a method.</td>
</tr>
<tr>
<td><code>model_pointer</code></td>
<td>Model block to be used by a method.</td>
</tr>
</tbody>
</table>

### Description

This is a duplicated keyword. Please use `dot` instead.

### See Also

These keywords may also be of interest:

- `bfgs`

### max_iterations

- `Keywords Area`
- `method`
- `dot_bfgs`
- `max_iterations`

Number of iterations allowed for optimizers and adaptive UQ methods

### Topics

This keyword is related to the topics:

- `method.independent.controls`
CHAPTER 6. KEYWORDS AREA

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence} / efficient_global: 25+n)

**Description**

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed \texttt{max_iterations} iterations. See also \texttt{max_function_evaluations}.

**Default Behavior**

Default value is 100.

**convergence_tolerance**

- Keywords Area
- method
- dot_bfgs
- convergence_tolerance

Stopping criterion based on convergence of the objective function or statistics

**Topics**

This keyword is related to the topics:

- method_independent_controls

**Specification**

**Alias:** none

**Argument(s):** REAL

**Default:** 1.e-4

**Description**

The \texttt{convergence_tolerance} specification provides a real value for controlling the termination of iteration. For optimization, it is most commonly a relative convergence tolerance for the objective function: i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by \texttt{convergence_tolerance}, then this convergence criterion is satisfied on the current iteration.

Therefore, permissible values are between 0 and 1, non-inclusive.

**Behavior Varies by Package/Library**

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.
Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:
- DOT: must be satisfied for two consecutive iterations
- NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of convergence_tolerance approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., convergence_tolerance = 1.e-6 will result in approximately six digits of accuracy in the final objective function).
- NL2SOL: See nl2sol

### constraint_tolerance

- **Keywords Area**
- method
- dot_bfgs
- constraint_tolerance

The maximum allowable value of constraint violation still considered to be feasible

**Topics**

This keyword is related to the topics:
- method_independent_controls

**Specification**

**Alias:** none  
**Argument(s):** REAL  
**Default:** Library default

**Description**

The constraint_tolerance specification determines the maximum allowable value of infeasibility that any constraint in an optimization problem may possess and still be considered to be satisfied.

If a constraint function is greater than this value then it is considered to be violated by the optimization algorithm. This specification gives some control over how tightly the constraints will be satisfied at convergence of the algorithm. However, if the value is set too small the algorithm may terminate with one or more constraints being violated.

This specification is currently meaningful for the NPSOL, NLSSOL, DOT and CONMIN constrained optimizers.

**Defaults**

Defaults can vary depending on the method.
- DOT constrained optimizers: 0.003
- NPSOL: dependent upon the machine precision, typically on the order of 1.e-8 for double precision computations
speculative

- Keywords Area
- method
- dot_bfgs
- speculative

Compute speculative gradients

Topics

This keyword is related to the topics:

- method
- independent
- controls

Specification

Alias: none

Argument(s): none

Default: no speculation

Description

When performing gradient-based optimization in parallel, speculative gradients can be selected to address the load imbalance that can occur between gradient evaluation and line search phases. In a typical gradient-based optimization, the line search phase consists primarily of evaluating the objective function and any constraints at a trial point, and then testing the trial point for a sufficient decrease in the objective function value and/or constraint violation. If a sufficient decrease is not observed, then one or more additional trial points may be attempted sequentially. However, if the trial point is accepted then the line search phase is complete and the gradient evaluation phase begins. By speculating that the gradient information associated with a given line search trial point will be used later, additional coarse grained parallelism can be introduced by computing the gradient information (either by finite difference or analytically) in parallel, at the same time as the line search phase trial-point function values. This balances the total amount of computation to be performed at each design point and allows for efficient utilization of multiple processors. While the total amount of work performed will generally increase (since some speculative gradients will not be used when a trial point is rejected in the line search phase), the run time will usually decrease (since gradient evaluations needed at the start of each new optimization cycle were already performed in parallel during the line search phase). Refer to [14] for additional details. The speculative specification is implemented for the gradient-based optimizers in the DOT, CONMIN, and OPT++ libraries, and it can be used with dakota numerical or analytic gradient selections in the responses specification (refer to responses gradient section for information on these specifications). It should not be selected with vendor numerical gradients since vendor internal finite difference algorithms have not been modified for this purpose.

In full-Newton approaches, the Hessian is also computed speculatively. NPSOL and NLSSOL do not support speculative gradients, as their gradient-based line search in user-supplied gradient mode (dakota numerical or analytic gradients) is a superior approach for load-balanced parallel execution.

The speculative specification enables speculative computation of gradient and/or Hessian information, where applicable, for parallel optimization studies. By speculating that the derivative information at the current point will be used later, the complete data set (all available gradient/Hessian information) can be computed on every function evaluation. While some of these computations will be wasted, the positive effects are a consistent parallel load balance and usually shorter wall clock time. The speculative specification is applicable
only when parallelism in the gradient calculations can be exploited by Dakota (it will be ignored for vendor numerical gradients).

**max_function_evaluations**

- **Keywords Area**
- **method**
- **dot_bfgs**
- **max_function_evaluations**

Number of function evaluations allowed for optimizers

**Topics**

This keyword is related to the topics:

- **method_independent_controls**

**Specification**

**Alias:** none
**Argument(s):** INTEGER
**Default:** 1000

**Description**

The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed `max_function_evaluations` evaluations. See also `max_iterations`.

**Default Behavior**

Default value is 1000.

**scaling**

- **Keywords Area**
- **method**
- **dot_bfgs**
- **scaling**

Turn on scaling for variables, responses, and constraints

**Topics**

This keyword is related to the topics:

- **method_independent_controls**
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none
Argument(s): none
Default: no scaling

Description

Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by by providing the scaling keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the method, variables, and responses blocks. When the scaling keyword is omitted, all _scale_types and *scales specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.

- a *scales keyword, which gives characteristic values
- a *scale_type keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

Scale Types

There are four scale types:
1. none (default) - no scaling, value of *scales keyword is ignored
2. value - multiplicative scaling
3. auto - automatic scaling
   First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:
   - two-sided bounds scaled into the interval [0,1];
   - one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
   - no bounds or targets: no automatic scaling possible, therefore no scaling for this component
   Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into [0,1].
4. log - logarithmic scaling
   First, any characteristic values from the optional *scales specification are applied. Then logarithm base 10 scaling is applied.
   Logarithmic scaling is not available for linear constraints.
   When continuous design variables are log scaled, linear constraints are not allowed.
6.2. METHOD

Scales
The *scales keywords are used to specify the characteristic values. These must be non-zero real numbers. The numbers are used according to the corresponding *scale_type, as described above. Depending on the scale type, the characteristic values may be required or optional.

- none, auto, log - optional
- value - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than $1.0 \times 10^{-10}$ DBL_MIN. User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.

Examples
The two examples below are equivalent:

```
responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value"
  primary_scales = 1 1 100

responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value" "value" "value"
  primary_scales = 1 1 100
```

model_pointer

- Keywords Area
- method
- dot_bfgs
- model_pointer

Identifier for model block to be used by a method

Topics
This keyword is related to the topics:

- block_pointer

Specification
Alias: none
Argument(s): STRING
Default: method use of last model parsed (or use of default model if none parsed)
CHAPTER 6. KEYWORDS AREA

Description

The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.

Usage Tips

When doing advanced analyses that involve using multiple methods and multiple models, defining a model-pointer for each method is imperative.

See block_pointer for details about pointers.

Examples

environment
  tabular_graphics_data
  method_pointer = 'UQ'

method
  id_method = 'UQ'
  model_pointer = 'SURR'
  sampling,
    samples = 10
    seed = 98765 rng rnum2
    response_levels = 0.1 0.2 0.6
      0.1 0.2 0.6
      0.1 0.2 0.6
  sample_type lhs
  distribution cumulative

model
  id_model = 'SURR'
  surrogate global,
    dace_method_pointer = 'DACE'
    polynomial quadratic

method
  id_method = 'DACE'
  model_pointer = 'DACE_M'
  sampling sample_type lhs
    samples = 121 seed = 5034 rng rnum2

model
  id_model = 'DACE_M'
  single
  interface_pointer = 'I1'

variables
  uniform_uncertain = 2
    lower_bounds = 0. 0.
    upper_bounds = 1. 1.
    descriptors = 'x1' 'x2'

interface
  id_interface = 'I1'
  system asynch evaluation_concurrency = 5
    analysis_driver = 'text_book'

responses
6.2. **METHOD**

response_functions = 3
no_gradients
no_hessians

6.2.13 **dot_slp**

- Keywords Area
- method
- dot_slp

Sequential Linear Programming

**Specification**

**Alias:** none  
**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/- Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>max_iterations</td>
<td>max_iterations</td>
<td>Number of iterations allowed for optimizers and adaptive UQ methods</td>
</tr>
<tr>
<td>Optional</td>
<td>convergence_-tolerance</td>
<td>convergence_-tolerance</td>
<td>Stopping criterion based on convergence of the objective function or statistics</td>
</tr>
<tr>
<td>Optional</td>
<td>constraint_-tolerance</td>
<td>constraint_-tolerance</td>
<td>The maximum allowable value of constraint violation still considered to be feasible</td>
</tr>
<tr>
<td>Optional</td>
<td>speculative</td>
<td>speculative</td>
<td>Compute speculative gradients</td>
</tr>
<tr>
<td>Optional</td>
<td>max_function_-evaluations</td>
<td>max_function_-evaluations</td>
<td>Number of function evaluations allowed for optimizers</td>
</tr>
</tbody>
</table>
CHAPTER 6. KEYWORDS AREA

| Optional | scaling  | Turn on scaling for variables, responses, and constraints |
| Optional | model_pointer | Identifier for model block to be used by a method |

Description

This is a duplicated keyword. Please use dot instead.

See Also

These keywords may also be of interest:

- slp

max_iterations

- Keywords Area
- method
- dot_slp
- max_iterations

Number of iterations allowed for optimizers and adaptive UQ methods

Topics

This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none

Argument(s): INTEGER

Default: 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence} / efficient_global: 25*n)

Description

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed \texttt{max_iterations} iterations. See also \texttt{max_function_evaluations}.

Default Behavior

Default value is 100.
6.2. METHOD

**convergence_tolerance**

- **Keywords Area**
- **method**
- **dot_slp**
- **convergence_tolerance**

Stopping criterion based on convergence of the objective function or statistics

**Topics**

This keyword is related to the topics:

- **method_independent_controls**

**Specification**

**Alias:** none

**Argument(s):** REAL

**Default:** 1.e-4

**Description**

The `convergence_tolerance` specification provides a real value for controlling the termination of iteration. For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by convergence_tolerance, then this convergence criterion is satisfied on the current iteration.

Therefore, permissible values are between 0 and 1, non-inclusive.

**Behavior Varies by Package/Library**

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- **DOT:** must be satisfied for two consecutive iterations

- **NPSOL:** defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of `convergence_tolerance` approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., `convergence_tolerance = 1.e-6` will result in approximately six digits of accuracy in the final objective function).

- **NL2SOL:** See `nl2sol`
constraint_tolerance

- Keywords Area
- method
- dot_slp
- constraint_tolerance

The maximum allowable value of constraint violation still considered to be feasible

Topics

This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none

Argument(s): REAL

Default: Library default

Description

The `constraint_tolerance` specification determines the maximum allowable value of infeasibility that any constraint in an optimization problem may possess and still be considered to be satisfied. If a constraint function is greater than this value then it is considered to be violated by the optimization algorithm. This specification gives some control over how tightly the constraints will be satisfied at convergence of the algorithm. However, if the value is set too small the algorithm may terminate with one or more constraints being violated. This specification is currently meaningful for the NPSOL, NLSSOL, DOT and CONMIN constrained optimizers.

Defaults

Defaults can vary depending on the method.

- DOT constrained optimizers: 0.003
- NPSOL: dependent upon the machine precision, typically on the order of 1.e-8 for double precision computations

speculative

- Keywords Area
- method
- dot_slp
- speculative

Compute speculative gradients
6.2. METHOD

Topics
This keyword is related to the topics:

- method
- independent
- controls

Specification
Alias: none
Argument(s): none
Default: no speculation

Description
When performing gradient-based optimization in parallel, speculative gradients can be selected to address the load imbalance that can occur between gradient evaluation and line search phases. In a typical gradient-based optimization, the line search phase consists primarily of evaluating the objective function and any constraints at a trial point, and then testing the trial point for a sufficient decrease in the objective function value and/or constraint violation. If a sufficient decrease is not observed, then one or more additional trial points may be attempted sequentially. However, if the trial point is accepted then the line search phase is complete and the gradient evaluation phase begins. By speculating that the gradient information associated with a given line search trial point will be used later, additional coarse grained parallelism can be introduced by computing the gradient information (either by finite difference or analytically) in parallel, at the same time as the line search phase trial-point function values. This balances the total amount of computation to be performed at each design point and allows for efficient utilization of multiple processors. While the total amount of work performed will generally increase (since some speculative gradients will not be used when a trial point is rejected in the line search phase), the run time will usually decrease (since gradient evaluations needed at the start of each new optimization cycle were already performed in parallel during the line search phase). Refer to [14] for additional details. The speculative specification is implemented for the gradient-based optimizers in the DOT, CONMIN, and OPT++ libraries, and it can be used with dakota numerical or analytic gradient selections in the responses specification (refer to responses gradient section for information on these specifications). It should not be selected with vendor numerical gradients since vendor internal finite difference algorithms have not been modified for this purpose.

In full-Newton approaches, the Hessian is also computed speculatively. NPSOL and NLSSOL do not support speculative gradients, as their gradient-based line search in user-supplied gradient mode (dakota numerical or analytic gradients) is a superior approach for load-balanced parallel execution.

The speculative specification enables speculative computation of gradient and/or Hessian information, where applicable, for parallel optimization studies. By speculating that the derivative information at the current point will be used later, the complete data set (all available gradient/Hessian information) can be computed on every function evaluation. While some of these computations will be wasted, the positive effects are a consistent parallel load balance and usually shorter wall clock time. The speculative specification is applicable only when parallelism in the gradient calculations can be exploited by Dakota (it will be ignored for vendor numerical gradients).

max_function_evaluations

- Keywords Area
- method
- dot_slp
- max_function_evaluations
Number of function evaluations allowed for optimizers

**Topics**

This keyword is related to the topics:

- method_independent_controls

**Specification**

Alias: none

Argument(s): INTEGER

Default: 1000

**Description**

The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed \texttt{max.function_evaluations} evaluations. See also \texttt{max.iterations}.

**Default Behavior**

Default value is 1000.

**scaling**

- Keywords Area
- method
- dot_slp
- scaling

Turn on scaling for variables, responses, and constraints

**Topics**

This keyword is related to the topics:

- method_independent_controls

**Specification**

Alias: none

Argument(s): none

Default: no scaling
6.2. METHOD

Description
Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by providing the scaling keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the method, variables, and responses blocks. When the scaling keyword is omitted, all _scale_types and *_scales specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.

- a *scales keyword, which gives characteristic values
- a *scale_type keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

Scale Types
There are four scale types:

1. none (default) - no scaling, value of *scales keyword is ignored
2. value - multiplicative scaling
3. auto - automatic scaling
   First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:
   - two-sided bounds scaled into the interval [0,1];
   - one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
   - no bounds or targets: no automatic scaling possible, therefore no scaling for this component
   Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into [0,1].
4. log - logarithmic scaling
   First, any characteristic values from the optional _scales specification are applied. Then logarithm base 10 scaling is applied.
   Logarithmic scaling is not available for linear constraints.
   When continuous design variables are log scaled, linear constraints are not allowed.

Scales
The *scales keywords are used to specify the characteristic values. These must be non-zero real numbers. The numbers are used according to the corresponding *scale_type, as described above.
Depending on the scale type, the characteristic values may be required or optional.
CHAPTER 6. KEYWORDS AREA

- none, auto, log - optional
- value - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than $1.0e10 \times DBL_MIN$. User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.

Examples

The two examples below are equivalent:

```plaintext
responses
 objective_functions 3
  sense "maximize"
  primary_scale_types = "value"
  primary_scales = 1 1 100

responses
 objective_functions 3
  sense "maximize"
  primary_scale_types = "value" "value" "value"
  primary_scales = 1 1 100
```

**model_pointer**

- Keywords Area
- method
- dot_slp
- model_pointer

Identifier for model block to be used by a method

Topics

This keyword is related to the topics:

- block_pointer

Specification

Alias: none

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)

Description

The **model_pointer** is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.
6.2. METHOD

Usage Tips
When doing advanced analyses that involve using multiple methods and multiple models, defining a model-pointer for each method is imperative. See block_pointer for details about pointers.

Examples

```
environment
    tabular_graphics_data
    method_pointer = 'UQ'

method
    id_method = 'UQ'
    model_pointer = 'SURR'
    sampling,
        samples = 10
        seed = 98765 rng rnum2
        response_levels = 0.1 0.2 0.6
        0.1 0.2 0.6
        0.1 0.2 0.6
    sample_type lhs
    distribution cumulative

model
    id_model = 'SURR'
    surrogate global,
    dace_method_pointer = 'DACE'
    polynomial quadratic

method
    id_method = 'DACE'
    model_pointer = 'DACE_M'
    sampling sample_type lhs
    samples = 121 seed = 5034 rng rnum2

model
    id_model = 'DACE_M'
    single
    interface_pointer = 'I1'

variables
    uniform_uncertain = 2
    lower_bounds = 0. 0.
    upper_bounds = 1. 1.
    descriptors = 'x1' 'x2'

interface
    id_interface = 'I1'
    system async evaluation_concurrency = 5
    analysis_driver = 'text_book'

responses
    response_functions = 3
    no_gradients
    no_hessians

6.2.14 dot_sqp

- Keywords Area
- method
- dot_sqp

Sequential Quadratic Program

**Specification**

**Alias:** none

**Argument(s):** none

| Required/- | Description of | Dakota Keyword | Dakota Keyword Description |
| Thin | Group | | |
| Optional | | max_iterations | Number of iterations allowed for optimizers and adaptive UQ methods |
| Optional | convergence_-tolerance | | Stopping criterion based on convergence of the objective function or statistics |
| Optional | constraint_-tolerance | | The maximum allowable value of constraint violation still considered to be feasible |
| Optional | speculative | | Compute speculative gradients |
| Optional | max_function_-evaluations | | Number of function evaluations allowed for optimizers |
| Optional | scaling | | Turn on scaling for variables, responses, and constraints |
6.2. METHOD

Optional

| model_pointer | Identifier for model block to be used by a method |

**Description**

This is a duplicated keyword. Please use dot instead.

**See Also**

These keywords may also be of interest:

- sqp

**max_iterations**

- Keywords Area
- method
- dot_sqp
- max_iterations

Number of iterations allowed for optimizers and adaptive UQ methods

**Topics**

This keyword is related to the topics:

- method_independent_controls

**Specification**

**Alias:** none  
**Argument(s):** INTEGER  
**Default:** 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence} / efficient_global: 25*n)

**Description**

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed max_iterations iterations. See also max_function_evaluations.

**Default Behavior**

Default value is 100.
**convergence_tolerance**

- Keywords Area
- method
- dot_sqp
- convergence_tolerance

Stopping criterion based on convergence of the objective function or statistics

**Topics**

This keyword is related to the topics:

- method

**Specification**

**Alias:** none

**Argument(s):** REAL

**Default:** 1.e-4

**Description**

The `convergence_tolerance` specification provides a real value for controlling the termination of iteration. For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by `convergence_tolerance`, then this convergence criterion is satisfied on the current iteration.

Therefore, permissible values are between 0 and 1, non-inclusive.

**Behavior Varies by Package/Library**

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- DOT: must be satisfied for two consecutive iterations

- NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of `convergence_tolerance` approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., `convergence_tolerance = 1.e-6` will result in approximately six digits of accuracy in the final objective function).

- NL2SOL: See nl2sol
constraint tolerance

- Keywords Area
- method
- dot_sqp
- constraint_tolerance

The maximum allowable value of constraint violation still considered to be feasible

Topics

This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none
Argument(s): REAL
Default: Library default

Description

The constraint_tolerance specification determines the maximum allowable value of infeasibility that any constraint in an optimization problem may possess and still be considered to be satisfied.

If a constraint function is greater than this value then it is considered to be violated by the optimization algorithm. This specification gives some control over how tightly the constraints will be satisfied at convergence of the algorithm. However, if the value is set too small the algorithm may terminate with one or more constraints being violated.

This specification is currently meaningful for the NPSOL, NLSSOL, DOT and CONMIN constrained optimizers.

Defaults
Defaults can vary depending on the method.

- DOT constrained optimizers: 0.003
- NPSOL: dependent upon the machine precision, typically on the order of $1.e^{-8}$ for double precision computations

speculative

- Keywords Area
- method
- dot_sqp
- speculative

Compute speculative gradients
CHAPTER 6. KEYWORDS AREA

Topics
This keyword is related to the topics:

- method_independent_controls

Specification
Alias: none
Argument(s): none
Default: no speculation

Description
When performing gradient-based optimization in parallel, speculative gradients can be selected to address the load imbalance that can occur between gradient evaluation and line search phases. In a typical gradient-based optimization, the line search phase consists primarily of evaluating the objective function and any constraints at a trial point, and then testing the trial point for a sufficient decrease in the objective function value and/or constraint violation. If a sufficient decrease is not observed, then one or more additional trial points may be attempted sequentially. However, if the trial point is accepted then the line search phase is complete and the gradient evaluation phase begins. By speculating that the gradient information associated with a given line search trial point will be used later, additional coarse grained parallelism can be introduced by computing the gradient information (either by finite difference or analytically) in parallel, at the same time as the line search phase trial-point function values. This balances the total amount of computation to be performed at each design point and allows for efficient utilization of multiple processors. While the total amount of work performed will generally increase (since some speculative gradients will not be used when a trial point is rejected in the line search phase), the run time will usually decrease (since gradient evaluations needed at the start of each new optimization cycle were already performed in parallel during the line search phase). Refer to [14] for additional details. The speculative specification is implemented for the gradient-based optimizers in the DOT, CONMIN, and OPT++ libraries, and it can be used with dakota numerical or analytic gradient selections in the responses specification (refer to responses gradient section for information on these specifications). It should not be selected with vendor numerical gradients since vendor internal finite difference algorithms have not been modified for this purpose. In full-Newton approaches, the Hessian is also computed speculatively. NPSOL and NLSSOL do not support speculative gradients, as their gradient-based line search in user-supplied gradient mode (dakota numerical or analytic gradients) is a superior approach for load-balanced parallel execution.

The speculative specification enables speculative computation of gradient and/or Hessian information, where applicable, for parallel optimization studies. By speculating that the derivative information at the current point will be used later, the complete data set (all available gradient/Hessian information) can be computed on every function evaluation. While some of these computations will be wasted, the positive effects are a consistent parallel load balance and usually shorter wall clock time. The speculative specification is applicable only when parallelism in the gradient calculations can be exploited by Dakota (it will be ignored for vendor numerical gradients).

max_function_evaluations

- Keywords Area
- method
- dot_sqp
- max_function_evaluations
6.2. METHOD

Number of function evaluations allowed for optimizers

Topics
This keyword is related to the topics:

- method-independent-controls

Specification
Alias: none
  
  Argument(s): INTEGER
  Default: 1000

Description
The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed \( \text{max}\_\text{function}\_\text{evaluations} \) evaluations. See also \( \text{max}\_\text{iterations} \).

  Default Behavior
  Default value is 1000.

scaling

- Keywords Area
- method
- dot_sqp
- scaling

Turn on scaling for variables, responses, and constraints

Topics
This keyword is related to the topics:

- method-independent-controls

Specification
Alias: none
  
  Argument(s): none
  Default: no scaling
CHAPTER 6. KEYWORDS AREA

Description

Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by providing the `scaling` keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the method, variables, and responses blocks. When the `scaling` keyword is omitted, all `_scale_types` and `*scales` specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.

- A `*scales` keyword, which gives characteristic values
- A `*scale_type` keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

Scale Types

There are four scale types:

1. **none** (default) - no scaling, value of `*scales` keyword is ignored
2. **value** - multiplicative scaling
3. **auto** - automatic scaling
4. **log** - logarithmic scaling

First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:

- Two-sided bounds scaled into the interval [0,1];
- One-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
- No bounds or targets: no automatic scaling possible, therefore no scaling for this component

Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into [0,1].

4. **log** - logarithmic scaling

First, any characteristic values from the optional `*scales` specification are applied. Then logarithm base 10 scaling is applied.

Logarithmic scaling is not available for linear constraints.

When continuous design variables are log scaled, linear constraints are not allowed.

Scales

The `*scales` keywords are used to specify the characteristic values. These must be non-zero real numbers.

The numbers are used according to the corresponding `*scale_type`, as described above.

Depending on the scale type, the characteristic values may be required or optional.
6.2. METHOD

- none, auto, log - optional
- value - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than \(1.0\times10^\text{DBL,MN}\). User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.

**Examples**

The two examples below are equivalent:

```plaintext
responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value"
  primary_scales = 1 1 100

responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value" "value" "value"
  primary_scales = 1 1 100
```

**model_pointer**

- **Keywords Area**
- **method**
- **dot_sqp**
- **model_pointer**

Identifier for model block to be used by a method

**Topics**

This keyword is related to the topics:

- **block_pointer**

**Specification**

**Alias:** none

**Argument(s):** STRING

**Default:** method use of last model parsed (or use of default model if none parsed)

**Description**

The **model_pointer** is used to specify which **model** block will be used to perform the function evaluations needed by the Dakota method.

**Default Behavior**

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a **model** block in the Dakota input file that has a corresponding **id_model** with the same name.
CHAPTER 6. KEYWORDS AREA

Usage Tips
When doing advanced analyses that involve using multiple methods and multiple models, defining a model-pointer for each method is imperative.

See block_pointer for details about pointers.

Examples

environment
  tabular_graphics_data
  method_pointer = 'UQ'

method
  id_method = 'UQ'
  model_pointer = 'SURR'
  sampling,
    samples = 10
    seed = 98765 rng rnum2
    response_levels = 0.1 0.2 0.6
    0.1 0.2 0.6
    0.1 0.2 0.6
  sample_type lhs
distribution cumulative

model
  id_model = 'SURR'
surrogate global,
  dace_method_pointer = 'DACE'
  polynomial quadratic

method
  id_method = 'DACE'
  model_pointer = 'DACE_M'
sampling sample_type lhs
  samples = 121 seed = 5034 rng rnum2

model
  id_model = 'DACE_M'
single
  interface_pointer = 'I1'

variables
  uniform_uncertain = 2
  lower_bounds = 0. 0.
  upper_bounds = 1. 1.
  descriptors = 'x1' 'x2'

interface
  id_interface = 'I1'
system asynch evaluation_concurrency = 5
  analysis_driver = 'text_book'

responses
  response_functions = 3
  no_gradients
  no_hessians

6.2.15 dot

- Keywords Area
6.2. METHOD

- method
- dot

Access to methods in the DOT package

Topics

This keyword is related to the topics:

- package.dot

Specification

Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required (Choose One)</td>
<td>Group 1</td>
<td>frcg</td>
<td>A conjugate gradient optimization method</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>mmlfd</td>
<td>Method of feasible directions</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>bfgs</td>
<td>A conjugate gradient optimization method</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>slp</td>
<td>Sequential Linear Programming</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>sqp</td>
<td>Sequential Quadratic Program</td>
</tr>
</tbody>
</table>

Optional

- max_iterations
- convergence_tolerance

Number of iterations allowed for optimizers and adaptive UQ methods

Stopping criterion based on convergence of the objective function or statistics
Optional constraint_tolerance The maximum allowable value of constraint violation still considered to be feasible

Optional speculative Compute speculative gradients

Optional max_function_evaluations Number of function evaluations allowed for optimizers

Optional scaling Turn on scaling for variables, responses, and constraints

Optional model_pointer Identifier for model block to be used by a method

Description

The DOT library [85] contains nonlinear programming optimizers, specifically the Broyden-Fletcher-Goldfarb-Shanno (Dakota’s dot_bfgs method) and Fletcher-Reeves conjugate gradient (Dakota’s dot_frcg method) methods for unconstrained optimization, and the modified method of feasible directions (Dakota’s dot_mmfd method), sequential linear programming (Dakota’s dot_slp method), and sequential quadratic programming (Dakota’s dot_sqp method) methods for constrained optimization.

Specialized handling of linear constraints is supported with DOT; linear constraint coefficients, bounds, and targets can be provided to DOT at start-up and tracked internally.

One of the five available methods in Group 1 must be specified.

All these methods take the same Optional Keywords, dealing with linear equality and inequality constraints.

Method Independent Controls - Stopping Criteria

Stopping criteria are set by:

- max_iterations
- max_function_evaluations
- convergence_tolerance
- constraint_tolerance

Note: The convergence_tolerance criterion must be satisfied for two consecutive iterations before DOT will terminate.

Method Independent Controls - Output

The output verbosity specification controls the amount of information generated by DOT: the silent and quiet settings result in header information, final results, and objective function, constraint, and parameter information on each iteration; whereas the verbose and debug settings add additional information on gradients, search direction, one-dimensional search results, and parameter scaling factors.
6.2. METHOD

Concurrency
DOT contains no parallel algorithms which can directly take advantage of concurrent evaluations. However, if numerical_gradients with method_source dakota is specified, then the finite difference function evaluations can be performed concurrently (using any of the parallel modes described in the Users Manual[4]). In addition, if speculative is specified, then gradients (dakota numerical or analytic gradients) will be computed on each line search evaluation in order to balance the load and lower the total run time in parallel optimization studies.

frcg

- Keywords Area
- method
- dot
- frcg

A conjugate gradient optimization method

Topics
This keyword is related to the topics:
- package_dot

Specification
Alias: none
Argument(s): none

Description
We here provide a caution regarding dot_frcg. In DOT Version 4.20, we have noticed inconsistent behavior of this algorithm across different versions of Linux. Our best assessment is that it is due to different treatments of uninitialized variables. As we do not know the intention of the code authors and maintaining DOT source code is outside of the Dakota project scope, we have not made nor are we recommending any code changes to address this. However, all users who use dot_frcg in DOT Version 4.20 should be aware that results may not be reliable.

See package_dot for information related to all DOT methods.

See Also
These keywords may also be of interest:
- bfgs
- mmfd
- slp
- sqp
mmfd

- Keywords Area
- method
- dot
- mmfd

Method of feasible directions

Topics

This keyword is related to the topics:

- package_dot

Specification

Alias: none
Argument(s): none

Description

See package_dot for information related to all DOT methods.

See Also

These keywords may also be of interest:

- bfgs
- frcg
- slp
- sqp

bfgs

- Keywords Area
- method
- dot
- bfgs

A conjugate gradient optimization method

Topics

This keyword is related to the topics:

- package_dot
Specification

Alias: none
  Argument(s): none

Description

See package dot for information related to all DOT methods.

See Also

These keywords may also be of interest:

- freg
- mmfd
- slp
- sqp

slp

- Keywords Area
- method
- dot
- slp

Sequential Linear Programming

Topics

This keyword is related to the topics:

- package dot

Specification

Alias: none
  Argument(s): none

Description

See package dot for information related to all DOT methods.
See Also

These keywords may also be of interest:

- bfgs
- frcg
- mmfd
- sqp

sqp

- Keywords Area
- method
- dot
- sqp

Sequential Quadratic Program

Topics

This keyword is related to the topics:

- package_dot

Specification

Alias: none

Argument(s): none

Description

See package_dot for information related to all DOT methods.

See Also

These keywords may also be of interest:

- bfgs
- frcg
- mmfd
- slp
max_iterations

- Keywords Area
- method
- dot
- max_iterations

Number of iterations allowed for optimizers and adaptive UQ methods

Topics

This keyword is related to the topics:
- method_independent_controls

Specification

Alias: none
Argument(s): INTEGER
Default: 100 (exceptions: fsu_cvt, local_reliability: 25; global.{reliability, interval_est, evidence} / efficient-global: 25*n)

Description

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed max_iterations iterations. See also max_function_evaluations.

Default Behavior
Default value is 100.

convergence_tolerance

- Keywords Area
- method
- dot
- convergence_tolerance

Stopping criterion based on convergence of the objective function or statistics

Topics

This keyword is related to the topics:
- method_independent_controls
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): REAL

Default: 1.e-4

Description

The convergence_tolerance specification provides a real value for controlling the termination of iteration.

For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by convergence_tolerance, then this convergence criterion is satisfied on the current iteration.

Therefore, permissible values are between 0 and 1, non-inclusive.

Behavior Varies by Package/Library

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- DOT: must be satisfied for two consecutive iterations
- NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of convergence_tolerance approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., convergence_tolerance = 1.e-6 will result in approximately six digits of accuracy in the final objective function).
- NL2SOL: See nl2sol

constraint_tolerance

- Keywords Area
- method
- dot

The maximum allowable value of constraint violation still considered to be feasible

Topics

This keyword is related to the topics:

- method_independent_controls
6.2. **METHOD**

**Specification**

Alias: none  
Argument(s): REAL  
Default: Library default

**Description**

The `constraint_tolerance` specification determines the maximum allowable value of infeasibility that any constraint in an optimization problem may possess and still be considered to be satisfied.

If a constraint function is greater than this value then it is considered to be violated by the optimization algorithm. This specification gives some control over how tightly the constraints will be satisfied at convergence of the algorithm. However, if the value is set too small the algorithm may terminate with one or more constraints being violated.

This specification is currently meaningful for the NPSOL, NLSSOL, DOT and CONMIN constrained optimizers.

**Defaults**

Defaults can vary depending on the method.

- DOT constrained optimizers: 0.003
- NPSOL: dependent upon the machine precision, typically on the order of $1 \times 10^{-8}$ for double precision computations

**speculative**

- Keywords Area
- method
- dot
- speculative

Compute speculative gradients

**Topics**

This keyword is related to the topics:

- method_independent_controls

**Specification**

Alias: none  
Argument(s): none  
Default: no speculation
Description

When performing gradient-based optimization in parallel, speculative gradients can be selected to address the load imbalance that can occur between gradient evaluation and line search phases. In a typical gradient-based optimization, the line search phase consists primarily of evaluating the objective function and any constraints at a trial point, and then testing the trial point for a sufficient decrease in the objective function value and/or constraint violation. If a sufficient decrease is not observed, then one or more additional trial points may be attempted sequentially. However, if the trial point is accepted then the line search phase is complete and the gradient evaluation phase begins. By speculating that the gradient information associated with a given line search trial point will be used later, additional coarse grained parallelism can be introduced by computing the gradient information (either by finite difference or analytically) in parallel, at the same time as the line search phase trial-point function values. This balances the total amount of computation to be performed at each design point and allows for efficient utilization of multiple processors. While the total amount of work performed will generally increase (since some speculative gradients will not be used when a trial point is rejected in the line search phase), the runtime will usually decrease (since gradient evaluations needed at the start of each new optimization cycle were already performed in parallel during the line search phase). Refer to [14] for additional details. The speculative specification is implemented for the gradient-based optimizers in the DOT, CONMIN, and OPT++ libraries, and it can be used with dakota numerical or analytic gradient selections in the responses specification (refer to responses gradient section for information on these specifications). It should not be selected with vendor numerical gradients since vendor internal finite difference algorithms have not been modified for this purpose.

In full-Newton approaches, the Hessian is also computed speculatively. NPSOL and NLSSOL do not support speculative gradients, as their gradient-based line search in user-supplied gradient mode (dakota numerical or analytic gradients) is a superior approach for load-balanced parallel execution.

The speculative specification enables speculative computation of gradient and/or Hessian information, where applicable, for parallel optimization studies. By speculating that the derivative information at the current point will be used later, the complete data set (all available gradient/Hessian information) can be computed on every function evaluation. While some of these computations will be wasted, the positive effects are a consistent parallel load balance and usually shorter wall clock time. The speculative specification is applicable only when parallelism in the gradient calculations can be exploited by Dakota (it will be ignored for vendor numerical gradients).

max_function_evaluations

- Keywords Area
- method
- dot
- max_function_evaluations

Number of function evaluations allowed for optimizers

Topics

This keyword is related to the topics:

- method_independent_controls
6.2. **METHOD**

**Specification**

**Alias:** none  
**Argument(s):** INTEGER  
**Default:** 1000

**Description**

The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed \texttt{max\_function\_evaluations} evaluations. See also \texttt{max\_iterations}.

**Default Behavior**  
Default value is 1000.

**scaling**

- **Keywords Area**
- **method**
- **dot**
- **scaling**

Turn on scaling for variables, responses, and constraints

**Topics**

This keyword is related to the topics:

- **method\_independent\_controls**

**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** no scaling

**Description**

Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by by providing the \texttt{scaling} keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the \texttt{method}, \texttt{variables}, and \texttt{responses} blocks. When the \texttt{scaling} keyword is omitted, all \_scale\_types and \_scales specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.
CHAPTER 6. KEYWORDS AREA

- a *scales keyword, which gives characteristic values
- a *scale_type keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

**Scale Types**
There are four scale types:

1. **none** (default) - no scaling, value of *scales keyword is ignored
2. **value** - multiplicative scaling
3. **auto** - automatic scaling
   First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:
   - two-sided bounds scaled into the interval [0,1];
   - one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
   - no bounds or targets: no automatic scaling possible, therefore no scaling for this component

Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into [0,1].

4. **log** - logarithmic scaling
   First, any characteristic values from the optional *scales specification are applied. Then logarithm base 10 scaling is applied.
   Logarithmic scaling is not available for linear constraints.
   When continuous design variables are log scaled, linear constraints are not allowed.

**Scales**
The *scales keywords are used to specify the characteristic values. These must be non-zero real numbers. The numbers are used according to the corresponding *scale_type, as described above.
Depending on the scale type, the characteristic values may be required or optional.

- none, auto, log - optional
- value - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than 1.0e10*DBL_MIN. User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.
Examples
The two examples below are equivalent:

```
responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value"
  primary_scales = 1 1 100

responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value" "value" "value"
  primary_scales = 1 1 100
```

model_pointer

- Keywords Area
- method
- dot
- model_pointer

Identifier for model block to be used by a method

Topics
This keyword is related to the topics:

- block_pointer

Specification

Alias: none

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)

Description
The `model_pointer` is used to specify which `model` block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior
If not specified, a Dakota method will use the last model block parsed. If specified, there must be a `model` block in the Dakota input file that has a corresponding `id_model` with the same name.

Usage Tips
When doing advanced analyses that involve using multiple methods and multiple models, defining a `model_pointer` for each method is imperative.

See `block_pointer` for details about pointers.
Examples

environment
tabular_graphics_data
method_pointer = 'UQ'

method
id_method = 'UQ'
model_pointer = 'SURR'
sampling,
samples = 10
seed = 98765 rng rnum2
response_levels = 0.1 0.2 0.6
0.1 0.2 0.6
0.1 0.2 0.6
sample_type lhs
distribution cumulative

model
id_model = 'SURR'
surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
id_method = 'DACE'
model_pointer = 'DACE_M'
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = 'DACE_M'
single
interface_pointer = 'I1'

variables
uniform_uncertain = 2
lower_bounds = 0. 0.
upper_bounds = 1. 1.
descriptors = 'x1' 'x2'

interface
id_interface = 'I1'
system asynch evaluation_concurrency = 5
analysis_driver = 'text_book'

responses
response_functions = 3
no_gradients
no_hessians

6.2.16 conmin_frcg

- Keywords Area
- method
- conmin_frcg

A conjugate gradient optimization method
### Specification

**Alias:** none  
**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>max_iterations</td>
<td>Number of iterations allowed for optimizers and adaptive UQ methods</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>convergence_-tolerance</td>
<td>Stopping criterion based on convergence of the objective function or statistics</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>constraint_-tolerance</td>
<td>The maximum allowable value of constraint violation still considered to be feasible</td>
</tr>
<tr>
<td>Optional</td>
<td>speculative</td>
<td>max_function_-evaluations</td>
<td>Compute speculative gradients</td>
</tr>
<tr>
<td>Optional</td>
<td>scaling</td>
<td>model_pointer</td>
<td>Number of function evaluations allowed for optimizers</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td></td>
<td>Turn on scaling for variables, responses, and constraints</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Identifier for model block to be used by a method</td>
</tr>
</tbody>
</table>

### Description

This is a duplicated keyword. Please use `conmin` instead.

### See Also

These keywords may also be of interest:

- `freg`
max_iterations

- Keywords Area
- method
- conmin_frcg
- max_iterations

Number of iterations allowed for optimizers and adaptive UQ methods

**Topics**

This keyword is related to the topics:

- method_independent_controls

**Specification**

*Alias: none*

*Argument(s):* INTEGER

*Default: 100 (exceptions: fsu_cvpt, local_reliability: 25; global_reliability, interval_est, evidence / efficient Whilst global: 25*n)*

**Description**

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed max_iterations iterations. See also max_function_evaluations.

**Default Behavior**

Default value is 100.

convergence_tolerance

- Keywords Area
- method
- conmin_frcg
- convergence_tolerance

Stopping criterion based on convergence of the objective function or statistics

**Topics**

This keyword is related to the topics:

- method_independent_controls
6.2. METHOD

Specification

Alias: none

Argument(s): REAL
Default: 1.e-4

Description

The convergence_tolerance specification provides a real value for controlling the termination of iteration. For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by convergence_tolerance, then this convergence criterion is satisfied on the current iteration.

Therefore, permissible values are between 0 and 1, non-inclusive.

Behavior Varies by Package/Library

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- DOT: must be satisfied for two consecutive iterations
- NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of convergence_tolerance approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., convergence_tolerance = 1.e-6 will result in approximately six digits of accuracy in the final objective function).
- NL2SOL: See nl2sol

constraint_tolerance

- Keywords Area
- method
- conmin_frcg
- constraint_tolerance

The maximum allowable value of constraint violation still considered to be feasible

Topics

This keyword is related to the topics:

- method_independent_controls
### Specification

**Alias:** none  
**Argument(s):** REAL  
**Default:** Library default

### Description

The `constraint_tolerance` specification determines the maximum allowable value of infeasibility that any constraint in an optimization problem may possess and still be considered to be satisfied.

If a constraint function is greater than this value then it is considered to be violated by the optimization algorithm. This specification gives some control over how tightly the constraints will be satisfied at convergence of the algorithm. However, if the value is set too small the algorithm may terminate with one or more constraints being violated.

This specification is currently meaningful for the NPSOL, NLSSOL, DOT and CONMIN constrained optimizers.

**Defaults**

Defaults can vary depending on the method.

- DOT constrained optimizers: 0.003
- NPSOL: dependent upon the machine precision, typically on the order of $1.e-8$ for double precision computations

### Topics

This keyword is related to the topics:

- `method_independent_controls`
Description

When performing gradient-based optimization in parallel, speculative gradients can be selected to address the load imbalance that can occur between gradient evaluation and line search phases. In a typical gradient-based optimization, the line search phase consists primarily of evaluating the objective function and any constraints at a trial point, and then testing the trial point for a sufficient decrease in the objective function value and/or constraint violation. If a sufficient decrease is not observed, then one or more additional trial points may be attempted sequentially. However, if the trial point is accepted then the line search phase is complete and the gradient evaluation phase begins. By speculating that the gradient information associated with a given line search trial point will be used later, additional coarse grained parallelism can be introduced by computing the gradient information (either by finite difference or analytically) in parallel, at the same time as the line search phase trial-point function values. This balances the total amount of computation to be performed at each design point and allows for efficient utilization of multiple processors. While the total amount of work performed will generally increase (since some speculative gradients will not be used when a trial point is rejected in the line search phase), the run time will usually decrease (since gradient evaluations needed at the start of each new optimization cycle were already performed in parallel during the line search phase). Refer to [14] for additional details. The speculative specification is implemented for the gradient-based optimizers in the DOT, CONMIN, and OPT++ libraries, and it can be used with dakota numerical or analytic gradient selections in the responses specification (refer to responses gradient section for information on these specifications). It should not be selected with vendor numerical gradients since vendor internal finite difference algorithms have not been modified for this purpose. In full-Newton approaches, the Hessian is also computed speculatively. NPSOL and NLSSOL do not support speculative gradients, as their gradient-based line search in user-supplied gradient mode (dakota numerical or analytic gradients) is a superior approach for load-balanced parallel execution.

The speculative specification enables speculative computation of gradient and/or Hessian information, where applicable, for parallel optimization studies. By speculating that the derivative information at the current point will be used later, the complete data set (all available gradient/Hessian information) can be computed on every function evaluation. While some of these computations will be wasted, the positive effects are a consistent parallel load balance and usually shorter wall clock time. The speculative specification is applicable only when parallelism in the gradient calculations can be exploited by Dakota (it will be ignored for vendor numerical gradients).

max_function_evaluations

- Keywords Area
- method
- conmin_frcg
- max_function_evaluations

Number of function evaluations allowed for optimizers

Topics

This keyword is related to the topics:

- method_independent_controls
CHAPTER 6. KEYWORDS AREA

CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): INTEGER

Default: 1000

Description

The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criterion first, the optimizer will stop after it has performed \textit{max\_function\_evaluations} evaluations. See also \textit{max\_iterations}.

Default Behavior

Default value is 1000.

scaling

- Keywords Area
- method
- conmin\_frcg
- scaling

Turn on scaling for variables, responses, and constraints

Topics

This keyword is related to the topics:

- \textit{method\_independent\_controls}

Specification

Alias: none

Argument(s): none

Default: no scaling

Description

Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by by providing the \textit{scaling} keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the \textit{method}, \textit{variables}, and \textit{responses} blocks. When the \textit{scaling} keyword is omitted, all \textit{\_scale\_types} and \textit{\_*scales} specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.
6.2. METHOD

- a *scales* keyword, which gives characteristic values
- a *scale_type* keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

**Scale Types**
There are four scale types:

1. none (default) - no scaling, value of *scales* keyword is ignored
2. value - multiplicative scaling
3. auto - automatic scaling
   First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:
   - two-sided bounds scaled into the interval [0,1];
   - one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
   - no bounds or targets: no automatic scaling possible, therefore no scaling for this component

   Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Futher, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into [0,1].
4. log - logarithmic scaling
   First, any characteristic values from the optional *scales* specification are applied. Then logarithm base 10 scaling is applied.
   Logarithmic scaling is not available for linear constraints.
   When continuous design variables are log scaled, linear constraints are not allowed.

**Scales**
The *scales* keywords are used to specify the characteristic values. These must be non-zero real numbers.
The numbers are used according to the corresponding *scale_type*, as described above.
Depending on the scale type, the characteristic values may be required or optional.

- none, auto, log - optional
- value - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than 1.0e10*DBL_MIN*. User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.
Examples
The two examples below are equivalent:

```plaintext
responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value"
  primary_scales = 1 1 100

responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value" "value" "value"
  primary_scales = 1 1 100
```

model_pointer

- Keywords Area
- method
- conmin_frcg
- model_pointer

Identifier for model block to be used by a method

Topics
This keyword is related to the topics:

- block_pointer

Specification
Alias: none
Argument(s): STRING
Default: method use of last model parsed (or use of default model if none parsed)

Description
The `model_pointer` is used to specify which `model` block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior
If not specified, a Dakota method will use the last model block parsed. If specified, there must be a `model` block in the Dakota input file that has a corresponding `id_model` with the same name.

Usage Tips
When doing advanced analyses that involve using multiple methods and multiple models, defining a `model-pointer` for each method is imperative.
See `block_pointer` for details about pointers.
6.2. METHOD

Examples

environment
tabular_graphics_data
method_pointer = 'UQ'

method
id_method = 'UQ'
model_pointer = 'SRR'
sampling,
samples = 10
seed = 98765 rng rnum2
response_levels = 0.1 0.2 0.6
0.1 0.2 0.6
sample_type lhs
distribution cumulative

model
id_model = 'SRR'
surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
id_method = 'DACE'
model_pointer = 'DACE_M'
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = 'DACE_M'
single
interface_pointer = 'I1'

variables
uniform_uncertain = 2
lower_bounds = 0. 0.
upper_bounds = 1. 1.
descriptors = 'x1' 'x2'

interface
id_interface = 'I1'
system asynch evaluation_concurrency = 5
analysis_driver = 'text_book'

responses
response_functions = 3
no_gradients
no_hessians

6.2.17 conmin_mfd

- Keywords Area
- method
- conmin_mfd

Method of feasible directions
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): none

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>max_iterations</td>
<td>Number of iterations allowed for optimizers and adaptive UQ methods</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>convergence_-tolerance</td>
<td>Stopping criterion based on convergence of the objective function or statistics</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>constraint_-tolerance</td>
<td>The maximum allowable value of constraint violation still considered to be feasible</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>speculative</td>
<td>Compute speculative gradients</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>max_function_-evaluations</td>
<td>Number of function evaluations allowed for optimizers</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>scaling</td>
<td>Turn on scaling for variables, responses, and constraints</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>model_pointer</td>
<td>Identifier for model block to be used by a method</td>
</tr>
</tbody>
</table>

Description

This is a duplicated keyword. Please use conmin instead.

See Also

These keywords may also be of interest:

- mfd
6.2. METHOD

max_iterations

- Keywords Area
- method
- conmin_mfd
- max_iterations

Number of iterations allowed for optimizers and adaptive UQ methods

Topics

This keyword is related to the topics:
- method_independent_controls

Specification

Alias: none
Argument(s): INTEGER
Default: 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence} / efficient_global: 25*n)

Description

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed \textit{max.iterations} iterations. See also \textit{max.function.evaluations}.

Default Behavior

Default value is 100.

convergence.tolerance

- Keywords Area
- method
- conmin_mfd
- convergence.tolerance

Stopping criterion based on convergence of the objective function or statistics

Topics

This keyword is related to the topics:
- method_independent_controls
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none
Argument(s): REAL
Default: 1.e-4

Description

The convergence_tolerance specification provides a real value for controlling the termination of iteration.

For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by convergence_tolerance, then this convergence criterion is satisfied on the current iteration.

Therefore, permissible values are between 0 and 1, non-inclusive.

Behavior Varies by Package/Library

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- DOT: must be satisfied for two consecutive iterations
- NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of convergence_tolerance approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., convergence_tolerance = 1.e-6 will result in approximately six digits of accuracy in the final objective function).
- NL2SOL: See nl2sol

constraint_tolerance

- Keywords Area
- method
- conmin_mfd
- constraint_tolerance

The maximum allowable value of constraint violation still considered to be feasible

Topics

This keyword is related to the topics:

- method_independent_controls
6.2. METHOD

**Specification**

Alias: none

Argument(s): REAL

Default: Library default

**Description**

The `constraint_tolerance` specification determines the maximum allowable value of infeasibility that any constraint in an optimization problem may possess and still be considered to be satisfied.

If a constraint function is greater than this value then it is considered to be violated by the optimization algorithm. This specification gives some control over how tightly the constraints will be satisfied at convergence of the algorithm. However, if the value is set too small the algorithm may terminate with one or more constraints being violated.

This specification is currently meaningful for the NPSOL, NLSSOL, DOT and CONMIN constrained optimizers.

**Defaults**

Defaults can vary depending on the method.

- DOT constrained optimizers: 0.003
- NPSOL: dependent upon the machine precision, typically on the order of $1 \cdot 10^{-8}$ for double precision computations

**speculative**

- Keywords Area
- method
- conmin_mfd
- speculative

Compute speculative gradients

**Topics**

This keyword is related to the topics:

- `method_independent_controls`

**Specification**

Alias: none

Argument(s): none

Default: no speculation
Description

When performing gradient-based optimization in parallel, speculative gradients can be selected to address the load imbalance that can occur between gradient evaluation and line search phases. In a typical gradient-based optimization, the line search phase consists primarily of evaluating the objective function and any constraints at a trial point, and then testing the trial point for a sufficient decrease in the objective function value and/or constraint violation. If a sufficient decrease is not observed, then one or more additional trial points may be attempted sequentially. However, if the trial point is accepted then the line search phase is complete and the gradient evaluation phase begins. By speculating that the gradient information associated with a given line search trial point will be used later, additional coarse grained parallelism can be introduced by computing the gradient information (either by finite difference or analytically) in parallel, at the same time as the line search phase trial-point function values. This balances the total amount of computation to be performed at each design point and allows for efficient utilization of multiple processors. While the total amount of work performed will generally increase (since some speculative gradients will not be used when a trial point is rejected in the line search phase), the run time will usually decrease (since gradient evaluations needed at the start of each new optimization cycle were already performed in parallel during the line search phase). Refer to [14] for additional details. The speculative specification is implemented for the gradient-based optimizers in the DOT, CONMIN, and OPT++ libraries, and it can be used with dakota numerical or analytic gradient selections in the responses specification (refer to responses gradient section for information on these specifications). It should not be selected with vendor numerical gradients since vendor internal finite difference algorithms have not been modified for this purpose.

In full-Newton approaches, the Hessian is also computed speculatively. NPSOL and NLSSOL do not support speculative gradients, as their gradient-based line search in user-supplied gradient mode (dakota numerical or analytic gradients) is a superior approach for load-balanced parallel execution.

The speculative specification enables speculative computation of gradient and/or Hessian information, where applicable, for parallel optimization studies. By speculating that the derivative information at the current point will be used later, the complete data set (all available gradient/Hessian information) can be computed on every function evaluation. While some of these computations will be wasted, the positive effects are a consistent parallel load balance and usually shorter wall clock time. The speculative specification is applicable only when parallelism in the gradient calculations can be exploited by Dakota (it will be ignored for vendor numerical gradients).

max_function_evaluations

- Keywords Area
- method
- conmin_mfd
- max_function_evaluations

Number of function evaluations allowed for optimizers

Topics

This keyword is related to the topics:

- method_independent_controls
6.2. **METHOD**

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** 1000

**Description**

The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed `max_function_evaluations` evaluations. See also `max_iterations`.

**Default Behavior**

Default value is 1000.

**scaling**

- Keywords Area
- method
- `conmin_mfd`
- scaling

Turn on scaling for variables, responses, and constraints

**Topics**

This keyword is related to the topics:

- `method_independent_controls`

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no scaling

**Description**

Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by by providing the `scaling` keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the `method`, `variables`, and `responses` blocks. When the `scaling` keyword is omitted, all `_scale_types` and `*_scales` specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.
• a *scales keyword, which gives characteristic values

• a *scale_type keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

Scale Types
There are four scale types:

1. none (default) - no scaling, value of *scales keyword is ignored

2. value - multiplicative scaling

3. auto - automatic scaling
   First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:
   - two-sided bounds scaled into the interval [0,1];
   - one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
   - no bounds or targets: no automatic scaling possible, therefore no scaling for this component

Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into [0,1].

4. log - logarithmic scaling
   First, any characteristic values from the optional *scales specification are applied. Then logarithm base 10 scaling is applied.
   Logarithmic scaling is not available for linear constraints.
   When continuous design variables are log scaled, linear constraints are not allowed.

Scales
The *scales keywords are used to specify the characteristic values. These must be non-zero real numbers. The numbers are used according to the corresponding *scale_type, as described above.
Depending on the scale type, the characteristic values may be required or optional.

• none, auto, log - optional

• value - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than 1.0e10*DBL_MIN. User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.
6.2. METHOD

Examples
The two examples below are equivalent:

```plaintext
responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value"
  primary_scales = 1 1 100

responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value" "value" "value"
  primary_scales = 1 1 100
```

model_pointer

- Keywords Area
- method
- conmin_mfd
- model_pointer

Identifier for model block to be used by a method

Topics
This keyword is related to the topics:

- block_pointer

Specification
Alias: none

Argument(s): STRING
Default: method use of last model parsed (or use of default model if none parsed)

Description
The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior
If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.

Usage Tips
When doing advanced analyses that involve using multiple methods and multiple models, defining a model_pointer for each method is imperative.

See block_pointer for details about pointers.
Examples

environment
  tabular_graphics_data
  method_pointer = 'UQ'

method
  id_method = 'UQ'
  model_pointer = 'SURR'
  sampling,
    samples = 10
    seed = 98765 rng rnum2
    response_levels = 0.1 0.2 0.6
      0.1 0.2 0.6
      0.1 0.2 0.6
    sample_type lhs
  distribution cumulative

model
  id_model = 'SURR'
    surrogate global,
    dace_method_pointer = 'DACE'
    polynomial quadratic

method
  id_method = 'DACE'
  model_pointer = 'DACE_M'
  sampling sample_type lhs
    samples = 121 seed = 5034 rng rnum2

model
  id_model = 'DACE_M'
    single
    interface_pointer = 'I1'

variables
  uniform_uncertain = 2
    lower_bounds = 0. 0.
    upper_bounds = 1. 1.
    descriptors = 'x1' 'x2'

interface
  id_interface = 'I1'
  system asynch evaluation_concurrency = 5
    analysis_driver = 'text_book'

responses
  response_functions = 3
  no_gradients
  no_hessians

6.2.18 conmin

- Keywords Area
- method
- conmin

Access to methods in the CONMIN library
6.2. METHOD

Topics

This keyword is related to the topics:

- package_conmin

Specification

Alias: none

Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional Required (Choose One)</th>
<th>Description of Group Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<td></td>
<td></td>
<td>freg</td>
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</tr>
<tr>
<td>Optional</td>
<td></td>
<td>mfd</td>
<td>Method of feasible directions</td>
</tr>
<tr>
<td>Optional</td>
<td>max_iterations</td>
<td></td>
<td>Number of iterations allowed for optimizers and adaptive UQ methods</td>
</tr>
<tr>
<td>Optional</td>
<td>convergence_-tolerance</td>
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<td>Stopping criterion based on convergence of the objective function or statistics</td>
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<td>Optional</td>
<td>constraint_-tolerance</td>
<td></td>
<td>The maximum allowable value of constraint violation still considered to be feasible</td>
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<tr>
<td>Optional</td>
<td>speculative</td>
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<td>Compute speculative gradients</td>
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<tr>
<td>Optional</td>
<td>max_function_evaluations</td>
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<table>
<thead>
<tr>
<th>Optional</th>
<th>scaling</th>
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<tr>
<td>Optional</td>
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<tr>
<td></td>
<td>Turn on scaling for variables, responses, and constraints Identifier for model block to be used by a method</td>
</tr>
</tbody>
</table>

### Description

The CONMIN library\[83\] is a public domain library of nonlinear programming optimizers, specifically the Fletcher-Reeves conjugate gradient (Dakota’s `conmin_frcg` method) method for unconstrained optimization, and the method of feasible directions (Dakota’s `conmin_mfd` method) for constrained optimization. As CONMIN was a predecessor to the DOT commercial library, the algorithm controls are very similar.

One of the two available methods in Group 1 must be specified.

All these methods take the same Optional Keywords, dealing with linear equality and inequality constraints.

### See Also

These keywords may also be of interest:

- `dot`

### frcg

- Keywords Area
- method
- conmin
- frcg

A conjugate gradient optimization method

### Topics

This keyword is related to the topics:

- `package_conmin`

### Specification

**Alias:** none

**Argument(s):** none

### Description

The interpretations of the method independent controls for CONMIN are essentially identical to those for DOT.

See `package_dot` for information related to CONMIN methods.
6.2. METHOD

See Also
These keywords may also be of interest:

- mfd
- freg

mfd

- Keywords Area
- method
- conmin
- mfd

Method of feasible directions

Topics
This keyword is related to the topics:

- package_conmin

Specification

Alias: none

Argument(s): none

Description
The interpretations of the method independent controls for CONMIN are essentially identical to those for DOT. See package_dot for information related to CONMIN methods.

See Also
These keywords may also be of interest:

- freg
- mmfd

max_iterations

- Keywords Area
- method
- conmin
- max_iterations

Number of iterations allowed for optimizers and adaptive UQ methods
CHAPTER 6. KEYWORDS AREA

Topics

This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none

Argument(s): INTEGER

Default: 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence} / efficient_global: 25*n)

Description

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed max_iterations iterations. See also max_function_evaluations.

Default Behavior

Default value is 100.

corvergence_tolerance

- Keywords Area
- method
- conmin
- convergence_tolerance

Stopping criterion based on convergence of the objective function or statistics

Topics

This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none

Argument(s): REAL

Default: 1.e-4

Description

The convergence_tolerance specification provides a real value for controlling the termination of iteration.

For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by convergence_tolerance, then this convergence criterion is satisfied on the current iteration.
Therefore, permissible values are between 0 and 1, non-inclusive.

**Behavior Varies by Package/Library**

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- DOT: must be satisfied for two consecutive iterations
- NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of `convergence_tolerance` approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., `convergence_tolerance = 1.e-6` will result in approximately six digits of accuracy in the final objective function).
- NL2SOL: See `nl2sol`

**constraint_tolerance**

- **Keywords Area**
- **method**
- **conmin**
- **constraint_tolerance**

The maximum allowable value of constraint violation still considered to be feasible

**Topics**

This keyword is related to the topics:

- **method_independent_controls**

**Specification**

**Alias:** none

**Argument(s):** REAL

**Default:** Library default

**Description**

The `constraint_tolerance` specification determines the maximum allowable value of infeasibility that any constraint in an optimization problem may possess and still be considered to be satisfied.

If a constraint function is greater than this value then it is considered to be violated by the optimization algorithm. This specification gives some control over how tightly the constraints will be satisfied at convergence of the algorithm. However, if the value is set too small the algorithm may terminate with one or more constraints being violated.
This specification is currently meaningful for the NPSOL, NLSSOL, DOT and CONMIN constrained optimizers.

**Defaults**

Defaults can vary depending on the method.

- DOT constrained optimizers: 0.003
- NPSOL: dependent upon the machine precision, typically on the order of $1.e-8$ for double precision computations

**speculative**

- **Keywords Area**
- **method**
- **conmin**
- **speculative**

Compute speculative gradients

**Topics**

This keyword is related to the topics:

- **method_independent_controls**

**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** no speculation

**Description**

When performing gradient-based optimization in parallel, **speculative** gradients can be selected to address the load imbalance that can occur between gradient evaluation and line search phases. In a typical gradient-based optimization, the line search phase consists primarily of evaluating the objective function and any constraints at a trial point, and then testing the trial point for a sufficient decrease in the objective function value and/or constraint violation. If a sufficient decrease is not observed, then one or more additional trial points may be attempted sequentially. However, if the trial point is accepted then the line search phase is complete and the gradient evaluation phase begins. By speculating that the gradient information associated with a given line search trial point will be used later, additional coarse grained parallelism can be introduced by computing the gradient information (either by finite difference or analytically) in parallel, at the same time as the line search phase trial-point function values. This balances the total amount of computation to be performed at each design point and allows for efficient utilization of multiple processors. While the total amount of work performed will generally increase (since some speculative gradients will not be used when a trial point is rejected in the line search phase), the run time will usually decrease (since gradient evaluations needed at the start of each new optimization cycle were already performed in parallel during the line search phase). Refer to [14] for additional details. The speculative specification is implemented for the gradient-based optimizers in the DOT, CONMIN, and OPT++ libraries, and it can be used with dakota numerical or analytic gradient selections in the responses specification (refer
to responses gradient section for information on these specifications). It should not be selected with vendor numerical gradients since vendor internal finite difference algorithms have not been modified for this purpose. In full-Newton approaches, the Hessian is also computed speculatively. NPSOL and NLSSOL do not support speculative gradients, as their gradient-based line search in user-supplied gradient mode (dakota numerical or analytic gradients) is a superior approach for load-balanced parallel execution.

The **speculative** specification enables speculative computation of gradient and/or Hessian information, where applicable, for parallel optimization studies. By speculating that the derivative information at the current point will be used later, the complete data set (all available gradient/Hessian information) can be computed on every function evaluation. While some of these computations will be wasted, the positive effects are a consistent parallel load balance and usually shorter wall clock time. The **speculative** specification is applicable only when parallelism in the gradient calculations can be exploited by Dakota (it will be ignored for vendor numerical gradients).

**max_function_evaluations**

- **Keywords Area**
- **method**
- **conmin**
- **max_function_evaluations**

Number of function evaluations allowed for optimizers

**Topics**

This keyword is related to the topics:

- **method_independent_controls**

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** 1000

**Description**

The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed **max_function_evaluations** evaluations. See also **max_iterations**.

**Default Behavior**

Default value is 1000.

**scaling**

- **Keywords Area**
- **method**
- **conmin**
• scaling

Turn on scaling for variables, responses, and constraints

Topics

This keyword is related to the topics:

• method_independent_controls

Specification

Alias: none

Argument(s): none

Default: no scaling

Description

Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by by providing the scaling keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the method, variables, and responses blocks. When the scaling keyword is omitted, all _scale_types and *_scales specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.

• a *scales keyword, which gives characteristic values

• a *scale_type keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

Scale Types

There are four scale types:

1. none (default) - no scaling, value of *scales keyword is ignored

2. value - multiplicative scaling

3. auto - automatic scaling

First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:

• two-sided bounds scaled into the interval [0,1];

• one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
6.2. METHOD

- no bounds or targets: no automatic scaling possible, therefore no scaling for this component

Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into [0,1].

4. log - logarithmic scaling

First, any characteristic values from the optional *scales specification are applied. Then logarithm base 10 scaling is applied.

Logarithmic scaling is not available for linear constraints.

When continuous design variables are log scaled, linear constraints are not allowed.

Scales

The *scales keywords are used to specify the characteristic values. These must be non-zero real numbers. The numbers are used according to the corresponding *scale_type, as described above.

Depending on the scale type, the characteristic values may be required or optional.

- none, auto, log - optional
- value - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than 1.0e10*DBL_MIN. User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.

Examples

The two examples below are equivalent:

```
responses
objective_functions 3
sense "maximize"
primary_scale_types = "value"
primary_scales = 1 1 100
```

```
responses
objective_functions 3
sense "maximize"
primary_scale_types = "value" "value" "value"
primary_scales = 1 1 100
```

model_pointer

- Keywords Area
- method
- conmin
- model_pointer

Identifier for model block to be used by a method
CHAPTER 6. KEYWORDS AREA

Topics
This keyword is related to the topics:

- block_pointer

Specification
Alias: none

Argument(s): STRING
Default: method use of last model parsed (or use of default model if none parsed)

Description
The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior
If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.

Usage Tips
When doing advanced analyses that involve using multiple methods and multiple models, defining a model_pointer for each method is imperative.

See block_pointer for details about pointers.

Examples

```
environment
  tabular_graphics_data
  method_pointer = 'UQ'

method
  id_method = 'UQ'
  model_pointer = 'SURR'
  sampling,
    samples = 10
    seed = 98765 rng rnum2
    response_levels = 0.1 0.2 0.6
      0.1 0.2 0.6
      0.1 0.2 0.6
    sample_type lhs
    distribution cumulative

model
  id_model = 'SURR'
  surrogate global,
  dace_method_pointer = 'DACE'
  polynomial quadratic

method
  id_method = 'DACE'
  model_pointer = 'DACE_M'
  sampling sample_type lhs
    samples = 121 seed = 5034 rng rnum2

model
  id_model = 'DACE_M'
  single
```
6.2. METHOD

interface_pointer = 'I1'

variables
uniform_uncertain = 2
lower_bounds = 0. 0.
upper_bounds = 1. 1.
descriptors = 'x1' 'x2'

interface
id_interface = 'I1'
system asynch evaluation_concurrency = 5
analysis_driver = 'text_book'

responses
response_functions = 3
no_gradients
no_hessians

6.2.19 dl_solver

- Keywords Area
- method
- dl Solver

(Experimental) Dynamically-loaded solver

Topics

This keyword is related to the topics:

- optimization_and_calibration

Specification

Alias: none
Argument(s): STRING

| Required/- | Description of | Dakota Keyword |
| Optional Optional | Group | max_function_evaluations |
| Number of | function | evaluations |
| evaluations allowed for optimizers |
CHAPTER 6. KEYWORDS AREA

| Optional | scaling | Turn on scaling for variables, responses, and constraints
| Optional | model_pointer | Identifier for model block to be used by a method |

**Description**

This keyword specifies a dynamically-loaded optimization solver library, an experimental Dakota feature that is not enabled by default.

**max_function_evaluations**

- Keywords Area
- method
- dl_solver
- max_function_evaluations

Number of function evaluations allowed for optimizers

**Topics**

This keyword is related to the topics:

- method_independent_controls

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** 1000

**Description**

The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed max_function_evaluations evaluations. See also max_iterations.

**Default Behavior**

Default value is 1000.

**scaling**

- Keywords Area
- method
- dl_solver
6.2. METHOD

- **scaling**
  
  Turn on scaling for variables, responses, and constraints

**Topics**

This keyword is related to the topics:

- method-independent_controls

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no scaling

**Description**

Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by providing the `scaling` keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the method, variables, and responses blocks. When the `scaling` keyword is omitted, all `*scales` and `*_scale_type` specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.

- a `*scales` keyword, which gives characteristic values
- a `*_scale_type` keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

**Scale Types**

There are four scale types:

1. `none` (default) - no scaling, value of `*scales` keyword is ignored
2. `value` - multiplicative scaling
3. `auto` - automatic scaling

First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:

- two-sided bounds scaled into the interval \([0,1]\);
- one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into \([0,1]\).

4. \textit{log} - logarithmic scaling

First, any characteristic values from the optional \texttt{*scales} specification are applied. Then logarithm base 10 scaling is applied.

Logarithmic scaling is not available for linear constraints.

When continuous design variables are log scaled, linear constraints are not allowed.

\textbf{Scales}

The \texttt{*scales} keywords are used to specify the characteristic values. These must be non-zero real numbers. The numbers are used according to the corresponding \texttt{*scale_type}, as described above.

Depending on the scale type, the characteristic values may be required or optional.

- \texttt{none, auto, log} - optional

- \texttt{value} - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than \(1.0\times10^{10}\). User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.

\textbf{Examples}

The two examples below are equivalent:

\begin{verbatim}
responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value"
  primary_scales = 1 1 100

responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value" "value" "value"
  primary_scales = 1 1 100
\end{verbatim}

\textbf{model_pointer}

- \texttt{Keywords Area}

- \texttt{method}

- \texttt{dl_solver}

- \texttt{model_pointer}

Identifier for model block to be used by a method
6.2. METHOD

Topics
This keyword is related to the topics:

- block_pointer

Specification
Alias: none
Argument(s): STRING
Default: method use of last model parsed (or use of default model if none parsed)

Description
The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior
If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.

Usage Tips
When doing advanced analyses that involve using multiple methods and multiple models, defining a model_pointer for each method is imperative.
See block_pointer for details about pointers.

Examples

```
environment
  tabular_graphics_data
  method_pointer = 'UQ'

method
  id_method = 'UQ'
  model_pointer = 'SURR'
  sampling,
    samples = 10
    seed = 98765 rng rnum2
    response_levels = 0.1 0.2 0.6
    sample_type lhs
    distribution cumulative

model
  id_model = 'SURR'
  surrogate global,
  dace_method_pointer = 'DACE'
  polynomial quadratic

method
  id_method = 'DACE'
  model_pointer = 'DACE_M'
  sampling sample_type lhs
  samples = 121 seed = 5034 rng rnum2

model
  id_model = 'DACE_M'
  single
```
interface_pointer = 'I1'

variables
 uniform_uncertain = 2
 lower_bounds = 0. 0.
 upper_bounds = 1. 1.
 descriptors = 'x1' 'x2'

interface
 id_interface = 'I1'
 system asynch evaluation_concurrency = 5
 analysis_driver = 'text_book'

responses
 response_functions = 3
 no_gradients
 no_hessians

6.2.20  npsol_sqp

• Keywords Area
• method
• npsol_sqp

Sequential Quadratic Program

Topics
This keyword is related to the topics:
• package_npsol
• sequential_quadratic_programming
• local_optimization_methods

Specification
Alias: none
Argument(s): none

<p>| Required/-  | Description of         | Dakota Keyword     | Dakota Keyword  |
| Optional   | Group                  | verify_level       | Description     |
|            |                        |                    | Verify the quality of analytic gradients |</p>
<table>
<thead>
<tr>
<th>Optional</th>
<th>function_precision</th>
<th>Specify the maximum precision of the analysis code responses</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>linesearch_-tolerance</td>
<td>Choose how accurately the algorithm will compute the minimum in a line search</td>
</tr>
<tr>
<td>Optional</td>
<td>convergence_-tolerance</td>
<td>Stopping criterion based on convergence of the objective function or statistics</td>
</tr>
<tr>
<td>Optional</td>
<td>max_iterations</td>
<td>Number of iterations allowed for optimizers and adaptive UQ methods</td>
</tr>
<tr>
<td>Optional</td>
<td>constraint_-tolerance</td>
<td>The maximum allowable value of constraint violation still considered to be feasible</td>
</tr>
<tr>
<td>Optional</td>
<td>speculative</td>
<td>Compute speculative gradients</td>
</tr>
<tr>
<td>Optional</td>
<td>max_function_-_evaluations</td>
<td>Number of function evaluations allowed for optimizers</td>
</tr>
<tr>
<td>Optional</td>
<td>scaling</td>
<td>Turn on scaling for variables, responses, and constraints</td>
</tr>
</tbody>
</table>
CHAPTER 6. KEYWORDS AREA

| Optional | model_pointer | Identifier for model block to be used by a method |

Description

NPSOL provides an implementation of sequential quadratic programming that can be accessed with npsol_sqp.

Stopping Criteria

The method independent controls for max_iterations and max_function_evaluations limit the number of major SQP iterations and the number of function evaluations that can be performed during an NPSOL optimization. The convergence_tolerance control defines NPSOL’s internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of convergence_tolerance approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., convergence_tolerance = 1.e-6 will result in approximately six digits of accuracy in the final objective function). The constraint_tolerance control defines how tightly the constraint functions are satisfied at convergence. The default value is dependent upon the machine precision of the platform in use, but is typically on the order of 1.e-8 for double precision computations. Extremely small values for constraint_tolerance may not be attainable. The output verbosity setting controls the amount of information generated at each major SQP iteration: the silent and quiet settings result in only one line of diagnostic output for each major iteration and print the final optimization solution, whereas the verbose and debug settings add additional information on the objective function, constraints, and variables at each major iteration.

Concurrency

NPSOL is not a parallel algorithm and cannot directly take advantage of concurrent evaluations. However, if numerical_gradients with method_source dakota is specified, then the finite difference function evaluations can be performed concurrently (using any of the parallel modes described in the Users Manual [4]).

An important related observation is the fact that NPSOL uses two different line searches depending on how gradients are computed. For either analytic_gradients or numerical_gradients with method_source dakota, NPSOL is placed in user-supplied gradient mode (NPSOL’s ”Derivative Level” is set to 3) and it uses a gradient-based line search (the assumption is that user-supplied gradients are inexpensive). On the other hand, if numerical_gradients are selected with method_source vendor, then NPSOL is computing finite differences internally and it will use a value-based line search (the assumption is that finite differencing on each line search evaluation is too expensive). The ramifications of this are: (1) performance will vary between method_source dakota and method_source vendor for numerical_gradients, and (2) gradient speculation is unnecessary when performing optimization in parallel since the gradient-based line search in user-supplied gradient mode is already load balanced for parallel execution. Therefore, a speculative specification will be ignored by NPSOL, and optimization with numerical_gradients should select method_source dakota for load balanced parallel operation and method_source vendor for efficient serial operation.

Linear constraints

Lastly, NPSOL supports specialized handling of linear inequality and equality constraints. By specifying the coefficients and bounds of the linear inequality constraints and the coefficients and targets of the linear equality constraints, this information can be provided to NPSOL at initialization and tracked internally, removing the need for the user to provide the values of the linear constraints on every function evaluation.

verify_level

- Keywords Area
- method
6.2. METHOD

- **npsol_sqp**
- **verify_level**

Verify the quality of analytic gradients

**Specification**

**Alias:** none
**Argument(s):** INTEGER
**Default:** -1 (no gradient verification)

**Description**

*verify_level* instructs the NPSOL and NLSSOL algorithms to perform their own finite difference verification of the gradients provided by Dakota. Typically these are used to verify *analytic_gradients* produced by a simulation code, though the option can be used with other Dakota-supplied gradient types including numerical or mixed.

Level 1 will verify the objective gradients, level 2, the nonlinear constraint gradients, and level 3, both. See the Optional Input Parameters section of the NPSOL manual[33] for additional information, including options to verify at the user-supplied initial point vs. first feasible point.

**function_precision**

- **Keywords Area**
- **method**
- **npsol_sqp**
- **function_precision**

Specify the maximum precision of the analysis code responses

**Specification**

**Alias:** none
**Argument(s):** REAL
**Default:** 1.0e-10

**Description**

The *function_precision* control provides the algorithm with an estimate of the accuracy to which the problem functions can be computed. This is used to prevent the algorithm from trying to distinguish between function values that differ by less than the inherent error in the calculation.
linesearch_tolerance

- Keywords Area
- method
- npsol_sqp
- linesearch_tolerance

Choose how accurately the algorithm will compute the minimum in a line search

**Specification**

**Alias:** none

**Argument(s):** REAL

**Default:** 0.9 (inaccurate line search)

**Description**

The *linesearch_tolerance* setting controls the accuracy of the line search. The smaller the value (between 0 and 1), the more accurately the algorithm will attempt to compute a precise minimum along the search direction.

convergence_tolerance

- Keywords Area
- method
- npsol_sqp
- convergence_tolerance

Stopping criterion based on convergence of the objective function or statistics

**Topics**

This keyword is related to the topics:

- method_independent_controls

**Specification**

**Alias:** none

**Argument(s):** REAL

**Default:** 1.e-4
Description

The `convergence_tolerance` specification provides a real value for controlling the termination of iteration. For optimization, it is most commonly a **relative convergence tolerance** for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by convergence_tolerance, then this convergence criterion is satisfied on the current iteration.

Therefore, permissible values are between 0 and 1, non-inclusive.

**Behavior Varies by Package/Library**

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- DOT: must be satisfied for two consecutive iterations
- NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of convergence_tolerance approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., `convergence_tolerance = 1.e-6` will result in approximately six digits of accuracy in the final objective function).
- NL2SOL: See `nl2sol`

**max_iterations**

- Keywords Area
- method
- npsol_sqp
- max_iterations

Number of iterations allowed for optimizers and adaptive UQ methods

**Topics**

This keyword is related to the topics:

- **method_independent_controls**

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability , interval_est , evidence} / efficient_{global: 25*n})
Description

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed \( \text{max\_iterations} \) iterations. See also \text{max\_function\_evaluations}.

Default Behavior
Default value is 100.

\text{constraint\_tolerance}

- Keywords Area
- method
- npsol_sqp
- constraint\_tolerance

The maximum allowable value of constraint violation still considered to be feasible

Topics

This keyword is related to the topics:
- method\_independent\_controls

Specification

Alias: none

Argument(s): REAL

Default: Library default

Description

The \text{constraint\_tolerance} specification determines the maximum allowable value of infeasibility that any constraint in an optimization problem may possess and still be considered to be satisfied.

If a constraint function is greater than this value then it is considered to be violated by the optimization algorithm. This specification gives some control over how tightly the constraints will be satisfied at convergence of the algorithm. However, if the value is set too small the algorithm may terminate with one or more constraints being violated.

This specification is currently meaningful for the NPSOL, NLSSOL, DOT and CONMIN constrained optimizers.

Defaults
Defaults can vary depending on the method.

- DOT constrained optimizers: 0.003
- NPSOL: dependent upon the machine precision, typically on the order of \(1.e-8\) for double precision computations
speculative

- Keywords Area
- method
- npsol_sqp
- speculative

Compute speculative gradients

Topics

This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none

Argument(s): none

Default: no speculation

Description

When performing gradient-based optimization in parallel, speculative gradients can be selected to address the load imbalance that can occur between gradient evaluation and line search phases. In a typical gradient-based optimization, the line search phase consists primarily of evaluating the objective function and any constraints at a trial point, and then testing the trial point for a sufficient decrease in the objective function value and/or constraint violation. If a sufficient decrease is not observed, then one or more additional trial points may be attempted sequentially. However, if the trial point is accepted then the line search phase is complete and the gradient evaluation phase begins. By speculating that the gradient information associated with a given line search trial point will be used later, additional coarse grained parallelism can be introduced by computing the gradient information (either by finite difference or analytically) in parallel, at the same time as the line search phase trial-point function values. This balances the total amount of computation to be performed at each design point and allows for efficient utilization of multiple processors. While the total amount of work performed will generally increase (since some speculative gradients will not be used when a trial point is rejected in the line search phase), the run time will usually decrease (since gradient evaluations needed at the start of each new optimization cycle were already performed in parallel during the line search phase). Refer to [14] for additional details. The speculative specification is implemented for the gradient-based optimizers in the DOT, CONMIN, and OPT++ libraries, and it can be used with dakota numerical or analytic gradient selections in the responses specification (refer to responses gradient section for information on these specifications). It should not be selected with vendor numerical gradients since vendor internal finite difference algorithms have not been modified for this purpose. In full-Newton approaches, the Hessian is also computed speculatively. NPSOL and NLSSOL do not support speculative gradients, as their gradient-based line search in user-supplied gradient mode (dakota numerical or analytic gradients) is a superior approach for load-balanced parallel execution.

The speculative specification enables speculative computation of gradient and/or Hessian information, where applicable, for parallel optimization studies. By speculating that the derivative information at the current point will be used later, the complete data set (all available gradient/Hessian information) can be computed on every function evaluation. While some of these computations will be wasted, the positive effects are a consistent parallel load balance and usually shorter wall clock time. The speculative specification is applicable
only when parallelism in the gradient calculations can be exploited by Dakota (it will be ignored for vendor numerical gradients).

**max_function_evaluations**

- Keywords Area
- method
- npsol_sqp
- max_function_evaluations

Number of function evaluations allowed for optimizers

**Topics**

This keyword is related to the topics:

- method_independent_controls

**Specification**

Alias: none  
Argument(s): INTEGER  
Default: 1000

**Description**

The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed max_function_evaluations evaluations. See also max_iterations.

**Default Behavior**

Default value is 1000.

**scaling**

- Keywords Area
- method
- npsol_sqp
- scaling

Turn on scaling for variables, responses, and constraints

**Topics**

This keyword is related to the topics:

- method_independent_controls
6.2. METHOD

Specification

Alias: none
Argument(s): none
Default: no scaling

Description

Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by by providing the scaling keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the method, variables, and responses blocks. When the scaling keyword is omitted, all _scale_types and *scales specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.

- a *scales keyword, which gives characteristic values
- a *scale_type keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

Scale Types

There are four scale types:

1. none (default) - no scaling, value of *scales keyword is ignored
2. value - multiplicative scaling
3. auto - automatic scaling
   
   First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:
   
   - two-sided bounds scaled into the interval [0,1];
   - one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
   - no bounds or targets: no automatic scaling possible, therefore no scaling for this component

   Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into [0,1].

4. log - logarithmic scaling
   
   First, any characteristic values from the optional _scales specification are applied. Then logarithm base 10 scaling is applied.

   Logarithmic scaling is not available for linear constraints.

   When continuous design variables are log scaled, linear constraints are not allowed.
Scales
The *scales keywords are used to specify the characteristic values. These must be non-zero real numbers. The numbers are used according to the corresponding *scale_type, as described above. Depending on the scale type, the characteristic values may be required or optional.

- none, auto, log - optional
- value - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than 1.0e10*DBL_MIN. User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.

Examples
The two examples below are equivalent:

```plaintext
responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value"
  primary_scales = 1 1 100
```

```plaintext
responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value" "value" "value"
  primary_scales = 1 1 100
```

model_pointer
- Keywords Area
- method
- npsol_sqp
- model_pointer

Identifier for model block to be used by a method

Topics
This keyword is related to the topics:

- block_pointer

Specification
Alias: none
Argument(s): STRING
Default: method use of last model parsed (or use of default model if none parsed)
6.2. METHOD

Description

The `model_pointer` is used to specify which `model` block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a `model` block in the Dakota input file that has a corresponding `id_model` with the same name.

Usage Tips

When doing advanced analyses that involve using multiple methods and multiple models, defining a `model-pointer` for each method is imperative.

See `block_pointer` for details about pointers.

Examples

```plaintext
environment
tabular_graphics_data
  method_pointer = 'UQ'

method
  id_method = 'UQ'
  model_pointer = 'SRR'
  sampling,
    samples = 10
    seed = 98765 rng rnum2
    response_levels = 0.1 0.2 0.6
    0.1 0.2 0.6
    0.1 0.2 0.6
  sample_type lhs
distribution cumulative

model
  id_model = 'SRR'
  surrogate global,
    dace_method_pointer = 'DACE'
    polynomial quadratic

method
  id_method = 'DACE'
  model_pointer = 'DACE_M'
  sampling sample_type lhs
    samples = 121 seed = 5034 rng rnum2

model
  id_model = 'DACE_M'
  single
  interface_pointer = 'I1'

variables
  uniform_uncertain = 2
    lower_bounds = 0. 0.
    upper_bounds = 1. 1.
    descriptors = 'x1' 'x2'

interface
  id_interface = 'I1'
  system async evaluation_concurrency = 5
  analysis_driver = 'text_book'

responses
```
response_functions = 3
no_gradients
no_hessians

6.2.21 nlssol_sqp

- Keywords Area
- method
- nlssol_sqp

Sequential Quadratic Program for nonlinear least squares

Topics
This keyword is related to the topics:
- sequential_quadratic_programming
- nonlinear_least_squares

Specification

Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<td>verify_level</td>
<td></td>
<td>Verify the quality of analytic gradients</td>
</tr>
<tr>
<td>Optional</td>
<td>function_precision</td>
<td></td>
<td>Specify the maximum precision of the analysis code responses</td>
</tr>
<tr>
<td>Optional</td>
<td>linesearch_-tolerance</td>
<td></td>
<td>Choose how accurately the algorithm will compute the minimum in a line search</td>
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</table>
### Description

NLSSOL is available as `nlssol_sqp` and supports unconstrained, bound-constrained, and generally-constrained problems. It exploits the structure of a least squares objective function through the periodic use of Gauss-Newton Hessian approximations to accelerate the SQP algorithm.

**Stopping Criteria**

The method independent controls for `max_iterations` and `max_function_evaluations` limit the number of major SQP iterations and the number of function evaluations that can be performed during an NPSOL optimization. The `convergence_tolerance` control defines NPSOL's internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of `convergence_tolerance` approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., `convergence_tolerance = 1.e-6` will result in approximately six digits of accuracy in the final objective function). The `constraint_tolerance` control defines how tightly the constraint functions are satisfied at convergence. The default value is dependent upon the machine precision of the platform in use, but is typically on the order of `1.e-8` for double precision computations. Extremely small

<table>
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<tbody>
<tr>
<td>Optional</td>
<td>max_iterations</td>
<td>Number of iterations allowed for optimizers and adaptive UQ methods</td>
</tr>
<tr>
<td>Optional</td>
<td>constraint_tolerance</td>
<td>The maximum allowable value of constraint violation still considered to be feasible</td>
</tr>
<tr>
<td>Optional</td>
<td>speculative</td>
<td>Compute speculative gradients</td>
</tr>
<tr>
<td>Optional</td>
<td>max_function_evaluations</td>
<td>Number of function evaluations allowed for optimizers</td>
</tr>
<tr>
<td>Optional</td>
<td>scaling</td>
<td>Turn on scaling for variables, responses, and constraints</td>
</tr>
<tr>
<td>Optional</td>
<td>model_pointer</td>
<td>Identifier for model block to be used by a method</td>
</tr>
</tbody>
</table>
values for constraint_tolerance may not be attainable.

See Also

These keywords may also be of interest:

- npsol_sqp
- nl2sol
- optpp_g_newton
- field_calibration_terms

verify_level

- Keywords Area
- method
- nlssol_sqp
- verify_level

Verify the quality of analytic gradients

Specification

Alias: none
Argument(s): INTEGER
Default: -1 (no gradient verification)

Description

verify_level instructs the NPSOL and NLSSOL algorithms to perform their own finite difference verification of the gradients provided by Dakota. Typically these are used to verify analytic_gradients produced by a simulation code, though the option can be used with other Dakota-supplied gradient types including numerical or mixed.

Level 1 will verify the objective gradients, level 2, the nonlinear constraint gradients, and level 3, both. See the Optional Input Parameters section of the NPSOL manual[33] for additional information, including options to verify at the user-supplied initial point vs. first feasible point.

function_precision

- Keywords Area
- method
- nlssol_sqp
- function_precision

Specify the maximum precision of the analysis code responses
6.2. METHOD

Specification

Alias: none

Argument(s): REAL
Default: 1.0e-10

Description

The function_precision control provides the algorithm with an estimate of the accuracy to which the problem functions can be computed. This is used to prevent the algorithm from trying to distinguish between function values that differ by less than the inherent error in the calculation.

linesearch_tolerance

- Keywords Area
- method
- nlssol_sqp
- linesearch_tolerance

Choose how accurately the algorithm will compute the minimum in a line search

Specification

Alias: none

Argument(s): REAL
Default: 0.9 (inaccurate line search)

Description

The linesearch_tolerance setting controls the accuracy of the line search. The smaller the value (between 0 and 1), the more accurately the algorithm will attempt to compute a precise minimum along the search direction.

convergence_tolerance

- Keywords Area
- method
- nlssol_sqp
- convergence_tolerance

Stopping criterion based on convergence of the objective function or statistics

Topics

This keyword is related to the topics:

- method_independent_controls
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): REAL
Default: 1.e-4

Description

The convergence_tolerance specification provides a real value for controlling the termination of iteration. For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by convergence_tolerance, then this convergence criterion is satisfied on the current iteration.

Therefore, permissible values are between 0 and 1, non-inclusive.

Behavior Varies by Package/Library

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- DOT: must be satisfied for two consecutive iterations
- NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of convergence_tolerance approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., convergence_tolerance = 1.e-6 will result in approximately six digits of accuracy in the final objective function).
- NL2SOL: See nl2sol

max_iterations

- Keywords Area
- method
- nlssol_sqp
- max_iterations

Number of iterations allowed for optimizers and adaptive UQ methods

Topics

This keyword is related to the topics:

- method_independent_controls
6.2. METHOD

Specification

Alias: none
Argument(s): INTEGER
Default: 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence} / efficient_global: 25*n)

Description

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed max_iterations iterations. See also max_function_evaluations.

Default Behavior
Default value is 100.

constraint_tolerance

- Keywords Area
- method
- nlssol_sqp
- constraint_tolerance

The maximum allowable value of constraint violation still considered to be feasible

Topics

This keyword is related to the topics:
- method_independent_controls

Specification

Alias: none
Argument(s): REAL
Default: Library default

Description

The constraint_tolerance specification determines the maximum allowable value of infeasibility that any constraint in an optimization problem may possess and still be considered to be satisfied.

If a constraint function is greater than this value then it is considered to be violated by the optimization algorithm. This specification gives some control over how tightly the constraints will be satisfied at convergence of the algorithm. However, if the value is set too small the algorithm may terminate with one or more constraints being violated.

This specification is currently meaningful for the NPSOL, NLSSOL, DOT and CONMIN constrained optimizers.

Defaults
Defaults can vary depending on the method.

- DOT constrained optimizers: 0.003

• NPSOL: dependent upon the machine precision, typically on the order of $1.e^{-8}$ for double precision computations.

**speculative**

- **Keywords Area**
- **method**
- **nlssol_sqp**
- **speculative**

Compute speculative gradients

**Topics**

This keyword is related to the topics:

- **method_independent_controls**

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no speculation

**Description**

When performing gradient-based optimization in parallel, speculative gradients can be selected to address the load imbalance that can occur between gradient evaluation and line search phases. In a typical gradient-based optimization, the line search phase consists primarily of evaluating the objective function and any constraints at a trial point, and then testing the trial point for a sufficient decrease in the objective function value and/or constraint violation. If a sufficient decrease is not observed, then one or more additional trial points may be attempted sequentially. However, if the trial point is accepted then the line search phase is complete and the gradient evaluation phase begins. By speculating that the gradient information associated with a given line search trial point will be used later, additional coarse grained parallelism can be introduced by computing the gradient information (either by finite difference or analytically) in parallel, at the same time as the line search phase trial-point function values. This balances the total amount of computation to be performed at each design point and allows for efficient utilization of multiple processors. While the total amount of work performed will generally increase (since some speculative gradients will not be used when a trial point is rejected in the line search phase), the run time will usually decrease (since gradient evaluations needed at the start of each new optimization cycle were already performed in parallel during the line search phase). Refer to [14] for additional details. The speculative specification is implemented for the gradient-based optimizers in the DOT, CONMIN, and OPT++ libraries, and it can be used with dakota numerical or analytic gradient selections in the responses specification (refer to responses gradient section for information on these specifications). It should not be selected with vendor numerical gradients since vendor internal finite difference algorithms have not been modified for this purpose. In full-Newton approaches, the Hessian is also computed speculatively. NPSOL and NLSSOL do not support speculative gradients, as their gradient-based line search in user-supplied gradient mode (dakota numerical or analytic gradients) is a superior approach for load-balanced parallel execution.

The **speculative** specification enables speculative computation of gradient and/or Hessian information, where applicable, for parallel optimization studies. By speculating that the derivative information at the current
point will be used later, the complete data set (all available gradient/Hessian information) can be computed on every function evaluation. While some of these computations will be wasted, the positive effects are a consistent parallel load balance and usually shorter wall clock time. The speculative specification is applicable only when parallelism in the gradient calculations can be exploited by Dakota (it will be ignored for vendor numerical gradients).

**max_function_evaluations**

- **Keywords Area**
- **method**
- **nlssol_sqp**
- **max_function_evaluations**

Number of function evaluations allowed for optimizers

**Topics**

This keyword is related to the topics:

- **method_independent_controls**

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** 1000

**Description**

The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed max_function_evaluations evaluations. See also **max_iterations**.

**Default Behavior**

Default value is 1000.

**scaling**

- **Keywords Area**
- **method**
- **nlssol_sqp**
- **scaling**

Turn on scaling for variables, responses, and constraints

**Topics**

This keyword is related to the topics:

- **method_independent_controls**
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none
Argument(s): none
Default: no scaling

Description

Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by by providing the scaling keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the method, variables, and responses blocks. When the scaling keyword is omitted, all _scale_types and _scales specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.

• a _scales keyword, which gives characteristic values
• a _scale_type keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

Scale Types

There are four scale types:

1. none (default) - no scaling, value of _scales keyword is ignored
2. value - multiplicative scaling
3. auto - automatic scaling
   First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:
   • two-sided bounds scaled into the interval [0,1];
   • one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
   • no bounds or targets: no automatic scaling possible, therefore no scaling for this component

Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into [0,1].

4. log - logarithmic scaling
   First, any characteristic values from the optional _scales specification are applied. Then logarithm base 10 scaling is applied.

Logarithmic scaling is not available for linear constraints.
When continuous design variables are log scaled, linear constraints are not allowed.
6.2. METHOD

**Scales**

The `*scales` keywords are used to specify the characteristic values. These must be non-zero real numbers. The numbers are used according to the corresponding `*scale_type`, as described above. Depending on the scale type, the characteristic values may be required or optional.

- `none, auto, log` - optional
- `value` - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than `1.0e10*DBL_MIN`. User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.

**Examples**

The two examples below are equivalent:

```plaintext
responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value"
  primary_scales = 1 1 100

responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value" "value" "value"
  primary_scales = 1 1 100
```

**model_pointer**

- **Keywords Area**
- **method**
- **nlssol_sqp**
- **model_pointer**

Identifier for model block to be used by a method

**Topics**

This keyword is related to the topics:

- **block_pointer**

**Specification**

**Alias:** none

**Argument(s):** STRING

**Default:** method use of last model parsed (or use of default model if none parsed)
**Description**

The **model_pointer** is used to specify which **model** block will be used to perform the function evaluations needed by the Dakota method.

**Default Behavior**

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a **model** block in the Dakota input file that has a corresponding **id_model** with the same name.

**Usage Tips**

When doing advanced analyses that involve using multiple methods and multiple models, defining a **model_pointer** for each method is imperative.

See **block_pointer** for details about pointers.

**Examples**

```plaintext
environment
   tabular_graphics_data
   method_pointer = 'UQ'

method
   id_method = 'UQ'
   model_pointer = 'SURR'
   sampling,
      samples = 10
      seed = 98765 rng rnum2
      response_levels = 0.1 0.2 0.6
      0.1 0.2 0.6
      0.1 0.2 0.6
   sample_type lhs
   distribution cumulative

model
   id_model = 'SURR'
   surrogate global,
   dace_method_pointer = 'DACE'
   polynomial quadratic

method
   id_method = 'DACE'
   model_pointer = 'DACE_M'
   sampling sample_type lhs
   samples = 121 seed = 5034 rng rnum2

model
   id_model = 'DACE_M'
   single
   interface_pointer = 'I1'

variables
   uniform_uncertain = 2
      lower_bounds = 0. 0.
      upper_bounds = 1. 1.
   descriptors = 'x1' 'x2'

interface
   id_interface = 'I1'
   system async evaluation_concurrency = 5
   analysis_driver = 'text_book'

responses
```
response_functions = 3
no_gradients
no_hessians

6.2.22 stanford

- Keywords Area
- method
- stanford

Select methods from the Stanford package

**Specification**

**Alias:** none

**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/Optional Required (Choose One)</th>
<th>Description of Group Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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</table>
|                                        |                              | npsol          | Duplicate of method-npsol-
sqp                       |
| Optional                               | npsol                        |                | Duplicate of method-nlssol-
sqp                       |
| Optional                               | verify_level                 |                | Verify the quality of analytic gradients               |
| Optional                               | function_precision          |                | Specify the maximum precision of the analysis code responses |
| Optional                               | linesearch_tolerance         |                | Choose how accurately the algorithm will compute the minimum in a line search |
## Description

This is a duplicate. See the method pages here:

- `nlsol_sqp`
- `npsol_sqp`

### npsol

- **Keywords Area**
- **method**
- **stanford**
- **npsol**
6.2. METHOD

Duplicate of method-npsol_sqp

Specification

Alias: none
Argument(s): none

Description

See the page for npsol_sqp

nlssol

• Keywords Area

• method

• stanford

• nlssol

Duplicate of method-nlssol_sqp

Specification

Alias: none
Argument(s): none

Description

See the page for nlssol_sqp

verify_level

• Keywords Area

• method

• stanford

• verify_level

Verify the quality of analytic gradients

Specification

Alias: none
Argument(s): INTEGER
Default: -1 (no gradient verification)
Description

verify_level instructs the NPSOL and NLSSOL algorithms to perform their own finite difference verification of the gradients provided by Dakota. Typically these are used to verify analytic_gradients produced by a simulation code, though the option can be used with other Dakota-supplied gradient types including numerical or mixed.

Level 1 will verify the objective gradients, level 2, the nonlinear constraint gradients, and level 3, both. See the Optional Input Parameters section of the NPSOL manual[33] for additional information, including options to verify at the user-supplied initial point vs. first feasible point.

function_precision

- Keywords Area
- method
- stanford
- function_precision

Specify the maximum precision of the analysis code responses

Specification

Alias: none

Argument(s): REAL

Default: 1.0e-10

Description

The function_precision control provides the algorithm with an estimate of the accuracy to which the problem functions can be computed. This is used to prevent the algorithm from trying to distinguish between function values that differ by less than the inherent error in the calculation.

line_search_tolerance

- Keywords Area
- method
- stanford
- line_search_tolerance

Choose how accurately the algorithm will compute the minimum in a line search

Specification

Alias: none

Argument(s): REAL

Default: 0.9 (inaccurate line search)
6.2. METHOD

Description

The linesearch_tolerance setting controls the accuracy of the line search. The smaller the value (between 0 and 1), the more accurately the algorithm will attempt to compute a precise minimum along the search direction.

convergence_tolerance

- Keywords Area
- method
- stanford
- convergence_tolerance

Stopping criterion based on convergence of the objective function or statistics

Topics

This keyword is related to the topics:

- method-independent_controls

Specification

Alias: none

Argument(s): REAL

Default: 1.e-4

Description

The convergence_tolerance specification provides a real value for controlling the termination of iteration.

For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by convergence_tolerance, then this convergence criterion is satisfied on the current iteration.

Therefore, permissible values are between 0 and 1, non-inclusive.

Behavior Varies by Package/Library

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- DOT: must be satisfied for two consecutive iterations
- NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of convergence_tolerance approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., convergence_tolerance = 1.e-6 will result in approximately six digits of accuracy in the final objective function).
- NL2SOL: See nl2sol
max_iterations

- Keywords Area
- method
- stanford
- max_iterations

Number of iterations allowed for optimizers and adaptive UQ methods

Topics
This keyword is related to the topics:
- method_independent_controls

Specification

Alias: none

Argument(s): INTEGER

Default: 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence} / efficient-global: 25*n)

Description
The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed max_iterations iterations. See also max_function_evaluations.

Default Behavior
Default value is 100.

constraint_tolerance

- Keywords Area
- method
- stanford
- constraint_tolerance

The maximum allowable value of constraint violation still considered to be feasible

Topics
This keyword is related to the topics:
- method_independent_controls
6.2. METHOD

Specification

Alias: none

Argument(s): REAL
Default: Library default

Description

The constraint_tolerance specification determines the maximum allowable value of infeasibility that any constraint in an optimization problem may possess and still be considered to be satisfied.

If a constraint function is greater than this value then it is considered to be violated by the optimization algorithm. This specification gives some control over how tightly the constraints will be satisfied at convergence of the algorithm. However, if the value is set too small the algorithm may terminate with one or more constraints being violated.

This specification is currently meaningful for the NPSOL, NLSSOL, DOT and CONMIN constrained optimizers.

Defaults

Defaults can vary depending on the method.

- DOT constrained optimizers: 0.003
- NPSOL: dependent upon the machine precision, typically on the order of $1.e-8$ for double precision computations

speculative

- Keywords Area
- method
- stanford
- speculative

Compute speculative gradients

Topics

This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none

Argument(s): none
Default: no speculation
CHAPTER 6. KEYWORDS AREA

Description

When performing gradient-based optimization in parallel, speculative gradients can be selected to address the load imbalance that can occur between gradient evaluation and line search phases. In a typical gradient-based optimization, the line search phase consists primarily of evaluating the objective function and any constraints at a trial point, and then testing the trial point for a sufficient decrease in the objective function value and/or constraint violation. If a sufficient decrease is not observed, then one or more additional trial points may be attempted sequentially. However, if the trial point is accepted then the line search phase is complete and the gradient evaluation phase begins. By speculating that the gradient information associated with a given line search trial point will be used later, additional coarse grained parallelism can be introduced by computing the gradient information (either by finite difference or analytically) in parallel, at the same time as the line search phase trial-point function values. This balances the total amount of computation to be performed at each design point and allows for efficient utilization of multiple processors. While the total amount of work performed will generally increase (since some speculative gradients will not be used when a trial point is rejected in the line search phase), the run time will usually decrease (since gradient evaluations needed at the start of each new optimization cycle were already performed in parallel during the line search phase). Refer to [14] for additional details. The speculative specification is implemented for the gradient-based optimizers in the DOT, CONMIN, and OPT++ libraries, and it can be used with dakota numerical or analytic gradient selections in the responses specification (refer to responses gradient section for information on these specifications). It should not be selected with vendor numerical gradients since vendor internal finite difference algorithms have not been modified for this purpose.

In full-Newton approaches, the Hessian is also computed speculatively. NPSOL and NLSSOL do not support speculative gradients, as their gradient-based line search in user-supplied gradient mode (dakota numerical or analytic gradients) is a superior approach for load-balanced parallel execution.

The speculative specification enables speculative computation of gradient and/or Hessian information, where applicable, for parallel optimization studies. By speculating that the derivative information at the current point will be used later, the complete data set (all available gradient/Hessian information) can be computed on every function evaluation. While some of these computations will be wasted, the positive effects are a consistent parallel load balance and usually shorter wall clock time. The speculative specification is applicable only when parallelism in the gradient calculations can be exploited by Dakota (it will be ignored for vendor numerical gradients).

max_function_evaluations

- Keywords Area
- method
- stanford
- max_function_evaluations

Number of function evaluations allowed for optimizers

Topics

This keyword is related to the topics:

- method_independent_controls
6.2. METHOD

Specification
Alias: none
Argument(s): INTEGER
Default: 1000

Description
The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed \( \text{max\_function\_evaluations} \) evaluations. See also \( \text{max\_iterations} \).

Default Behavior
Default value is 1000.

scaling

- Keywords Area
- method
- stanford
- scaling

Turn on scaling for variables, responses, and constraints

Topics
This keyword is related to the topics:
- method\_independent\_controls

Specification
Alias: none
Argument(s): none
Default: no scaling

Description
Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by by providing the scaling keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the method, variables, and responses blocks. When the scaling keyword is omitted, all \_scale\_types and \_*\_scales\_specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.
• a *scales keyword, which gives characteristic values

• a *scale_type keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

Scale Types

There are four scale types:

1. none (default) - no scaling, value of *scales keyword is ignored

2. value - multiplicative scaling

3. auto - automatic scaling

First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:

• two-sided bounds scaled into the interval [0,1];
• one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
• no bounds or targets: no automatic scaling possible, therefore no scaling for this component

Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into [0,1].

4. log - logarithmic scaling

First, any characteristic values from the optional *scales specification are applied. Then logarithm base 10 scaling is applied.

Logarithmic scaling is not available for linear constraints.

When continuous design variables are log scaled, linear constraints are not allowed.

Scales

The *scales keywords are used to specify the characteristic values. These must be non-zero real numbers. The numbers are used according to the corresponding *scale_type, as described above.

Depending on the scale type, the characteristic values may be required or optional.

• none, auto, log - optional

• value - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than 1.0e10*DBL_MIN. User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.
6.2. METHOD

Examples
The two examples below are equivalent:

```plaintext
responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value"
  primary_scales = 1 1 100

responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value" "value" "value"
  primary_scales = 1 1 100
```

**model_pointer**

- Keywords Area
- method
- stanford
- model_pointer

Identifier for model block to be used by a method

Topics
This keyword is related to the topics:

- block_pointer

Specification

**Alias:** none

**Argument(s):** STRING

**Default:** method use of last model parsed (or use of default model if none parsed)

Description

The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

**Default Behavior**

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.

**Usage Tips**

When doing advanced analyses that involve using multiple methods and multiple models, defining a model-pointer for each method is imperative.

See block_pointer for details about pointers.
Examples

environment
tabular_graphics_data
method_pointer = 'UQ'

method
id_method = 'UQ'
model_pointer = 'SURR'
sampling,
samples = 10
seed = 98765 rng rnum2
response_levels = 0.1 0.2 0.6
       0.1 0.2 0.6
       0.1 0.2 0.6
sample_type lhs
distribution cumulative

model
id_model = 'SURR'
surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
id_method = 'DACE'
model_pointer = 'DACE_M'
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = 'DACE_M'
single
interface_pointer = 'I1'

variables
uniform_uncertain = 2
lower_bounds = 0. 0.
upper_bounds = 1. 1.
descriptors = 'x1' 'x2'

interface
id_interface = 'I1'
system asynch evaluation_concurrency = 5
analysis_driver = 'text_book'

responses
response_functions = 3
no_gradients
no_hessians

6.2.23 nlpql_sqp

- Keywords Area
- method
- nlpql_sqp

Sequential Quadratic Program
6.2. METHOD

Topics
This keyword is related to the topics:

- package_nlpql
- sequential_quadratic_programming
- local_optimization_methods

Specification
Alias: none
Argument(s): none

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<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>max_iterations</td>
<td>Number of iterations allowed for optimizers and adaptive UQ methods</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>convergence_-tolerance</td>
<td>Stopping criterion based on convergence of the objective function or statistics</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>max_function_evaluations</td>
<td>Number of function evaluations allowed for optimizers</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>scaling</td>
<td>Turn on scaling for variables, responses, and constraints</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>model_pointer</td>
<td>Identifier for model block to be used by a method</td>
</tr>
</tbody>
</table>

Description
NLPQL provides an implementation of sequential quadratic programming through nlpql_sqp. The particular SQP implementation in nlpql_sqp uses a variant with distributed and non-monotone line search. Thus, this variant is designed to be more robust in the presence of inaccurate or noisy gradients common in many engineering applications.

The method independent controls for maximum iterations and output verbosity are mapped to NLPQL controls MAXIT and IPRINT, respectively. The maximum number of function evaluations is enforced within the NLPQL-LPOptimizer class.
**max_iterations**

- **Keywords Area**
- **method**
- **nlpql_sqp**
- **max_iterations**

Number of iterations allowed for optimizers and adaptive UQ methods

**Topics**

This keyword is related to the topics:

- **method_independent_controls**

**Specification**

**Alias:** none  
**Argument(s):** INTEGER  
**Default:** 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence} / efficient_global: 25*n)

**Description**

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed max_iterations iterations. See also max_function_evaluations.

**Default Behavior**

Default value is 100.

**convergence_tolerance**

- **Keywords Area**
- **method**
- **nlpql_sqp**
- **convergence_tolerance**

Stopping criterion based on convergence of the objective function or statistics

**Topics**

This keyword is related to the topics:

- **method_independent_controls**
6.2. METHOD

Specification

Alias: none

Argument(s): REAL

Default: 1.e-4

Description

The convergence_tolerance specification provides a real value for controlling the termination of iteration. For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by convergence_tolerance, then this convergence criterion is satisfied on the current iteration.

Therefore, permissible values are between 0 and 1, non-inclusive.

Behavior Varies by Package/Library

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- DOT: must be satisfied for two consecutive iterations
- NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of convergence_tolerance approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., convergence_tolerance = 1.e-6 will result in approximately six digits of accuracy in the final objective function).
- NL2SOL: See nl2sol

max_function_evaluations

- Keywords Area
- method
- nlpl_sqp
- max_function_evaluations

Number of function evaluations allowed for optimizers

Topics

This keyword is related to the topics:

- method_independent_controls
CHAPTER 6. KEYWORDS AREA

**Specification**

Alias: none

- **Argument(s):** INTEGER
  - **Default:** 1000

**Description**

The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed \( \text{max\_function\_evaluations} \)
evaluations. See also \( \text{max\_iterations} \).

**Default Behavior**

Default value is 1000.

**scaling**

- Keywords Area
- method
- nlpql_sqp
- scaling

Turn on scaling for variables, responses, and constraints

**Topics**

This keyword is related to the topics:

- method\_independent\_controls

**Specification**

Alias: none

- **Argument(s):** none
  - **Default:** no scaling

**Description**

Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by by providing the \text{scaling} keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the method, variables, and responses blocks. When the \text{scaling} keyword is omitted, all \_scale\_types and *\_scales specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.
6.2. METHOD

- a *scales keyword, which gives characteristic values
- a *scale_type keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

**Scale Types**

There are four scale types:

1. **none** (default) - no scaling, value of *scales keyword is ignored
2. **value** - multiplicative scaling
3. **auto** - automatic scaling

First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:

- two-sided bounds scaled into the interval [0,1];
- one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
- no bounds or targets: no automatic scaling possible, therefore no scaling for this component

Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into [0,1].

4. **log** - logarithmic scaling

First, any characteristic values from the optional *scales specification are applied. Then logarithm base 10 scaling is applied.

Logarithmic scaling is not available for linear constraints.

When continuous design variables are log scaled, linear constraints are not allowed.

**Scales**

The *scales keywords are used to specify the characteristic values. These must be non-zero real numbers. The numbers are used according to the corresponding *scale_type, as described above. Depending on the scale type, the characteristic values may be required or optional.

- none, auto, log - optional
- value - required

A warning is issued if scaling would result in division by a value smaller in magnitude than 1.0e10*DBL_MIN. User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.
Examples

The two examples below are equivalent:

```
responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value"
  primary_scales = 1 1 100
```

```
responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value" "value" "value"
  primary_scales = 1 1 100
```

**model_pointer**

- **Keywords Area**
- **method**
- **nlpql_sqp**
- **model_pointer**

Identifier for model block to be used by a method

Topics

This keyword is related to the topics:

- **block_pointer**

Specification

**Alias:** none

**Argument(s):** STRING

**Default:** method use of last model parsed (or use of default model if none parsed)

Description

The `model_pointer` is used to specify which `model` block will be used to perform the function evaluations needed by the Dakota method.

**Default Behavior**

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a `model` block in the Dakota input file that has a corresponding `id_model` with the same name.

**Usage Tips**

When doing advanced analyses that involve using multiple methods and multiple models, defining a `model_pointer` for each method is imperative. See `block_pointer` for details about pointers.
6.2. METHOD

Examples

environment
tabular_graphics_data
method_pointer = 'UQ'

method
id_method = 'UQ'
model_pointer = 'Surr'
sampling,
samples = 10
seed = 98765 rng rnum2
response_levels = 0.1 0.2 0.6
0.1 0.2 0.6
0.1 0.2 0.6
sample_type lhs
distribution cumulative

model
id_model = 'Surr'
surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
id_method = 'DACE'
model_pointer = 'DACE_M'
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = 'DACE_M'
single
interface_pointer = 'I1'

variables
uniform_uncertain = 2
lower_bounds = 0. 0.
upper_bounds = 1. 1.
descriptors = 'x1' 'x2'

interface
id_interface = 'I1'
system asynch evaluation_concurrency = 5
analysis_driver = 'text_book'

responses
response_functions = 3
no_gradients
no_hessians

6.2.24 optpp_cg

- Keywords Area

- method

- optpp_cg

A conjugate gradient optimization method
### Topics
This keyword is related to the topics:

- package_optpp
- local_optimization_methods

### Specification

**Alias:** none
**Argument(s):** none

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<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
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<tbody>
<tr>
<td>Optional</td>
<td>max_step</td>
<td>max_step</td>
<td>Max change in design point</td>
</tr>
<tr>
<td>Optional</td>
<td>gradient_tolerance</td>
<td>gradient_tolerance</td>
<td>Stopping criteria based on L2 norm of gradient</td>
</tr>
<tr>
<td>Optional</td>
<td>max_iterations</td>
<td>max_iterations</td>
<td>Number of iterations allowed for optimizers and adaptive UQ methods</td>
</tr>
<tr>
<td>Optional</td>
<td>convergence_-tolerance</td>
<td>convergence_-tolerance</td>
<td>Stopping criterion based on convergence of the objective function or statistics</td>
</tr>
<tr>
<td>Optional</td>
<td>speculative</td>
<td>speculative</td>
<td>Compute speculative gradients</td>
</tr>
<tr>
<td>Optional</td>
<td>max_function_-evaluations</td>
<td>max_function_-evaluations</td>
<td>Number of function evaluations allowed for optimizers</td>
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6.2. METHOD

<table>
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<th>Optional</th>
<th>scaling</th>
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</thead>
<tbody>
<tr>
<td>Optional</td>
<td>model_pointer</td>
</tr>
<tr>
<td></td>
<td>Turn on scaling for variables, responses, and constraints</td>
</tr>
<tr>
<td></td>
<td>Identifier for model block to be used by a method</td>
</tr>
</tbody>
</table>

### Description

The conjugate gradient method is an implementation of the Polak-Ribiere approach and handles only unconstrained problems.

See package_optpp for info related to all optpp methods.

### See Also

These keywords may also be of interest:

- optpp_g_newton
- optpp_pds
- optpp_fd_newton
- optpp_newton
- optpp_g_newton

**max_step**

- Keywords Area
- method
- optpp_cg
- max_step

Max change in design point

### Specification

**Alias:** none

**Argument(s):** REAL

**Default:** 1000.

### Description

The `max_step` control specifies the maximum step that can be taken when computing a change in the current design point (e.g., limiting the Newton step computed from current gradient and Hessian information). It is equivalent to a move limit or a maximum trust region size. The `gradient_tolerance` control defines the threshold value on the L2 norm of the objective function gradient that indicates convergence to an unconstrained minimum (no active constraints). The `gradient_tolerance` control is defined for all gradient-based optimizers.
**gradient_tolerance**

- Keywords Area
- method
- optpp_cg
- gradient_tolerance

Stopping criteria based on L2 norm of gradient

**Specification**

**Alias:** none

**Argument(s):** REAL

**Default:** 1.e-4

**Description**

The *gradient_tolerance* control defines the threshold value on the L2 norm of the objective function gradient that indicates convergence to an unconstrained minimum (no active constraints). The *gradient_tolerance* control is defined for all gradient-based optimizers.

**max_iterations**

- Keywords Area
- method
- optpp_cg
- max_iterations

Number of iterations allowed for optimizers and adaptive UQ methods

**Topics**

This keyword is related to the topics:

- method_independent_controls

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** 100 (exceptions: fsu_cvt, local_reliability: 25; global{reliability, interval_est, evidence} / efficient_global: 25*n)
6.2. METHOD

Description

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed \textit{max.\_iterations} iterations. See also \textit{max.\_function\_evaluations}.

Default Behavior

Default value is 100.

\textbf{convergence\_tolerance}

- Keywords Area
- \textit{method}
- \textit{optpp\_cg}
- \textit{convergence\_tolerance}

Stopping criterion based on convergence of the objective function or statistics

Topics

This keyword is related to the topics:

- \textit{method\_independent\_controls}

Specification

Alias: none

\begin{itemize}
  \item \textit{Argument(s):} REAL
  \item \textit{Default:} 1.e-4
\end{itemize}

Description

The \textit{convergence\_tolerance} specification provides a real value for controlling the termination of iteration. For optimization, it is most commonly a \textit{relative convergence tolerance} for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by \textit{convergence\_tolerance}, then this convergence criterion is satisfied on the current iteration.

Therefore, permissible values are between 0 and 1, non-inclusive.

Behavior Varies by Package/Library

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- DOT: must be satisfied for two consecutive iterations
• NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of convergence_tolerance approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., convergence_tolerance = 1.e-6 will result in approximately six digits of accuracy in the final objective function).

• NL2SOL: See nl2sol

speculative

• Keywords Area
  • method
  • optpp_cg
  • speculative

Compute speculative gradients

Topics

This keyword is related to the topics:

• methodIndependent_controls

Specification

Alias: none
  Argument(s): none
  Default: no speculation

Description

When performing gradient-based optimization in parallel, speculative gradients can be selected to address the load imbalance that can occur between gradient evaluation and line search phases. In a typical gradient-based optimization, the line search phase consists primarily of evaluating the objective function and any constraints at a trial point, and then testing the trial point for a sufficient decrease in the objective function value and/or constraint violation. If a sufficient decrease is not observed, then one or more additional trial points may be attempted sequentially. However, if the trial point is accepted then the line search phase is complete and the gradient evaluation phase begins. By speculating that the gradient information associated with a given line search trial point will be used later, additional coarse grained parallelism can be introduced by computing the gradient information (either by finite difference or analytically) in parallel, at the same time as the line search phase trial-point function values. This balances the total amount of computation to be performed at each design point and allows for efficient utilization of multiple processors. While the total amount of work performed will generally increase (since some speculative gradients will not be used when a trial point is rejected in the line search phase), the run time will usually decrease (since gradient evaluations needed at the start of each new optimization cycle were already performed in parallel during the line search phase). Refer to [14] for additional details. The speculative specification is implemented for the gradient-based optimizers in the DOT, CONMIN, and OPT++ libraries, and it can be used with dakota numerical or analytic gradient selections in the responses specification (refer to responses gradient section for information on these specifications). It should not be selected with vendor numerical gradients since vendor internal finite difference algorithms have not been modified for this purpose.
In full-Newton approaches, the Hessian is also computed speculatively. NPSOL and NLSSOL do not support speculative gradients, as their gradient-based line search in user-supplied gradient mode (dakota numerical or analytic gradients) is a superior approach for load-balanced parallel execution.

The speculative specification enables speculative computation of gradient and/or Hessian information, where applicable, for parallel optimization studies. By speculating that the derivative information at the current point will be used later, the complete data set (all available gradient/Hessian information) can be computed on every function evaluation. While some of these computations will be wasted, the positive effects are a consistent parallel load balance and usually shorter wall clock time. The speculative specification is applicable only when parallelism in the gradient calculations can be exploited by Dakota (it will be ignored for vendor numerical gradients).

**max_function_evaluations**

- **Keywords Area**
- **method**
- **optpp.cg**
- **max_function_evaluations**

Number of function evaluations allowed for optimizers

**Topics**

This keyword is related to the topics:

- **method_independent_controls**

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** 1000

**Description**

The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed **max_function_evaluations** evaluations. See also **max_iterations**.

**Default Behavior**

Default value is 1000.

**scaling**

- **Keywords Area**
- **method**
- **optpp.cg**
- **scaling**

Turn on scaling for variables, responses, and constraints
Topics

This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none
Argument(s): none
Default: no scaling

Description

Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by by providing the scaling keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the method, variables, and responses blocks. When the scaling keyword is omitted, all .scale_type and *_scales specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.

- a *scales keyword, which gives characteristic values
- a *scale_type keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

Scale Types

There are four scale types:

1. none (default) - no scaling, value of *scales keyword is ignored
2. value - multiplicative scaling
3. auto - automatic scaling

First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:

- two-sided bounds scaled into the interval [0,1];
- one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
- no bounds or targets: no automatic scaling possible, therefore no scaling for this component

Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into [0,1].
4. \textit{log} - logarithmic scaling

First, any characteristic values from the optional *scales specification are applied. Then logarithm base 10 scaling is applied.

Logarithmic scaling is not available for linear constraints.

When continuous design variables are log scaled, linear constraints are not allowed.

\textbf{Scales}

The *scales keywords are used to specify the characteristic values. These must be non-zero real numbers. The numbers are used according to the corresponding *scale_type, as described above. Depending on the scale type, the characteristic values may be required or optional.

- none, auto, log - optional
- value - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than $1.0 \times 10^{10} \times \text{DBL_MIN}$. User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.

\textbf{Examples}

The two examples below are equivalent:

```
responses
 objective_functions 3
  sense "maximize"
  primary_scale_types = "value"
  primary_scales = 1 1 100

responses
 objective_functions 3
  sense "maximize"
  primary_scale_types = "value" "value" "value"
  primary_scales = 1 1 100
```

\textbf{model_pointer}

- Keywords Area
- method
- optpp_cg
- model_pointer

Identifier for model block to be used by a method

\textbf{Topics}

This keyword is related to the topics:

- block_pointer
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)

Description

The `model_pointer` is used to specify which `model` block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a `model` block in the Dakota input file that has a corresponding `id_model` with the same name.

Usage Tips

When doing advanced analyses that involve using multiple methods and multiple models, defining a `model_pointer` for each method is imperative.

See `block_pointer` for details about pointers.

Examples

```dakota
environment
tabular_graphics_data
method_pointer = 'UQ'

method
id_method = 'UQ'
model_pointer = 'SURR'
sampling,
samples = 10
seed = 98765 rng rnum2
response_levels = 0.1 0.2 0.6
0.1 0.2 0.6
0.1 0.2 0.6
sample_type lhs
distribution cumulative

model
id_model = 'SURR'
surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
id_method = 'DACE'
model_pointer = 'DACE_M'
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = 'DACE_M'
single
interface_pointer = 'I1'

variables
uniform_uncertain = 2
lower_bounds = 0. 0.
upper_bounds = 1. 1.
descriptors = 'x1' 'x2'
```
6.2. METHOD

interface
  id_interface = 'I1'
system async evaluation_concurrency = 5
  analysis_driver = 'text_book'

responses
  response_functions = 3
  no_gradients
  no_hessians

6.2.25 optpp_q_newton

- Keywords Area
  - method
  - optpp_q_newton

  Quasi-Newton optimization method

Topics

This keyword is related to the topics:

- package_optpp
- local_optimization_methods

Specification

Alias: none
  Argument(s): none

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Optional</td>
<td>search_method</td>
<td></td>
<td>Select a search method for Newton-based optimizers</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>merit_function</td>
<td></td>
<td>Balance goals of reducing objective function and satisfying constraints</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>steplength_to_boundary</td>
<td></td>
<td>Controls how close to the boundary of the feasible region the algorithm is allowed to move</td>
</tr>
</tbody>
</table>
### Description

This is a Newton method that expects a gradient and computes a low-rank approximation to the Hessian. Each of the Newton-based methods are automatically bound to the appropriate OPT++ algorithm based on the user constraint specification (unconstrained, bound-constrained, or generally-constrained). In the generally-constrained case, the Newton methods use a nonlinear interior-point approach to manage the constraints.

See package\_optpp for info related to all optpp methods.
6.2. METHOD

search_method

- Keywords Area
- method
- optpp_q_newton
- search_method

Select a search method for Newton-based optimizers

Specification

Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required(Choose One)</td>
<td>Group 1</td>
<td>value_based_line_search</td>
<td>Use only function values for line search</td>
</tr>
<tr>
<td>gradient_based_line_search</td>
<td></td>
<td>Set the search method to use the gradient</td>
<td></td>
</tr>
<tr>
<td>trust_region</td>
<td></td>
<td>Use trust region as the globalization strategy.</td>
<td></td>
</tr>
<tr>
<td>tr_pds</td>
<td></td>
<td>Use direct search as the local search in a trust region method</td>
<td></td>
</tr>
</tbody>
</table>

Description

The search_method control is defined for all Newton-based optimizers and is used to select between trust_region, gradient_based_line_search, and value_based_line_search methods. The gradient_based_line_search option uses the line search method proposed by[61]. This option satisfies sufficient decrease and curvature conditions; whereas, value_based_line_search only satisfies the sufficient decrease condition. At each line search iteration, the gradient_based_line_search method computes the function and gradient at the trial point. Consequently, given expensive function evaluations, the value_based_line_search method is preferred to the gradient_based_line_search method. Each of these Newton methods additionally supports the tr_pds selection for unconstrained problems. This option performs a robust trust region search using pattern search techniques. Use of a line search is the default for bound-constrained and generally-constrained problems, and use of a trust_region search method is the default for unconstrained problems.

value_based_line_search

- Keywords Area
- method
• optpp_q_newton

• search_method

• value_based_line_search

Use only function values for line search

**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** trust_region (unconstrained), value_based_line_search (bound/general constraints)

**Description**

The `search_method` control is defined for all Newton-based optimizers and is used to select between trust-region, gradient_based_line_search, and value_based_line_search methods. The gradient_based_line_search option uses the line search method proposed by[61]. This option satisfies sufficient decrease and curvature conditions; whereas, value_based_line_search only satisfies the sufficient decrease condition. At each line search iteration, the gradient_based_line_search method computes the function and gradient at the trial point. Consequently, given expensive function evaluations, the value_based_line_search method is preferred to the gradient_based_line_search method. Each of these Newton methods additionally supports the tr_pds selection for unconstrained problems. This option performs a robust trust region search using pattern search techniques. Use of a line search is the default for bound-constrained and generally-constrained problems, and use of a trust_region search method is the default for unconstrained problems.

**gradient_based_line_search**

• Keywords Area

• method

• optpp_q_newton

• search_method

• gradient_based_line_search

Set the search method to use the gradient

**Specification**

**Alias:** none  
**Argument(s):** none
6.2. METHOD

Description

The search_method control is defined for all Newton-based optimizers and is used to select between trust_region, gradient_based_line_search, and value_based_line_search methods. The gradient_based_line_search option uses the line search method proposed by[61]. This option satisfies sufficient decrease and curvature conditions; whereas, value_base_line_search only satisfies the sufficient decrease condition. At each line search iteration, the gradient_based_line_search method computes the function and gradient at the trial point. Consequently, given expensive function evaluations, the value_based_line_search method is preferred to the gradient_based_line_search method. Each of these Newton methods additionally supports the tr_pds selection for unconstrained problems. This option performs a robust trust region search using pattern search techniques. Use of a line search is the default for bound-constrained and generally-constrained problems, and use of a trust_region search method is the default for unconstrained problems.

trust_region

- Keywords Area
- method
- optpp_q_newton
- search_method
- trust_region

Use trust region as the globalization strategy.

Specification

Alias: none
Argument(s): none

Description

The trust_region optional group specification can be used to specify the initial size of the trust region (using initial_size) relative to the total variable bounds, the minimum size of the trust region (using minimum_size), the contraction factor for the trust region size (using contraction_factor) used when the surrogate model is performing poorly, and the expansion factor for the trust region size (using expansion_factor) used when the surrogate model is performing well. Two additional commands are the trust region size contraction threshold (using contract_threshold) and the trust region size expansion threshold (using expand_threshold). These two commands are related to what is called the trust region ratio, which is the actual decrease in the truth model divided by the predicted decrease in the truth model in the current trust region. The command contract_threshold sets the minimum acceptable value for the trust region ratio, i.e., values below this threshold cause the trust region to shrink for the next SBL iteration. The command expand_threshold determines the trust region value above which the trust region will expand for the next SBL iteration.

tr_pds

- Keywords Area
- method
• optpp_q_newton
• search_method
• tr_pds

Use direct search as the local search in a trust region method

Specification

Alias: none
Argument(s): none

Description

The search_method control is defined for all Newton-based optimizers and is used to select between trust_region, gradient_based_line_search, and value_based_line_search methods. The gradient_based_line_search option uses the line search method proposed by[61]. This option satisfies sufficient decrease and curvature conditions; whereas, value_base_line_search only satisfies the sufficient decrease condition. At each line search iteration, the gradient_based_line_search method computes the function and gradient at the trial point. Consequently, given expensive function evaluations, the value_based_line_search method is preferred to the gradient_based_line_search method. Each of these Newton methods additionally supports the tr_pds selection for unconstrained problems. This option performs a robust trust region search using pattern search techniques. Use of a line search is the default for bound-constrained and generally-constrained problems, and use of a trust_region search method is the default for unconstrained problems.

merit_function

• Keywords Area
• method
• optpp_q_newton
• merit_function

Balance goals of reducing objective function and satisfying constraints

Specification

Alias: none
Argument(s): none
Default: argaez_tapia

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required (Choose One)</td>
<td>Group 1</td>
<td>el_bakry</td>
<td>El-Bakry merit function</td>
</tr>
</tbody>
</table>
Description

A merit function is a function in constrained optimization that attempts to provide joint progress toward reducing the objective function and satisfying the constraints.

el_bakry

- Keywords Area
- method
- optpp_q_newton
- merit_function
- el_bakry

El-Bakry merit function

Specification

Alias: none
Argument(s): none

Description

The "el_bakry" merit function is the L2-norm of the first order optimality conditions for the nonlinear programming problem. The cost per linesearch iteration is n+1 function evaluations. For more information, see[20].

argaez_tapia

- Keywords Area
- method
- optpp_q_newton
- merit_function
- argaez_tapia

The merit function by Tapia and Argaez

Specification

Alias: none
Argument(s): none
Description

The "argaez_tapia" merit function can be classified as a modified augmented Lagrangian function. The augmented Lagrangian is modified by adding to its penalty term a potential reduction function to handle the perturbed complementarity condition. The cost per linesearch iteration is one function evaluation. For more information, see [80].

If the function evaluation is expensive or noisy, set the merit_function to "argaez_tapia" or "van_shanno".

van_shanno

- Keywords Area
- method
- optpp_q_newton
- merit_function
- van_shanno

The merit function by Vanderbei and Shanno

Specification

Alias: none
Argument(s): none

Description

The "van_shanno" merit function can be classified as a penalty function for the logarithmic barrier formulation of the nonlinear programming problem. The cost per linesearch iteration is one function evaluation. For more information see[82].

If the function evaluation is expensive or noisy, set the merit_function to "argaez_tapia" or "van_shanno".

steplength_to_boundary

- Keywords Area
- method
- optpp_q_newton
- steplength_to_boundary

Controls how close to the boundary of the feasible region the algorithm is allowed to move

Specification

Alias: none
Argument(s): REAL
Default: Merit function dependent: 0.8 (el_bakry), 0.99995 (argaez_tapia), 0.95 (van_shanno)
6.2. METHOD

Description

The steplength_to_boundary specification is a parameter (between 0 and 1) that controls how close to the boundary of the feasible region the algorithm is allowed to move. A value of 1 means that the algorithm is allowed to take steps that may reach the boundary of the feasible region. If the user wishes to maintain strict feasibility of the design parameters this value should be less than 1. Default values are .8, .99995, and .95 for the el_bakry, argaez_tapia, and van_shanno merit functions, respectively.

centering_parameter

- Keywords Area
- method
- optpp_q_newton
- centering_parameter

Controls how closely the algorithm should follow the "central path”

Specification

Alias: none
Argument(s): REAL
Default: Merit function dependent: 0.2 (el_bakry), 0.2 (argaez_tapia), 0.1 (van_shanno)

Description

The centering_parameter specification is a parameter (between 0 and 1) that controls how closely the algorithm should follow the "central path”. See[89] for the definition of central path. The larger the value, the more closely the algorithm follows the central path, which results in small steps. A value of 0 indicates that the algorithm will take a pure Newton step. Default values are .2, .2, and .1 for the el_bakry, argaez_tapia, and van_shanno merit functions, respectively.

max_step

- Keywords Area
- method
- optpp_q_newton
- max_step

Max change in design point

Specification

Alias: none
Argument(s): REAL
Default: 1000.
CHAPTER 6. KEYWORDS AREA

Description

The `max_step` control specifies the maximum step that can be taken when computing a change in the current design point (e.g., limiting the Newton step computed from current gradient and Hessian information). It is equivalent to a move limit or a maximum trust region size. The `gradient_tolerance` control defines the threshold value on the L2 norm of the objective function gradient that indicates convergence to an unconstrained minimum (no active constraints). The `gradient_tolerance` control is defined for all gradient-based optimizers.

`gradient_tolerance`

- Keywords Area
- method
- `optpp_q_newton`
- `gradient_tolerance`

Stopping criteria based on L2 norm of gradient

Specification

Alias: none

Argument(s): REAL

Default: 1.e-4

Description

The `gradient_tolerance` control defines the threshold value on the L2 norm of the objective function gradient that indicates convergence to an unconstrained minimum (no active constraints). The `gradient_tolerance` control is defined for all gradient-based optimizers.

`max_iterations`

- Keywords Area
- method
- `optpp_q_newton`
- `max_iterations`

Number of iterations allowed for optimizers and adaptive UQ methods

Topics

This keyword is related to the topics:

- `method_independent_controls`
6.2. METHOD

Specification

Alias: none
Argument(s): INTEGER
Default: 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence} / efficient_globals: 25*n)

Description

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed max_iterations iterations. See also max_function_evaluations.

Default Behavior

Default value is 100.

convergence_tolerance

- Keywords Area
- method
- optpp_q_newton
- convergence_tolerance

Stopping criterion based on convergence of the objective function or statistics

Topics

This keyword is related to the topics:
- method_independent_controls

Specification

Alias: none
Argument(s): REAL
Default: 1.e-4

Description

The convergence_tolerance specification provides a real value for controlling the termination of iteration. For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by convergence_tolerance, then this convergence criterion is satisfied on the current iteration.

Therefore, permissible values are between 0 and 1, non-inclusive.

Behavior Varies by Package/Library

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.
Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- DOT: must be satisfied for two consecutive iterations
- NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of convergence_tolerance approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., convergence_tolerance = 1.e-6 will result in approximately six digits of accuracy in the final objective function).
- NL2SOL: See nl2sol

speculative

- Keywords Area
- method
- optpp_q_newton
- speculative

Compute speculative gradients

Topics

This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none

Argument(s): none

Default: no speculation

Description

When performing gradient-based optimization in parallel, speculative gradients can be selected to address the load imbalance that can occur between gradient evaluation and line search phases. In a typical gradient-based optimization, the line search phase consists primarily of evaluating the objective function and any constraints at a trial point, and then testing the trial point for a sufficient decrease in the objective function value and/or constraint violation. If a sufficient decrease is not observed, then one or more additional trial points may be attempted sequentially. However, if the trial point is accepted then the line search phase is complete and the gradient evaluation phase begins. By speculating that the gradient information associated with a given line search trial point will be used later, additional coarse grained parallelism can be introduced by computing the gradient information (either by finite difference or analytically) in parallel, at the same time as the line search phase trial-point function values. This balances the total amount of computation to be performed at each design point and allows for efficient utilization of multiple processors. While the total amount of work performed will generally increase (since some speculative gradients will not be used when a trial point is rejected in the line search phase), the run
time will usually decrease (since gradient evaluations needed at the start of each new optimization cycle were already performed in parallel during the line search phase). Refer to [14] for additional details. The speculative specification is implemented for the gradient-based optimizers in the DOT, CONMIN, and OPT++ libraries, and it can be used with dakota numerical or analytic gradient selections in the responses specification (refer to responses gradient section for information on these specifications). It should not be selected with vendor numerical gradients since vendor internal finite difference algorithms have not been modified for this purpose. In full-Newton approaches, the Hessian is also computed speculatively. NPSOL and NLSSOL do not support speculative gradients, as their gradient-based line search in user-supplied gradient mode (dakota numerical or analytic gradients) is a superior approach for load-balanced parallel execution.

The speculative specification enables speculative computation of gradient and/or Hessian information, where applicable, for parallel optimization studies. By speculating that the derivative information at the current point will be used later, the complete data set (all available gradient/Hessian information) can be computed on every function evaluation. While some of these computations will be wasted, the positive effects are a consistent parallel load balance and usually shorter wall clock time. The speculative specification is applicable only when parallelism in the gradient calculations can be exploited by Dakota (it will be ignored for vendor numerical gradients).

**max_function_evaluations**

- **Keywords Area**
- method
- optpp_q Newton
- max_function_evaluations

Number of function evaluations allowed for optimizers

**Topics**

This keyword is related to the topics:

- method.independent.controls

**Specification**

**Alias**: none

**Argument(s)**: INTEGER

**Default**: 1000

**Description**

The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed max.function_evaluations evaluations. See also max_iterations.

**Default Behavior**

Default value is 1000.
TURN ON SCALING FOR VARIABLES, RESPONSES, AND CONSTRAINTS

Topics
This keyword is related to the topics:

- method_independent_controls

Specification
Alias: none

Argument(s): none
Default: no scaling

Description
Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by providing the `scaling` keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the method, variables, and responses blocks. When the `scaling` keyword is omitted, all `scale_types` and `scales` specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.

- a `scales` keyword, which gives characteristic values
- a `scale_type` keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

Scale Types
There are four scale types:

1. `none` (default) - no scaling, value of `scales` keyword is ignored
2. `value` - multiplicative scaling
3. **auto** - automatic scaling

First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:

- two-sided bounds scaled into the interval \([0,1]\);
- one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
- no bounds or targets: no automatic scaling possible, therefore no scaling for this component

Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into \([0,1]\).

4. **log** - logarithmic scaling

First, any characteristic values from the optional \(*_scales\) specification are applied. Then logarithm base 10 scaling is applied.

Logarithmic scaling is not available for linear constraints.

When continuous design variables are log scaled, linear constraints are not allowed.

**Scales**

The \(*_scales\) keywords are used to specify the characteristic values. These must be non-zero real numbers. The numbers are used according to the corresponding \(*_scale\_type\), as described above.

Depending on the scale type, the characteristic values may be required or optional.

- **none, auto, log** - optional
- **value** - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than \(1.0e10*DBL\_MIN\). User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.

**Examples**

The two examples below are equivalent:

```plaintext
responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value"
  primary_scales = 1 1 100

responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value" "value" "value"
  primary_scales = 1 1 100
```
model_pointer

- Keywords Area
- method
- optpp.q_newton
- model_pointer

Identifier for model block to be used by a method

Topics

This keyword is related to the topics:

- block_pointer

Specification

Alias: none

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)

Description

The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.

Usage Tips

When doing advanced analyses that involve using multiple methods and multiple models, defining a model-pointer for each method is imperative.

See block_pointer for details about pointers.

Examples

```plaintext
environment
   tabular_graphics_data
   method_pointer = 'UQ'

method
   id_method = 'UQ'
   model_pointer = 'SURR'
   sampling,
      samples = 10
      seed = 98765 rng rnum2
      response_levels = 0.1 0.2 0.6
      0.1 0.2 0.6
      0.1 0.2 0.6
      sample_type lhs
      distribution cumulative

model
   id_model = 'SURR'
```
6.2. METHOD

surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
id_method = 'DACE'
model_pointer = 'DACE_M'
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = 'DACE_M'
single
interface_pointer = 'I1'

variables
uniform_uncertain = 2
lower_bounds = 0.0.
upper_bounds = 1.1.
descriptors = 'x1' 'x2'

interface
id_interface = 'I1'
system asynch evaluation_concurrency = 5
analysis_driver = 'text_book'

responses
response_functions = 3
no_gradients
no_hessians

6.2.26 optpp_fd_newton

- Keywords Area
- method
- optpp_fd_newton

Finite Difference Newton optimization method

Topics
This keyword is related to the topics:
- package_optpp
- local_optimization_methods

Specification
Alias: none

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>search_method</td>
<td>Select a search method for Newton-based optimizers</td>
<td></td>
</tr>
<tr>
<td>----------</td>
<td>---------------</td>
<td>--------------------------------------------------</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>merit_function</td>
<td>Balance goals of reducing objective function and satisfying constraints</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>steplength_to_boundary</td>
<td>Controls how close to the boundary of the feasible region the algorithm is allowed to move</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>centering_parameter</td>
<td>Controls how closely the algorithm should follow the &quot;central path&quot;</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>max_step</td>
<td>Max change in design point</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>gradient_tolerance</td>
<td>Stopping criteria based on L2 norm of gradient</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>max_iterations</td>
<td>Number of iterations allowed for optimizers and adaptive UQ methods</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>convergence_tolerance</td>
<td>Stopping criterion based on convergence of the objective function or statistics</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>speculative</td>
<td>Compute speculative gradients</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>max_function_evaluations</td>
<td>Number of function evaluations allowed for optimizers</td>
<td></td>
</tr>
</tbody>
</table>
6.2. METHOD

<table>
<thead>
<tr>
<th>Optional</th>
<th>scaling</th>
<th>Turn on scaling for variables, responses, and constraints</th>
</tr>
</thead>
<tbody>
<tr>
<td>model_point</td>
<td>model_pointer</td>
<td>Identifier for model block to be used by a method</td>
</tr>
</tbody>
</table>

**Description**

This is a Newton method that expects a gradient and computes a finite-difference approximation to the Hessian. Each of the Newton-based methods are automatically bound to the appropriate OPT++ algorithm based on the user constraint specification (unconstrained, bound-constrained, or generally-constrained). In the generally-constrained case, the Newton methods use a nonlinear interior-point approach to manage the constraints.

See package_optpp for info related to all optpp methods.

**See Also**

These keywords may also be of interest:

- optpp_cg
- optpp_g_newton
- optpp_pds
- optpp_newton
- optpp_g_newton

**search_method**

- Keywords Area
- method
- optpp_fd_newton
- search_method

Select a search method for Newton-based optimizers

**Specification**

**Alias:** none

**Argument(s):** none
CHAPTER 6. KEYWORDS AREA

### Description

The `search_method` control is defined for all Newton-based optimizers and is used to select between `trust_region`, `gradient_based_line_search`, and `value_based_line_search` methods. The `gradient_based_line_search` option uses the line search method proposed by[61]. This option satisfies sufficient decrease and curvature conditions; whereas, `value_based_line_search` only satisfies the sufficient decrease condition. At each line search iteration, the `gradient_based_line_search` method computes the function and gradient at the trial point. Consequently, given expensive function evaluations, the `value_based_line_search` method is preferred to the `gradient_based_line_search` method. Each of these Newton methods additionally supports the `tr_pds` selection for unconstrained problems. This option performs a robust trust region search using pattern search techniques. Use of a line search is the default for bound-constrained and generally-constrained problems, and use of a `trust_region` search method is the default for unconstrained problems.

### value_based_line_search

- **Keywords Area**
- **method**
- **optpp_fd_newton**
- **search_method**
- **value_based_line_search**

Use only function values for line search

### Specification

**Alias:** none

**Argument(s):** none

**Default:** `trust_region` (unconstrained), `value_based_line_search` (bound/general constraints)
6.2. METHOD

Description

The search method control is defined for all Newton-based optimizers and is used to select between trust-region, gradient-based line search, and value-based line search methods. The gradient-based line_search option uses the line search method proposed by[61]. This option satisfies sufficient decrease and curvature conditions; whereas, value-based line_search only satisfies the sufficient decrease condition. At each line search iteration, the gradient_based_line_search method computes the function and gradient at the trial point. Consequently, given expensive function evaluations, the value_based_line_search method is preferred to the gradient_based_line_search method. Each of these Newton methods additionally supports the tr_pds selection for unconstrained problems. This option performs a robust trust region search using pattern search techniques. Use of a line search is the default for bound-constrained and generally-constrained problems, and use of a trust_region search method is the default for unconstrained problems.

gradient_based_line_search

- Keywords Area
- method
- optpp_Jd_newton
- search_method
- gradient_based_line_search

Set the search method to use the gradient

Specification

Alias: none

Argument(s): none

Description

The search method control is defined for all Newton-based optimizers and is used to select between trust-region, gradient-based line_search, and value-based line_search methods. The gradient-based line_search option uses the line search method proposed by[61]. This option satisfies sufficient decrease and curvature conditions; whereas, value_based_line_search only satisfies the sufficient decrease condition. At each line search iteration, the gradient_based_line_search method computes the function and gradient at the trial point. Consequently, given expensive function evaluations, the value_based_line_search method is preferred to the gradient_based_line_search method. Each of these Newton methods additionally supports the tr_pds selection for unconstrained problems. This option performs a robust trust region search using pattern search techniques. Use of a line search is the default for bound-constrained and generally-constrained problems, and use of a trust_region search method is the default for unconstrained problems.

trust_region

- Keywords Area
- method
Use trust region as the globalization strategy.

**Specification**

**Alias:** none  
**Argument(s):** none

**Description**

The `trust_region` optional group specification can be used to specify the initial size of the trust region (using `initial_size`) relative to the total variable bounds, the minimum size of the trust region (using `minimum_size`), the contraction factor for the trust region size (using `contraction_factor`) used when the surrogate model is performing poorly, and the expansion factor for the trust region size (using `expansion_factor`) used when the surrogate model is performing well. Two additional commands are the trust region size contraction threshold (using `contract_threshold`) and the trust region size expansion threshold (using `expand_threshold`). These two commands are related to what is called the trust region ratio, which is the actual decrease in the truth model divided by the predicted decrease in the truth model in the current trust region. The command `contract_threshold` sets the minimum acceptable value for the trust region ratio, i.e., values below this threshold cause the trust region to shrink for the next SBL iteration. The command `expand_threshold` determines the trust region value above which the trust region will expand for the next SBL iteration.

**tr_pds**

- Keywords Area
- method
- `optpp_fd_newton`
- `search_method`
- `tr_pds`

Use direct search as the local search in a trust region method

**Specification**

**Alias:** none  
**Argument(s):** none

**Description**

The `search_method` control is defined for all Newton-based optimizers and is used to select between `trust_region`, `gradient_based_line_search`, and `value_based_line_search` methods. The `gradient_based_line_search` option uses the line search method proposed by[61]. This option satisfies sufficient decrease and curvature conditions; whereas, `value_based_line_search` only satisfies the sufficient decrease condition. At each line search iteration, the `gradient_based_line_search` method computes the function
and gradient at the trial point. Consequently, given expensive function evaluations, the value_based_line_search method is preferred to the gradient_based_line_search method. Each of these Newton methods additionally supports the tr_pds selection for unconstrained problems. This option performs a robust trust region search using pattern search techniques. Use of a line search is the default for bound-constrained and generally-constrained problems, and use of a trust_region search method is the default for unconstrained problems.

**merit_function**

- **Keywords Area**
- **method**
- **optpp_fd_newton**
- **merit_function**

Balance goals of reducing objective function and satisfying constraints

**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** argaez_tapia

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword</th>
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<td>Optional</td>
<td>Group</td>
<td>Group 1</td>
<td>Description</td>
</tr>
<tr>
<td>Required (Choose One)</td>
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<td></td>
</tr>
<tr>
<td>argaez_tapia</td>
<td>The merit function by Tapia and Argaez</td>
<td></td>
<td></td>
</tr>
<tr>
<td>van_shanno</td>
<td>The merit function by Vanderbei and Shanno</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Description**

A merit_function is a function in constrained optimization that attempts to provide joint progress toward reducing the objective function and satisfying the constraints.

**el_bakry**

- **Keywords Area**
- **method**
- **optpp_fd_newton**
- **merit_function**
- **el_bakry**

El-Bakry merit function
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): none

Description

The "el_bakry" merit function is the L2-norm of the first order optimality conditions for the nonlinear programming problem. The cost per linesearch iteration is \( n+1 \) function evaluations. For more information, see\([20]\).

argaez_tapia

- Keywords Area
- method
- optpp_fd_newton
- merit_function
- argaez_tapia

The merit function by Tapia and Argaez

Specification

Alias: none

Argument(s): none

Description

The "argaez_tapia" merit function can be classified as a modified augmented Lagrangian function. The augmented Lagrangian is modified by adding to its penalty term a potential reduction function to handle the perturbed complementarity condition. The cost per linesearch iteration is one function evaluation. For more information, see\([80]\).

If the function evaluation is expensive or noisy, set the merit_function to "argaez_tapia" or "van_shanno".

van_shanno

- Keywords Area
- method
- optpp_fd_newton
- merit_function
- van_shanno

The merit function by Vanderbei and Shanno
6.2. METHOD

Specification

Alias: none
  Argument(s): none

Description

The "van_shanno" merit function can be classified as a penalty function for the logarithmic barrier formulation
of the nonlinear programming problem. The cost per linesearch iteration is one function evaluation. For more
information see[82].

If the function evaluation is expensive or noisy, set the merit.function to "argaez_tapia" or "van_shanno".

steplength_to_boundary

- Keywords Area
- method
- optpp_fd_newton
- steplength_to_boundary

Controls how close to the boundary of the feasible region the algorithm is allowed to move

Specification

Alias: none
  Argument(s): REAL
  Default: Merit function dependent: 0.8 (el_bakry), 0.99995 (argaez_tapia), 0.95 (van_shanno)

Description

The steplength_to_boundary specification is a parameter (between 0 and 1) that controls how close to the
boundary of the feasible region the algorithm is allowed to move. A value of 1 means that the algorithm is allowed
to take steps that may reach the boundary of the feasible region. If the user wishes to maintain strict feasibility of
the design parameters this value should be less than 1. Default values are .8, .99995, and .95 for the el_bakry,
argaez_tapia, and van_shanno merit functions, respectively.

centering_parameter

- Keywords Area
- method
- optpp_fd_newton
- centering_parameter

Controls how closely the algorithm should follow the "central path"
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): REAL

Default: Merit function dependent: 0.2 (el_bakry), 0.2 (argaez_tapia), 0.1 (van_shanno)

Description

The **centering parameter** specification is a parameter (between 0 and 1) that controls how closely the algorithm should follow the "central path". See[89] for the definition of central path. The larger the value, the more closely the algorithm follows the central path, which results in small steps. A value of 0 indicates that the algorithm will take a pure Newton step. Default values are .2, .2, and .1 for the el_bakry, argaez_tapia, and van_shanno merit functions, respectively.

**max_step**

- Keywords Area
- method
- optpp_fd_newton
- max_step

Max change in design point

Specification

Alias: none

Argument(s): REAL

Default: 1000.

Description

The **max_step** control specifies the maximum step that can be taken when computing a change in the current design point (e.g., limiting the Newton step computed from current gradient and Hessian information). It is equivalent to a move limit or a maximum trust region size. The **gradient_tolerance** control defines the threshold value on the L2 norm of the objective function gradient that indicates convergence to an unconstrained minimum (no active constraints). The **gradient_tolerance** control is defined for all gradient-based optimizers.

**gradient_tolerance**

- Keywords Area
- method
- optpp_fd_newton
- gradient_tolerance

Stopping criteria based on L2 norm of gradient
6.2. METHOD

Specification

Alias: none
Argument(s): REAL
Default: 1.e-4

Description

The *gradient_tolerance* control defines the threshold value on the L2 norm of the objective function gradient that indicates convergence to an unconstrained minimum (no active constraints). The *gradient_tolerance* control is defined for all gradient-based optimizers.

**max_iterations**

- **Keywords Area**
- method
- optpp_fd_newton
- max_iterations

Number of iterations allowed for optimizers and adaptive UQ methods

Topics

This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none
Argument(s): INTEGER
Default: 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence} / efficient-global: 25*n)

Description

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed \texttt{max_iterations} iterations. See also \texttt{max_function_evaluations}.

Default Behavior

Default value is 100.

**convergence_tolerance**

- **Keywords Area**
- method
- optpp_fd_newton
- convergence_tolerance

Stopping criterion based on convergence of the objective function or statistics
CHAPTER 6. KEYWORDS AREA

Topics

This keyword is related to the topics:

- method
- independent_controls

Specification

Alias: none
Argument(s): REAL
Default: 1.e-4

Description

The convergence_tolerance specification provides a real value for controlling the termination of iteration. For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by convergence_tolerance, then this convergence criterion is satisfied on the current iteration.

Therefore, permissible values are between 0 and 1, non-inclusive.

Behavior Varies by Package/Library

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- DOT: must be satisfied for two consecutive iterations
- NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of convergence_tolerance approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., convergence_tolerance = 1.e-6 will result in approximately six digits of accuracy in the final objective function).
- NL2SOL: See nl2sol

speculative

- Keywords Area
- method
- optpp_fd_newton
- speculative

Compute speculative gradients
6.2. METHOD

Topics
This keyword is related to the topics:

- method
- independent_controls

Specification
Alias: none

Argument(s): none

Default: no speculation

Description
When performing gradient-based optimization in parallel, speculative gradients can be selected to address the load imbalance that can occur between gradient evaluation and line search phases. In a typical gradient-based optimization, the line search phase consists primarily of evaluating the objective function and any constraints at a trial point, and then testing the trial point for a sufficient decrease in the objective function value and/or constraint violation. If a sufficient decrease is not observed, then one or more additional trial points may be attempted sequentially. However, if the trial point is accepted then the line search phase is complete and the gradient evaluation phase begins. By speculating that the gradient information associated with a given line search trial point will be used later, additional coarse grained parallelism can be introduced by computing the gradient information (either by finite difference or analytically) in parallel, at the same time as the line search phase trial-point function values. This balances the total amount of computation to be performed at each design point and allows for efficient utilization of multiple processors. While the total amount of work performed will generally increase (since some speculative gradients will not be used when a trial point is rejected in the line search phase), the run time will usually decrease (since gradient evaluations needed at the start of each new optimization cycle were already performed in parallel during the line search phase). Refer to [14] for additional details. The speculative specification is implemented for the gradient-based optimizers in the DOT, CONMIN, and OPT++ libraries, and it can be used with dakota numerical or analytic gradient selections in the responses specification (refer to responses gradient section for information on these specifications). It should not be selected with vendor numerical gradients since vendor internal finite difference algorithms have not been modified for this purpose.

In full-Newton approaches, the Hessian is also computed speculatively. NPSOL and NLSSOL do not support speculative gradients, as their gradient-based line search in user-supplied gradient mode (dakota numerical or analytic gradients) is a superior approach for load-balanced parallel execution.

The speculative specification enables speculative computation of gradient and/or Hessian information, where applicable, for parallel optimization studies. By speculating that the derivative information at the current point will be used later, the complete data set (all available gradient/Hessian information) can be computed on every function evaluation. While some of these computations will be wasted, the positive effects are a consistent parallel load balance and usually shorter wall clock time. The speculative specification is applicable only when parallelism in the gradient calculations can be exploited by Dakota (it will be ignored for vendor numerical gradients).

max_function_evaluations

- Keywords Area
- method
- optpp_fd_newton
- max_function_evaluations
CHAPTER 6. KEYSWORD AREA

Number of function evaluations allowed for optimizers

Topics
This keyword is related to the topics:

• method_independent_controls

Specification
Alias: none
Argument(s): INTEGER
Default: 1000

Description
The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed \texttt{max\_function\_evaluations} evaluations. See also \texttt{max\_iterations}.

Default Behavior
Default value is 1000.

scaling

• Keywords Area

• method

• optpp\_fd\_newton

• scaling

Turn on scaling for variables, responses, and constraints

Topics
This keyword is related to the topics:

• method_independent_controls

Specification
Alias: none
Argument(s): none
Default: no scaling
6.2. METHOD

Description

Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by providing the scaling keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the method, variables, and responses blocks. When the scaling keyword is omitted, all _scale_types and *scales specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.

- a *scales keyword, which gives characteristic values
- a *scale_type keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

Scale Types

There are four scale types:

1. none (default) - no scaling, value of *scales keyword is ignored
2. value - multiplicative scaling
3. auto - automatic scaling
4. log - logarithmic scaling

First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:

- two-sided bounds scaled into the interval [0,1];
- one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
- no bounds or targets: no automatic scaling possible, therefore no scaling for this component

Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into [0,1].

4. log - logarithmic scaling

First, any characteristic values from the optional _scales specification are applied. Then logarithm base 10 scaling is applied.
Logarithmic scaling is not available for linear constraints.

When continuous design variables are log scaled, linear constraints are not allowed.

Scales

The *scales keywords are used to specify the characteristic values. These must be non-zero real numbers. The numbers are used according to the corresponding *scale_type, as described above.

Depending on the scale type, the characteristic values may be required or optional.
Keywords Area

- none, auto, log - optional
- value - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than 1.0e10*DBL_MIN. User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.

Examples

The two examples below are equivalent:

```plaintext
responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value"
  primary_scales = 1 1 100

responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value" "value" "value"
  primary_scales = 1 1 100
```

**model_pointer**

- Keywords Area
- method
- optpp_fd_newton
- model_pointer

Identifier for model block to be used by a method

Topics

This keyword is related to the topics:

- block_pointer

Specification

Alias: none

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)

Description

The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.
Usage Tips

When doing advanced analyses that involve using multiple methods and multiple models, defining a `model_pointer` for each method is imperative. See `block_pointer` for details about pointers.

Examples

```plaintext
environment
  tabular_graphics_data
  method_pointer = 'UQ'

method
  id_method = 'UQ'
  model_pointer = 'SRR'
  sampling,
    samples = 10
    seed = 98765 rng rnum2
    response_levels = 0.1 0.2 0.6
    0.1 0.2 0.6
    0.1 0.2 0.6
    sample_type lhs
distribution cumulative

model
  id_model = 'SRR'
surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
  id_method = 'DACE'
  model_pointer = 'DACE_M'
  sampling sample_type lhs
  samples = 121 seed = 5034 rng rnum2

model
  id_model = 'DACE_M'
single
  interface_pointer = 'I1'

variables
  uniform_uncertain = 2
  lower_bounds = 0.0
  upper_bounds = 1.0
  descriptors = 'x1' 'x2'

interface
  id_interface = 'I1'
system async evaluation_concurrency = 5
  analysis_driver = 'text_book'

responses
  response_functions = 3
  no_gradients
  no_hessians
```

6.2.27 optpp.g_newton

- Keywords Area
• method
• optpp.g_newton

Newton method based least-squares calibration

Topics
This keyword is related to the topics:

• package_optpp
• local_optimization_methods

Specification

Alias: none

Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional Group</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>search_method</td>
<td></td>
<td>Select a search method for Newton-based optimizers</td>
</tr>
<tr>
<td>Optional</td>
<td>merit_function</td>
<td></td>
<td>Balance goals of reducing objective function and satisfying constraints</td>
</tr>
<tr>
<td>Optional</td>
<td>steplength_to-boundary</td>
<td></td>
<td>Controls how close to the boundary of the feasible region the algorithm is allowed to move</td>
</tr>
<tr>
<td>Optional</td>
<td>centering-parameter</td>
<td></td>
<td>Controls how closely the algorithm should follow the “central path”</td>
</tr>
<tr>
<td>Optional</td>
<td>max_step</td>
<td></td>
<td>Max change in design point</td>
</tr>
<tr>
<td>Optional</td>
<td>gradient_tolerance</td>
<td></td>
<td>Stopping criteria based on L2 norm of gradient</td>
</tr>
</tbody>
</table>
### Description

The Gauss-Newton algorithm is available as `optpp_g.newton` and supports unconstrained, bound-constrained, and generally-constrained problems. When interfaced with the unconstrained, bound-constrained, and nonlinear interior point full-Newton optimizers from the OPT++ library, it provides a Gauss-Newton least squares capability which – on zero-residual test problems – can exhibit quadratic convergence rates near the solution. (Real problems almost never have zero residuals, i.e., perfect fits.)

See package `optpp` for info related to all `optpp` methods.

### See Also

These keywords may also be of interest:

- `optpp_cg`
- `optpp_pds`
- `optpp_fd_newton`
- `optpp_newton`
- `optpp_g_newton`

---

<table>
<thead>
<tr>
<th>Optional</th>
<th>max_iterations</th>
<th>Number of iterations allowed for optimizers and adaptive UQ methods</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>convergence_tolerance</td>
<td>Stopping criterion based on convergence of the objective function or statistics</td>
</tr>
<tr>
<td>Optional</td>
<td>speculative</td>
<td>Compute speculative gradients</td>
</tr>
<tr>
<td>Optional</td>
<td>max_function_evaluations</td>
<td>Number of function evaluations allowed for optimizers</td>
</tr>
<tr>
<td>Optional</td>
<td>scaling</td>
<td>Turn on scaling for variables, responses, and constraints</td>
</tr>
<tr>
<td>Optional</td>
<td>model_pointer</td>
<td>Identifier for model block to be used by a method</td>
</tr>
</tbody>
</table>
• field_calibration_terms

search_method

• Keywords Area

• method

• optpp_g_newton

• search_method

Select a search method for Newton-based optimizers

Specification

Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required*(Choose One)*</td>
<td>Group 1</td>
<td>value_based_line_search</td>
<td>Use only function values for line search</td>
</tr>
<tr>
<td>gradient_based_line_search</td>
<td>Set the search method to use the gradient</td>
<td></td>
<td></td>
</tr>
<tr>
<td>trust_region</td>
<td>Use trust region as the globalization strategy</td>
<td></td>
<td></td>
</tr>
<tr>
<td>tr_pds</td>
<td>Use direct search as the local search in a trust region method</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Description

The search_method control is defined for all Newton-based optimizers and is used to select between trust_region, gradient_based_line_search, and value_based_line_search methods. The gradient_based_line_search option uses the line search method proposed by[61]. This option satisfies sufficient decrease and curvature conditions; whereas, value_base_line_search only satisfies the sufficient decrease condition. At each line search iteration, the gradient_based_line_search method computes the function and gradient at the trial point. Consequently, given expensive function evaluations, the value_based_line_search method is preferred to the gradient_based_line_search method. Each of these Newton methods additionally supports the tr_pds selection for unconstrained problems. This option performs a robust trust region search using pattern search techniques. Use of a line search is the default for bound-constrained and generally-constrained problems, and use of a trust_region search method is the default for unconstrained problems.
6.2. METHOD

value_based_line_search

- Keywords Area
- method
- optpp.g_newton
- search_method
- value_based_line_search

Use only function values for line search

Specification

Alias: none
Argument(s): none
Default: trust_region (unconstrained), value_based_line_search (bound/general constraints)

Description

The search_method control is defined for all Newton-based optimizers and is used to select between trust_region, gradient_based_line_search, and value_based_line_search methods. The gradient_based_line_search option uses the line search method proposed by [61]. This option satisfies sufficient decrease and curvature conditions; whereas, value_base_line_search only satisfies the sufficient decrease condition. At each line search iteration, the gradient_based_line_search method computes the function and gradient at the trial point. Consequently, given expensive function evaluations, the value_based_line_search method is preferred to the gradient_based_line_search method. Each of these Newton methods additionally supports the tr_pds selection for unconstrained problems. This option performs a robust trust region search using pattern search techniques. Use of a line search is the default for bound-constrained and generally-constrained problems, and use of a trust_region search method is the default for unconstrained problems.

gradient_based_line_search

- Keywords Area
- method
- optpp.g_newton
- search_method
- gradient_based_line_search

Set the search method to use the gradient

Specification

Alias: none
Argument(s): none
CHAPTER 6. KEYWORDS AREA

Description

The search method control is defined for all Newton-based optimizers and is used to select between trust-region, gradient-based line search, and value-based line search methods. The gradient-based line search option uses the line search method proposed by[61]. This option satisfies sufficient decrease and curvature conditions; whereas, value-based line search only satisfies the sufficient decrease condition. At each line search iteration, the gradient-based line search method computes the function and gradient at the trial point. Consequently, given expensive function evaluations, the value-based line search method is preferred to the gradient-based line search method. Each of these Newton methods additionally supports the tr_pds selection for unconstrained problems. This option performs a robust trust region search using pattern search techniques. Use of a line search is the default for bound-constrained and generally-constrained problems, and use of a trust_region search method is the default for unconstrained problems.

trust_region

- Keywords Area
- method
- optpp_g_newton
- search_method
- trust_region

Use trust region as the globalization strategy.

Specification

Alias: none
Argument(s): none

Description

The trust_region optional group specification can be used to specify the initial size of the trust region (using initial_size) relative to the total variable bounds, the minimum size of the trust region (using minimum_size), the contraction factor for the trust region size (using contraction_factor) used when the surrogate model is performing poorly, and the expansion factor for the trust region size (using expansion_factor) used when the the surrogate model is performing well. Two additional commands are the trust region size contraction threshold (using contract_threshold) and the trust region size expansion threshold (using expand_threshold). These two commands are related to what is called the trust region ratio, which is the actual decrease in the truth model divided by the predicted decrease in the truth model in the current trust region. The command contract_threshold sets the minimum acceptable value for the trust region ratio, i.e., values below this threshold cause the trust region to shrink for the next SBL iteration. The command expand_threshold determines the trust region value above which the trust region will expand for the next SBL iteration.

tr_pds

- Keywords Area
- method
6.2. METHOD

- `optpp_g_newton`
- `search_method`
- `tr_pds`

Use direct search as the local search in a trust region method

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

The `search_method` control is defined for all Newton-based optimizers and is used to select between `trust_region`, `gradient_based_line_search`, and `value_based_line_search` methods. The `gradient_based_line_search` option uses the line search method proposed by [61]. This option satisfies sufficient decrease and curvature conditions; whereas, `value_based_line_search` only satisfies the sufficient decrease condition. At each line search iteration, the `gradient_based_line_search` method computes the function and gradient at the trial point. Consequently, given expensive function evaluations, the `value_based_line_search` method is preferred to the `gradient_based_line_search` method. Each of these Newton methods additionally supports the `tr_pds` selection for unconstrained problems. This option performs a robust trust region search using pattern search techniques. Use of a line search is the default for bound-constrained and generally-constrained problems, and use of a `trust_region` search method is the default for unconstrained problems.

**merit_function**

- **Keywords Area**
- **method**
- `optpp_g_newton`
- `merit_function`

Balance goals of reducing objective function and satisfying constraints

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** argaez_tapia

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Required (Choose One)</strong></td>
<td><strong>Group 1</strong></td>
<td><code>el_bakry</code></td>
<td>El-Bakry merit function</td>
</tr>
</tbody>
</table>
Description

A merit function is a function in constrained optimization that attempts to provide joint progress toward reducing the objective function and satisfying the constraints.

el_bakry

- Keywords Area
- method
- optpp.g.newton
- merit_function
- el_bakry

El-Bakry merit function

Specification

Alias: none
Argument(s): none

Description

The "el_bakry" merit function is the L2-norm of the first order optimality conditions for the nonlinear programming problem. The cost per linesearch iteration is n+1 function evaluations. For more information, see[20].

argaez_tapia

- Keywords Area
- method
- optpp.g.newton
- merit_function
- argaez_tapia

The merit function by Tapia and Argaez

Specification

Alias: none
Argument(s): none
6.2. METHOD

Description

The "argaez_tapia" merit function can be classified as a modified augmented Lagrangian function. The augmented Lagrangian is modified by adding to its penalty term a potential reduction function to handle the perturbed complementarity condition. The cost per linesearch iteration is one function evaluation. For more information, see [80].

If the function evaluation is expensive or noisy, set the merit function to "argaez_tapia" or "van_shanno".

van_shanno

- **Keywords Area**
- method
- optpp_g_newton
- merit_function
- van_shanno

The merit function by Vanderbei and Shanno

Specification

**Alias:** none

**Argument(s):** none

Description

The "van_shanno" merit function can be classified as a penalty function for the logarithmic barrier formulation of the nonlinear programming problem. The cost per linesearch iteration is one function evaluation. For more information see[82].

If the function evaluation is expensive or noisy, set the merit function to "argaez_tapia" or "van_shanno".

steplength_to_boundary

- **Keywords Area**
- method
- optpp_g_newton
- steplength_to_boundary

Controls how close to the boundary of the feasible region the algorithm is allowed to move

Specification

**Alias:** none

**Argument(s):** REAL

**Default:** Merit function dependent: 0.8 (el_bakry), 0.99995 (argaez_tapia), 0.95 (van_shanno)
CHAPTER 6. KEYWORDS AREA

Description

The `steplength_to_boundary` specification is a parameter (between 0 and 1) that controls how close to the boundary of the feasible region the algorithm is allowed to move. A value of 1 means that the algorithm is allowed to take steps that may reach the boundary of the feasible region. If the user wishes to maintain strict feasibility of the design parameters this value should be less than 1. Default values are .8, .99995, and .95 for the `el_bakry`, `argaez_tapia`, and `van_shanno` merit functions, respectively.

```
centering_parameter
  • Keywords Area
  • method
  • optpp_g_newton
  • centering_parameter

  Controls how closely the algorithm should follow the "central path"
```

Specification

Alias: none
Argument(s): REAL
Default: Merit function dependent: 0.2 (el_bakry), 0.2 (argaez_tapia), 0.1 (van_shanno)

Description

The `centering_parameter` specification is a parameter (between 0 and 1) that controls how closely the algorithm should follow the "central path". See[89] for the definition of central path. The larger the value, the more closely the algorithm follows the central path, which results in small steps. A value of 0 indicates that the algorithm will take a pure Newton step. Default values are .2, .2, and .1 for the `el_bakry`, `argaez_tapia`, and `van_shanno` merit functions, respectively.

```
max_step
  • Keywords Area
  • method
  • optpp_g_newton
  • max_step

  Max change in design point
```

Specification

Alias: none
Argument(s): REAL
Default: 1000.
6.2. METHOD

Description

The `max_step` control specifies the maximum step that can be taken when computing a change in the current design point (e.g., limiting the Newton step computed from current gradient and Hessian information). It is equivalent to a move limit or a maximum trust region size. The `gradient_tolerance` control defines the threshold value on the L2 norm of the objective function gradient that indicates convergence to an unconstrained minimum (no active constraints). The `gradient_tolerance` control is defined for all gradient-based optimizers.

`gradient_tolerance`

- **Keywords Area**
- **method**
- **optpp_g_newton**
- **gradient_tolerance**

Stopping critera based on L2 norm of gradient

Specification

**Alias:** none

**Argument(s):** REAL

**Default:** 1.e-4

Description

The `gradient_tolerance` control defines the threshold value on the L2 norm of the objective function gradient that indicates convergence to an unconstrained minimum (no active constraints). The `gradient_tolerance` control is defined for all gradient-based optimizers.

`max_iterations`

- **Keywords Area**
- **method**
- **optpp_g_newton**
- **max_iterations**

Number of iterations allowed for optimizers and adaptive UQ methods

Topics

This keyword is related to the topics:

- **method_independent_controls**
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none
Argument(s): INTEGER
Default: 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence} / efficient_global: 25*n)

Description

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed max_iterations iterations. See also max_function_evaluations.

Default Behavior
Default value is 100.

convergence_tolerance

- Keywords Area
- method
- optpp_g_newton
- convergence_tolerance

Stopping criterion based on convergence of the objective function or statistics

Topics

This keyword is related to the topics:
- method_independent_controls

Specification

Alias: none
Argument(s): REAL
Default: 1.e-4

Description

The convergence_tolerance specification provides a real value for controlling the termination of iteration. For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by convergence_tolerance, then this convergence criterion is satisfied on the current iteration.

Therefore, permissible values are between 0 and 1, non-inclusive.

Behavior Varies by Package/Library
This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.
Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- DOT: must be satisfied for two consecutive iterations
- NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of `convergence_tolerance` approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., `convergence_tolerance = 1.e-6` will result in approximately six digits of accuracy in the final objective function).
- NL2SOL: See `nl2sol`

**speculative**

- **Keywords Area**
- method
- `optpp_g_newton`
- speculative

Compute speculative gradients

**Topics**

This keyword is related to the topics:

- method_independent_controls

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no speculation

**Description**

When performing gradient-based optimization in parallel, `speculative` gradients can be selected to address the load imbalance that can occur between gradient evaluation and line search phases. In a typical gradient-based optimization, the line search phase consists primarily of evaluating the objective function and any constraints at a trial point, and then testing the trial point for a sufficient decrease in the objective function value and/or constraint violation. If a sufficient decrease is not observed, then one or more additional trial points may be attempted sequentially. However, if the trial point is accepted then the line search phase is complete and the gradient evaluation phase begins. By speculating that the gradient information associated with a given line search trial point will be used later, additional coarse grained parallelism can be introduced by computing the gradient information (either by finite difference or analytically) in parallel, at the same time as the line search phase trial-point function values. This balances the total amount of computation to be performed at each design point and allows for efficient utilization of multiple processors. While the total amount of work performed will generally increase (since some speculative gradients will not be used when a trial point is rejected in the line search phase), the run
time will usually decrease (since gradient evaluations needed at the start of each new optimization cycle were already performed in parallel during the line search phase). Refer to [14] for additional details. The speculative specification is implemented for the gradient-based optimizers in the DOT, CONMIN, and OPT++ libraries, and it can be used with dakota numerical or analytic gradient selections in the responses specification (refer to responses gradient section for information on these specifications). It should not be selected with vendor numerical gradients since vendor internal finite difference algorithms have not been modified for this purpose. In full-Newton approaches, the Hessian is also computed speculatively. NPSOL and NLSSOL do not support speculative gradients, as their gradient-based line search in user-supplied gradient mode (dakota numerical or analytic gradients) is a superior approach for load-balanced parallel execution.

The speculative specification enables speculative computation of gradient and/or Hessian information, where applicable, for parallel optimization studies. By speculating that the derivative information at the current point will be used later, the complete data set (all available gradient/Hessian information) can be computed on every function evaluation. While some of these computations will be wasted, the positive effects are a consistent parallel load balance and usually shorter wall clock time. The speculative specification is applicable only when parallelism in the gradient calculations can be exploited by Dakota (it will be ignored for vendor numerical gradients).

**max_function_evaluations**

- **Keywords Area**
- **method**
- **optpp_g_newton**
- **max_function_evaluations**

Number of function evaluations allowed for optimizers

**Topics**

This keyword is related to the topics:

- **method_independent_controls**

**Specification**

Alias: none

**Argument(s):** INTEGER

**Default:** 1000

**Description**

The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed `max_function_evaluations` evaluations. See also `max_iterations`.

**Default Behavior**

Default value is 1000.
6.2. METHOD

scaling

- Keywords Area
- method
- optpp_g_newton
- scaling

Turn on scaling for variables, responses, and constraints

Topics

This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none

Argument(s): none

Default: no scaling

Description

Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by by providing the `scaling` keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the method, variables, and responses blocks. When the `scaling` keyword is omitted, all _scale_types and *scales specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.

- a *scales keyword, which gives characteristic values
- a *scale_type keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

Scale Types

There are four scale types:

1. none (default) - no scaling, value of *scales keyword is ignored
2. value - multiplicative scaling
3. **auto** - automatic scaling

First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:

- two-sided bounds scaled into the interval \([0,1]\);
- one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
- no bounds or targets: no automatic scaling possible, therefore no scaling for this component

Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into \([0,1]\).

4. **log** - logarithmic scaling

First, any characteristic values from the optional \(\ast\_\text{scales}\) specification are applied. Then logarithm base 10 scaling is applied.

Logarithmic scaling is not available for linear constraints.

When continuous design variables are log scaled, linear constraints are not allowed.

**Scales**

The \(\ast\_\text{scales}\) keywords are used to specify the characteristic values. These must be non-zero real numbers. The numbers are used according to the corresponding \(\ast\_\text{scale_type}\), as described above.

Depending on the scale type, the characteristic values may be required or optional.

- none, auto, log - optional
- value - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than \(1.0e10\ast\text{DBL_MIN}\). User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.

**Examples**

The two examples below are equivalent:

```plaintext
responses
    objective_functions 3
    sense "maximize"
    primary_scale_types = "value"
    primary_scales = 1 1 100

responses
    objective_functions 3
    sense "maximize"
    primary_scale_types = "value" "value" "value"
    primary_scales = 1 1 100
```
6.2. METHOD

model_pointer

- Keywords Area
- method
- optpp_g_newton
- model_pointer

Identifier for model block to be used by a method

Topics

This keyword is related to the topics:

- block_pointer

Specification

Alias: none

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)

Description

The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.

Usage Tips

When doing advanced analyses that involve using multiple methods and multiple models, defining a model_pointer for each method is imperative.

See block_pointer for details about pointers.

Examples

environment
  tabular_graphics_data
  method_pointer = 'UQ'

method
  id_method = 'UQ'
  model_pointer = 'SURR'
  sampling,
  samples = 10
  seed = 98765 rng rnum2
  response_levels = 0.1 0.2 0.6
                  0.1 0.2 0.6
                  0.1 0.2 0.6
  sample_type lhs
  distribution cumulative

model
  id_model = 'SURR'
surrogate global,
dace_method_pointer = ’DACE’
polynomial quadratic

method
id_method = ’DACE’
model_pointer = ’DACE_M’
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = ’DACE_M’
single
interface_pointer = ’I1’

variables
uniform_uncertain = 2
lower_bounds = 0. 0.
upper_bounds = 1. 1.
descriptors = ’x1’ ’x2’

interface
id_interface = ’I1’
system asynch evaluation_concurrency = 5
analysis_driver = ’text_book’

responses
response_functions = 3
no_gradients
no_hessians

6.2.28 optpp_newton

- Keywords Area
- method
- optpp_newton

Newton method based optimization

Topics
This keyword is related to the topics:

- package_optpp
- local_optimization_methods

Specification
Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<tr>
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<tr>
<td>Optional</td>
<td>search_method</td>
<td>Select a search method for Newton-based optimizers</td>
<td></td>
</tr>
<tr>
<td>----------</td>
<td>---------------</td>
<td>---------------------------------------------------</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>merit_function</td>
<td>Balance goals of reducing objective function and satisfying constraints</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>steplength_to_boundary</td>
<td>Controls how close to the boundary of the feasible region the algorithm is allowed to move</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>centering_parameter</td>
<td>Controls how closely the algorithm should follow the &quot;central path&quot;</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>max_step</td>
<td>Max change in design point</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>gradient_tolerance</td>
<td>Stopping criteria based on L2 norm of gradient</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>max_iterations</td>
<td>Number of iterations allowed for optimizers and adaptive UQ methods</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>convergence_tolerance</td>
<td>Stopping criterion based on convergence of the objective function or statistics</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>speculative</td>
<td>Compute speculative gradients</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>max_function_evaluations</td>
<td>Number of function evaluations allowed for optimizers</td>
<td></td>
</tr>
</tbody>
</table>
Description
This is a full Newton method that expects a gradient and a Hessian. Each of the Newton-based methods are automatically bound to the appropriate OPT++ algorithm based on the user constraint specification (unconstrained, bound-constrained, or generally-constrained). In the generally-constrained case, the Newton methods use a nonlinear interior-point approach to manage the constraints.

See package_optpp for info related to all optpp methods.

See Also
These keywords may also be of interest:

- optpp_cg
- optpp_g_newton
- optpp_pds
- optpp_fd_newton
- optpp_g_newton

search_method

- Keywords Area
- method
- optpp_newton
- search_method

Select a search method for Newton-based optimizers

Specification
Alias: none
Argument(s): none
### Description

The search_method control is defined for all Newton-based optimizers and is used to select between trust_region, gradient_based_line_search, and value_based_line_search methods. The gradient_based_line_search option uses the line search method proposed by[61]. This option satisfies sufficient decrease and curvature conditions; whereas, value_based_line_search only satisfies the sufficient decrease condition. At each line search iteration, the gradient_based_line_search method computes the function and gradient at the trial point. Consequently, given expensive function evaluations, the value_based_line_search method is preferred to the gradient_based_line_search method. Each of these Newton methods additionally supports the tr_pds selection for unconstrained problems. This option performs a robust trust region search using pattern search techniques. Use of a line search is the default for bound-constrained and generally-constrained problems, and use of a trust_region search method is the default for unconstrained problems.

### value_based_line_search

- **Keywords** Area
  - method
  - optpp_newton
  - search_method
  - value_based_line_search

Use only function values for line search

### Specification

**Alias:** none

**Argument(s):** none

**Default:** trust_region (unconstrained), value_based_line_search (bound/general constraints)
CHAPTER 6. KEYWORDS AREA

Description

The search method control is defined for all Newton-based optimizers and is used to select between trust-region, gradient-based line search, and value-based line search methods. The gradient-based line search option uses the line search method proposed by [61]. This option satisfies sufficient decrease and curvature conditions; whereas, value-based line search only satisfies the sufficient decrease condition. At each line search iteration, the gradient-based line search method computes the function and gradient at the trial point. Consequently, given expensive function evaluations, the value-based line search method is preferred to the gradient-based line search method. Each of these Newton methods additionally supports the tr_pds selection for unconstrained problems. This option performs a robust trust region search using pattern search techniques. Use of a line search is the default for bound-constrained and generally-constrained problems, and use of a trust_region search method is the default for unconstrained problems.

\textbf{gradient\_based\_line\_search}

- Keywords Area
- method
- optpp_newton
- search_method
- gradient_based_line_search

Set the search method to use the gradient

Specification

Alias: none

Argument(s): none

Description

The search method control is defined for all Newton-based optimizers and is used to select between trust-region, gradient-based line search, and value-based line search methods. The gradient-based line search option uses the line search method proposed by [61]. This option satisfies sufficient decrease and curvature conditions; whereas, value-based line search only satisfies the sufficient decrease condition. At each line search iteration, the gradient-based line search method computes the function and gradient at the trial point. Consequently, given expensive function evaluations, the value-based line search method is preferred to the gradient-based line search method. Each of these Newton methods additionally supports the tr_pds selection for unconstrained problems. This option performs a robust trust region search using pattern search techniques. Use of a line search is the default for bound-constrained and generally-constrained problems, and use of a trust_region search method is the default for unconstrained problems.

\textbf{trust\_region}

- Keywords Area
- method
6.2. METHOD

- optpp_newton
- search_method
- trust_region

Use trust region as the globalization strategy.

Specification

Alias: none
Argument(s): none

Description

The trust_region optional group specification can be used to specify the initial size of the trust region (using initial_size) relative to the total variable bounds, the minimum size of the trust region (using minimum_size), the contraction factor for the trust region size (using contraction_factor) used when the surrogate model is performing poorly, and the expansion factor for the trust region size (using expansion_factor) used when the the surrogate model is performing well. Two additional commands are the trust region size contraction threshold (using contract_threshold) and the trust region size expansion threshold (using expand_threshold). These two commands are related to what is called the trust region ratio, which is the actual decrease in the truth model divided by the predicted decrease in the truth model in the current trust region. The command contract_threshold sets the minimum acceptable value for the trust region ratio, i.e., values below this threshold cause the trust region to shrink for the next SBL iteration. The command expand_threshold determines the trust region value above which the trust region will expand for the next SBL iteration.

tr_pds

- Keywords Area
- method
- optpp_newton
- search_method
- tr_pds

Use direct search as the local search in a trust region method

Specification

Alias: none
Argument(s): none

Description

The search_method control is defined for all Newton-based optimizers and is used to select between trust_region, gradient_based_line_search, and value_based_line_search methods. The gradient_based_line_search option uses the line search method proposed by[61]. This option satisfies sufficient decrease and curvature conditions; whereas, value_based_line_search only satisfies the sufficient decrease condition. At each line search iteration, the gradient_based_line_search method computes the function
and gradient at the trial point. Consequently, given expensive function evaluations, the `value_based_line_search` method is preferred to the `gradient_based_line_search` method. Each of these Newton methods additionally supports the `tr_pds` selection for unconstrained problems. This option performs a robust trust region search using pattern search techniques. Use of a line search is the default for bound-constrained and generally-constrained problems, and use of a `trust_region` search method is the default for unconstrained problems.

**merit_function**

- **Keywords Area**
- **method**
- **optpp_newton**
- **merit_function**

Balance goals of reducing objective function and satisfying constraints

**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** `argaez_tapia`

<table>
<thead>
<tr>
<th>Required/-Optional</th>
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<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<td>el_bakry</td>
<td>El-Bakry merit function</td>
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<tr>
<td>argaez_tapia</td>
<td>The merit function by Tapia and Argaez</td>
<td></td>
<td></td>
</tr>
<tr>
<td>van_shanno</td>
<td>The merit function by Vanderbei and Shanno</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Description**

A `merit_function` is a function in constrained optimization that attempts to provide joint progress toward reducing the objective function and satisfying the constraints.

**el_bakry**

- **Keywords Area**
- **method**
- **optpp_newton**
- **merit_function**
- **el_bakry**

El-Bakry merit function
6.2. METHOD

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

The "elbakry" merit function is the L2-norm of the first order optimality conditions for the nonlinear programming problem. The cost per linesearch iteration is \( n+1 \) function evaluations. For more information, see [20].

**argaez_tapia**

- **Keywords** Area
- **method**
- **optpp_newton**
- **merit_function**
- **argaez_tapia**

The merit function by Tapia and Argaez

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

The "argaez_tapia" merit function can be classified as a modified augmented Lagrangian function. The augmented Lagrangian is modified by adding to its penalty term a potential reduction function to handle the perturbed complementarity condition. The cost per linesearch iteration is one function evaluation. For more information, see [80].

If the function evaluation is expensive or noisy, set the **merit_function** to "argaez_tapia" or "van_shanno".

**van_shanno**

- **Keywords** Area
- **method**
- **optpp_newton**
- **merit_function**
- **van_shanno**

The merit function by Vanderbei and Shanno
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none
Argument(s): none

Description

The "van_shanno" merit function can be classified as a penalty function for the logarithmic barrier formulation of the nonlinear programming problem. The cost per linesearch iteration is one function evaluation. For more information see [82].

If the function evaluation is expensive or noisy, set the merit_function to "argaez_tapia" or "van_shanno".

steplength_to_boundary

- Keywords Area
- method
- optpp_newton
- steplength_to_boundary

Controls how close to the boundary of the feasible region the algorithm is allowed to move

Specification

Alias: none
Argument(s): REAL
Default: Merit function dependent: 0.8 (el_bakry), 0.99995 (argaez_tapia), 0.95 (van_shanno)

Description

The steplength_to_boundary specification is a parameter (between 0 and 1) that controls how close to the boundary of the feasible region the algorithm is allowed to move. A value of 1 means that the algorithm is allowed to take steps that may reach the boundary of the feasible region. If the user wishes to maintain strict feasibility of the design parameters this value should be less than 1. Default values are .8, .99995, and .95 for the el_bakry, argaez_tapia, and van_shanno merit functions, respectively.

centering_parameter

- Keywords Area
- method
- optpp_newton
- centering_parameter

Controls how closely the algorithm should follow the "central path"
6.2. METHOD

Specification

Alias: none

Argument(s): REAL

Default: Merit function dependent: 0.2 (el_bakry), 0.2 (argaez_tapia), 0.1 (van_shanno)

Description

The centering parameter specification is a parameter (between 0 and 1) that controls how closely the algorithm should follow the "central path". See [89] for the definition of central path. The larger the value, the more closely the algorithm follows the central path, which results in small steps. A value of 0 indicates that the algorithm will take a pure Newton step. Default values are .2, .2, and .1 for the el_bakry, argaez_tapia, and van_shanno merit functions, respectively.

max_step

- Keywords Area
- method
- optpp_newton
- max_step

Max change in design point

Specification

Alias: none

Argument(s): REAL

Default: 1000.

Description

The max_step control specifies the maximum step that can be taken when computing a change in the current design point (e.g., limiting the Newton step computed from current gradient and Hessian information). It is equivalent to a move limit or a maximum trust region size. The gradient_tolerance control defines the threshold value on the L2 norm of the objective function gradient that indicates convergence to an unconstrained minimum (no active constraints). The gradient_tolerance control is defined for all gradient-based optimizers.

gradient_tolerance

- Keywords Area
- method
- optpp_newton
- gradient_tolerance

Stopping criteria based on L2 norm of gradient
CHAPTER 6. KEYWORDS AREA

**Specification**

**Alias:** none  
**Argument(s):** REAL  
**Default:** 1.e-4

**Description**

The `gradient_tolerance` control defines the threshold value on the L2 norm of the objective function gradient that indicates convergence to an unconstrained minimum (no active constraints). The `gradient_tolerance` control is defined for all gradient-based optimizers.

**max_iterations**

- **Keywords Area**
- **method**
- **optpp_newton**
- **max_iterations**

Number of iterations allowed for optimizers and adaptive UQ methods

**Topics**

This keyword is related to the topics:

- **method_independent_controls**

**Specification**

**Alias:** none  
**Argument(s):** INTEGER  
**Default:** 100 (exceptions: fsu_cvt , local_reliability: 25; global_{reliability , interval_est , evidence} / efficient_global: 25+n)

**Description**

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed `max_iterations` iterations. See also `max_function_evaluations`.

**Default Behavior**

Default value is 100.

**convergence_tolerance**

- **Keywords Area**
- **method**
- **optpp_newton**
- **convergence_tolerance**

Stopping criterion based on convergence of the objective function or statistics
6.2. METHOD

Topics

This keyword is related to the topics:

- method
  - independent
  - controls

Specification

Alias: none
- Argument(s): REAL
- Default: 1.e-4

Description

The convergence_tolerance specification provides a real value for controlling the termination of iteration.

For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by convergence_tolerance, then this convergence criterion is satisfied on the current iteration.

Therefore, permissible values are between 0 and 1, non-inclusive.

Behavior Varies by Package/Library

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- DOT: must be satisfied for two consecutive iterations
- NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of convergence_tolerance approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., convergence_tolerance = 1.e-6 will result in approximately six digits of accuracy in the final objective function).
- NL2SOL: See nl2sol

speculative

- Keywords Area
- method
- optpp_newton
- speculative

Compute speculative gradients
CHAPTER 6. KEYWORDS AREA

Topics
This keyword is related to the topics:

- method_independent_controls

Specification
Alias: none
Argument(s): none
Default: no speculation

Description
When performing gradient-based optimization in parallel, speculative gradients can be selected to address the load imbalance that can occur between gradient evaluation and line search phases. In a typical gradient-based optimization, the line search phase consists primarily of evaluating the objective function and any constraints at a trial point, and then testing the trial point for a sufficient decrease in the objective function value and/or constraint violation. If a sufficient decrease is not observed, then one or more additional trial points may be attempted sequentially. However, if the trial point is accepted then the line search phase is complete and the gradient evaluation phase begins. By speculating that the gradient information associated with a given line search trial point will be used later, additional coarse grained parallelism can be introduced by computing the gradient information (either by finite difference or analytically) in parallel, at the same time as the line search phase trial-point function values. This balances the total amount of computation to be performed at each design point and allows for efficient utilization of multiple processors. While the total amount of work performed will generally increase (since some speculative gradients will not be used when a trial point is rejected in the line search phase), the run time will usually decrease (since gradient evaluations needed at the start of each new optimization cycle were already performed in parallel during the line search phase). Refer to [14] for additional details. The speculative specification is implemented for the gradient-based optimizers in the DOT, CONMIN, and OPT++ libraries, and it can be used with dakota numerical or analytic gradient selections in the responses specification (refer to responses gradient section for information on these specifications). It should not be selected with vendor numerical gradients since vendor internal finite difference algorithms have not been modified for this purpose. In full-Newton approaches, the Hessian is also computed speculatively. NPSOL and NLSSOL do not support speculative gradients, as their gradient-based line search in user-supplied gradient mode (dakota numerical or analytic gradients) is a superior approach for load-balanced parallel execution.

The speculative specification enables speculative computation of gradient and/or Hessian information, where applicable, for parallel optimization studies. By speculating that the derivative information at the current point will be used later, the complete data set (all available gradient/Hessian information) can be computed on every function evaluation. While some of these computations will be wasted, the positive effects are a consistent parallel load balance and usually shorter wall clock time. The speculative specification is applicable only when parallelism in the gradient calculations can be exploited by Dakota (it will be ignored for vendor numerical gradients).

max_function_evaluations

- Keywords Area
- method
- optpp_newton
- max_function_evaluations
6.2. METHOD

Number of function evaluations allowed for optimizers

Topics
This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none
Argument(s): INTEGER
Default: 1000

Description
The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed max_function_evaluations evaluations. See also max_iterations.

Default Behavior
Default value is 1000.

scaling

- Keywords Area
- method
- optpp_newton
- scaling

Turn on scaling for variables, responses, and constraints

Topics
This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none
Argument(s): none
Default: no scaling
**Description**

Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by providing the `scaling` keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the `method`, `variables`, and `responses` blocks. When the `scaling` keyword is omitted, all `_scale_types` and `*_scales` specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.

- a `*_scales` keyword, which gives characteristic values
- a `*_scale_type` keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

**Scale Types**

There are four scale types:

1. **none** (default) - no scaling, value of `*_scales` keyword is ignored
2. **value** - multiplicative scaling
3. **auto** - automatic scaling
   
   First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:
   
   - two-sided bounds scaled into the interval [0,1];
   - one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
   - no bounds or targets: no automatic scaling possible, therefore no scaling for this component

   Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into [0,1].

4. **log** - logarithmic scaling
   
   First, any characteristic values from the optional `*_scales` specification are applied. Then logarithm base 10 scaling is applied.

   Logarithmic scaling is not available for linear constraints.

   When continuous design variables are log scaled, linear constraints are not allowed.

**Scales**

The `*_scales` keywords are used to specify the characteristic values. These must be non-zero real numbers. The numbers are used according to the corresponding `*_scale_type`, as described above.

Depending on the scale type, the characteristic values may be required or optional.
6.2. METHOD

- none, auto, log - optional
- value - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than \(1.0 \times 10^{10} \times \text{DBL_MIN}\). User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.

Examples

The two examples below are equivalent:

```plaintext
responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value"
  primary_scales = 1 1 100

responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value" "value" "value"
  primary_scales = 1 1 100
```

model_pointer

- Keywords Area
- method
- optpp_newton
- model_pointer

Identifier for model block to be used by a method

Topics

This keyword is related to the topics:

- block_pointer

Specification

Alias: none

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)

Description

The `model_pointer` is used to specify which `model` block will be used to perform the function evaluations needed by the Dakota method.

**Default Behavior**

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a `model` block in the Dakota input file that has a corresponding `id_model` with the same name.
**Usage Tips**

When doing advanced analyses that involve using multiple methods and multiple models, defining a `model_pointer` for each method is imperative.

See `block_pointer` for details about pointers.

**Examples**

```plaintext
environment
  tabular_graphics_data
  method_pointer = 'UQ'

method
  id_method = 'UQ'
  model_pointer = 'SURR'
  sampling,
      samples = 10
      seed = 98765 rng rnum2
      response_levels = 0.1 0.2 0.6
      0.1 0.2 0.6
      0.1 0.2 0.6
  sample_type lhs
  distribution cumulative

model
  id_model = 'SURR'
  surrogate global,
  dace_method_pointer = 'DACE'
  polynomial quadratic

method
  id_method = 'DACE'
  model_pointer = 'DACE_M'
  sampling sample_type lhs
  samples = 121 seed = 5034 rng rnum2

model
  id_model = 'DACE_M'
  single
  interface_pointer = 'I1'

variables
  uniform_uncertain = 2
  lower_bounds = 0. 0.
  upper_bounds = 1. 1.
  descriptors = 'x1' 'x2'

interface
  id_interface = 'I1'
  system asynch evaluation_concurrency = 5
  analysis_driver = 'text_book'

responses
  response_functions = 3
  no_gradients
  no_hessians
```

6.2.29 optpp_pds

- Keywords Area
6.2. METHOD

- method
- optpp.pds

Simplex-based derivative free optimization method

Topics

This keyword is related to the topics:

- package.optpp

Specification

Alias: none

Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>search_scheme_size</td>
<td>max_iterations</td>
<td>Number of points to be used in the direct search template. Number of iterations allowed for optimizers and adaptive UQ methods.</td>
</tr>
<tr>
<td>Optional</td>
<td>convergence_tolerance</td>
<td>max_function_evaluations</td>
<td>Stopping criterion based on convergence of the objective function or statistics. Number of function evaluations allowed for optimizers.</td>
</tr>
</tbody>
</table>
**Description**

The direct search algorithm, PDS (parallel direct search method), supports bound constraints. The PDS method can directly exploit asynchronous evaluations; however, this capability has not yet been implemented in Dakota.

See package_optpp for info related to all optpp methods.

**See Also**

These keywords may also be of interest:

- optpp.cg
- optpp.g_newton
- optpp_fd_newton
- optpp.newton
- optpp.g_newton

**search_scheme_size**

- Keywords Area
- method
- optpp.pds
- search_scheme_size

Number of points to be used in the direct search template

**Specification**

**Alias:** none  
**Argument(s):** INTEGER  
**Default:** 32

**Description**

The search_scheme_size is defined for the PDS method to specify the number of points to be used in the direct search template.
6.2. METHOD

max_iterations

- Keywords Area
- method
- optpp_pds
- max.iterations

Number of iterations allowed for optimizers and adaptive UQ methods

Topics

This keyword is related to the topics:
- method.independent.controls

Specification

Alias: none

Argument(s): INTEGER

Default: 100 (exceptions: fsu_cvt, local.reliability: 25; global.{reliability, interval.est, evidence} / efficient-global: 25*n)

Description

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed max.iterations iterations. See also max.function_evaluations.

Default Behavior

Default value is 100.

convergence.tolerance

- Keywords Area
- method
- optpp_pds
- convergence.tolerance

Stopping criterion based on convergence of the objective function or statistics

Topics

This keyword is related to the topics:
- method.independent.controls
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): REAL

Default: 1.e-4

Description

The convergence_tolerance specification provides a real value for controlling the termination of iteration. For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by convergence_tolerance, then this convergence criterion is satisfied on the current iteration.

Therefore, permissible values are between 0 and 1, non-inclusive.

Behavior Varies by Package/Library

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- DOT: must be satisfied for two consecutive iterations

- NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of convergence_tolerance approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., convergence_tolerance = 1.e-6 will result in approximately six digits of accuracy in the final objective function).

- NL2SOL: See nl2sol

max_function_evaluations

- Keywords Area

- method

- optpp.pds

- max_function_evaluations

Number of function evaluations allowed for optimizers

Topics

This keyword is related to the topics:

- method_independent_controls
6.2. **METHOD**

### Specification

**Alias:** none

**Argument(s):** INTEGER
**Default:** 1000

**Description**

The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed \texttt{max.function_evaluations} evaluations. See also \texttt{max.iterations}.

**Default Behavior**

Default value is 1000.

#### scaling

- **Keywords Area**
- **method**
- **optpp.pds**
- **scaling**

Turn on scaling for variables, responses, and constraints.

### Topics

This keyword is related to the topics:

- **method\_independent\_controls**

### Specification

**Alias:** none

**Argument(s):** none
**Default:** no scaling

**Description**

Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by providing the \texttt{scaling} keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the method, variables, and responses blocks. When the \texttt{scaling} keyword is omitted, all \_\_scale\_types and *\_scales specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.
• a *scales keyword, which gives characteristic values

• a *scale_type keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

Scale Types
There are four scale types:

1. none (default) - no scaling, value of *scales keyword is ignored

2. value - multiplicative scaling

3. auto - automatic scaling

First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:

• two-sided bounds scaled into the interval [0,1];
• one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
• no bounds or targets: no automatic scaling possible, therefore no scaling for this component

Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into [0,1].

4. log - logarithmic scaling

First, any characteristic values from the optional *scales specification are applied. Then logarithm base 10 scaling is applied.

Logarithmic scaling is not available for linear constraints.

When continuous design variables are log scaled, linear constraints are not allowed.

Scales
The *scales keywords are used to specify the characteristic values. These must be non-zero real numbers. The numbers are used according to the corresponding *scale_type, as described above.

Depending on the scale type, the characteristic values may be required or optional.

• none, auto, log - optional

• value - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than 1.0e10*DBL_MIN. User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.
6.2. METHOD

Examples

The two examples below are equivalent:

```plaintext
responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value"
  primary_scales = 1 1 100

responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value" "value" "value"
  primary_scales = 1 1 100
```

**model_pointer**

- **Keywords Area**
- **method**
- **optpp.pds**
- **model_pointer**

Identifier for model block to be used by a method

**Topics**

This keyword is related to the topics:

- **block_pointer**

**Specification**

**Alias:** none

**Argument(s):** STRING

**Default:** method use of last model parsed (or use of default model if none parsed)

**Description**

The **model_pointer** is used to specify which **model** block will be used to perform the function evaluations needed by the Dakota method.

**Default Behavior**

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a **model** block in the Dakota input file that has a corresponding **id_model** with the same name.

**Usage Tips**

When doing advanced analyses that involve using multiple methods and multiple models, defining a **model-pointer** for each method is imperative.

See **block_pointer** for details about pointers.
Examples

environment
tabular_graphics_data
method_pointer = 'UQ'

method
id_method = 'UQ'
model_pointer = 'SURR'
sampling,
samples = 10
seed = 98765 rng rnum2
response_levels = 0.1 0.2 0.6
          0.1 0.2 0.6
          0.1 0.2 0.6
sample_type lhs
distribution cumulative

model
id_model = 'SURR'
surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
id_method = 'DACE'
model_pointer = 'DACE_M'
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = 'DACE_M'
single
interface_pointer = 'I1'

variables
uniform_uncertain = 2
  lower_bounds = 0. 0.
  upper_bounds = 1. 1.
  descriptors = 'x1' 'x2'

interface
id_interface = 'I1'
system asynch evaluation_concurrency = 5
  analysis_driver = 'text_book'

responses
response_functions = 3
no_gradients
no_hessians

6.2.30 asynch_pattern_search

- Keywords Area
- method
- asynch_pattern_search

Pattern search, derivative free optimization method
6.2. METHOD

Topics
This keyword is related to the topics:

- package_hopspack
- global_optimization_methods

Specification
**Alias:** coliny_apps
**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>initial_delta</td>
<td>contraction_factor</td>
<td>Amount by which step length is rescaled</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>threshold_delta</td>
<td>Step length-based stopping criteria for derivative-free optimizers</td>
</tr>
<tr>
<td>Optional</td>
<td>solution_target</td>
<td>synchroniztion</td>
<td>Select how Dakota schedules function evaluations in a pattern search</td>
</tr>
<tr>
<td>Optional</td>
<td>merit_function</td>
<td></td>
<td>Balance goals of reducing objective function and satisfying constraints</td>
</tr>
<tr>
<td>Optional</td>
<td>constraint_penalty</td>
<td></td>
<td>Multiplier for the penalty function</td>
</tr>
<tr>
<td>Optional</td>
<td>smoothing_factor</td>
<td></td>
<td>Smoothing value for smoothed penalty functions</td>
</tr>
</tbody>
</table>
### Description

The asynchronous parallel pattern search (APPS) algorithm [37] is a fully asynchronous pattern search technique in that the search along each offset direction continues without waiting for searches along other directions to finish.

Currently, APPS only supports coordinate bases with a total of $2n$ function evaluations in the pattern, and these patterns may only contract.

### Concurrency

APPS exploits parallelism through the use of Dakota’s concurrent function evaluations. The variant of the algorithm that is currently exposed, however, limits the amount of concurrency that can be exploited. In particular, APPS can leverage an evaluation concurrency level of at most twice the number of variables. More options that allow for greater evaluation concurrency may be exposed in future releases.

### Algorithm Behavior

- **initial_delta:** the initial step length, must be positive
- **threshold_delta:** step length used to determine convergence, must be greater than or equal to 4.4e-16
- **contraction_factor:** amount by which step length is rescaled after unsuccessful iterates, must be strictly between 0 and 1

### Merit Functions

APPS solves nonlinearly constrained problems by solving a sequence of linearly constrained merit function-base subproblems. There are several exact and smoothed exact penalty functions that can be specified with the `merit_function` control. The options are as follows:

- **merit_max:** based on $\ell_\infty$ norm
- **merit_max_smooth:** based on smoothed $\ell_\infty$ norm
- **merit1:** based on $\ell_1$ norm
6.2. METHOD

- merit1_smooth: based on smoothed $\ell_1$ norm
- merit2: based on $\ell_2$ norm
- merit2_smooth: based on smoothed $\ell_2$ norm
- merit2_squared: based on $\ell_2^2$ norm

The user can also specify the following to affect the merit functions:

- constraint_penalty
- smoothing_parameter

Method Independent Controls

The only method independent controls that are currently mapped to APPS are:

- max_function_evaluations
- constraint_tolerance
- output

Note that while APPS treats the constraint tolerance separately for linear and nonlinear constraints, we apply the same value to both if the user specifies constraint_tolerance.

The APPS internal display level is mapped to the Dakota output settings as follows:

- debug: display final solution, all input parameters, variable and constraint info, trial points, search directions, and execution details
- verbose: display final solution, all input parameters, variable and constraint info, and trial points
- normal: display final solution, all input parameters, variable and constraint summaries, and new best points
- quiet: display final solution and all input parameters
- silent: display final solution

**initial_delta**

- Keywords Area
- method
- asynch_pattern_search
- initial_delta

Initial step size for derivative-free optimizers

**Specification**

**Alias:** none

**Argument(s):** REAL

**Default:** 1.0
CHAPTER 6. KEYWORDS AREA

Description

The initial_delta keyword defines the size of the first search step in derivative-free optimization methods, specifically asynch_pattern_search, coliny_cobyla, coliny_pattern_search, coliny_solis_wets, and mesh_adaptive_search. It is applied in an absolute sense to all search directions.

Default Behavior

The default value is 1.0.

Usage Tips

It is recommended that initial_delta be the approximate distance from the initial point to the solution. If this distance is unknown, it is advisable to err on the side of choosing an initial_delta that is too large or to not specify it. Relative application of initial_delta is not available unless the user scales the problem accordingly.

Examples

Three example method input blocks appear below.

For asynch_pattern_search:

```
method
  asynch_pattern_search
  initial_delta = .5
  contraction_factor = 0.25
  merit_function merit1_smooth
  smoothing_factor = 1.0
  constraint_tolerance = 1.e-6
```

For coliny_pattern_search:

```
method
coliny_pattern_search
  initial_delta = .2
  threshold_delta = 1.e-4
  max_iterations 100
  solution_accuracy = 1.e-6
  seed = 1234
  max_function_evaluations = 1000
```

For mesh_adaptive_search

```
method
  mesh_adaptive_search
  initial_delta = 2.0
  seed = 1234
```

contraction_factor

- Keywords Area
- method
- asynch_pattern_search
- contraction_factor

Amount by which step length is rescaled
6.2. METHOD

**Specification**

**Alias:** none  
**Argument(s):** REAL  
**Default:** 0.5

**Description**

For pattern search methods, `contraction_factor` specifies the amount by which step length is rescaled after unsuccessful iterates, must be strictly between 0 and 1.

For methods that can expand the step length, the expansion is $1/\text{contraction\_factor}$

**threshold\_delta**  
- **Keywords Area**  
- **method**  
- **asynch\_pattern\_search**  
- **threshold\_delta**

Step length-based stopping criteria for derivative-free optimizers

**Specification**

**Alias:** none  
**Argument(s):** REAL  
**Default:** 0.01

**Description**

The `threshold\_delta` keyword defines the minimum step length allowed by the optimizer and is used to determine convergence. It is applicable to `asynch\_pattern\_search`, `coliny\_cobyla`, `coliny\_pattern\_search`, `coliny\_solis\_wets`, and `mesh\_adaptive\_search`.

**Default Behavior**

The default value varies according to method as follows:

- **asynch\_pattern\_search**: 1.0e-2  
- **coliny\_cobyla**: 1.0e-4  
- **coliny\_pattern\_search**: 1.0e-5  
- **coliny\_solis\_wets**: 1.0e-6  
- **mesh\_adaptive\_search**: 1.0e-6

**Usage Tips**

It is recommended that `threshold\_delta` be set to a value for which changes of that scale in parameter values cause negligible changes in the objective function.
Examples

Three example method input blocks appear below.

For asynch_pattern_search:

```plaintext
method asynch_pattern_search
  contraction_factor = 0.25
  threshold_delta = 1.e-4
  solution_target = 1.e-6
  max_function_evaluations = 500
  constraint_tolerance = 1.e-6
```

For coliny_pattern_search:

```plaintext
method coliny_pattern_search
  initial_delta = .2
  threshold_delta = 1.e-4
  max_iterations = 100
  solution_accuracy = 1.e-6
  seed = 1234
  max_function_evaluations = 1000
```

For mesh_adaptive_search:

```plaintext
method mesh_adaptive_search
  threshold_delta = 0.01
  seed = 1234
```

solution_target

- Keywords Area
- method
- asynch_pattern_search
- solution_target

Stopping criteria based on objective function value

Specification

Alias: solution_accuracy

Argument(s): REAL

Default: no target

Description

solution_target is a termination criterion. The algorithm will terminate when the function value falls below solution_target.
synchronization

- Keywords Area
- method
- asynch_pattern_search
- synchronization

Select how Dakota schedules function evaluations in a pattern search

### Specification

**Alias:** none
**Argument(s):** none
**Default:** nonblocking

<table>
<thead>
<tr>
<th>Required/Optional (Choose One)</th>
<th>Description of Group synchronization (Group 1)</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>nonblocking</td>
<td>Evaluate points in the pattern until an improving point is found</td>
</tr>
</tbody>
</table>

### Description

The synchronization specification can be used to specify the use of either blocking or nonblocking schedulers.

blocking

- Keywords Area
- method
- asynch_pattern_search
- synchronization
- blocking

Evaluate all points in a pattern

### Specification

**Alias:** none
**Argument(s):** none

### Description

In the blocking case, all points in the pattern are evaluated (in parallel), and if the best of these trial points is an improving point, then it becomes the next iterate. These runs are reproducible, assuming use of the same seed in the stochastic case.
nonblocking
  • Keywords Area
  • method
  • asynch_pattern_search
  • synchronization
  • nonblocking

Evaluate points in the pattern until an improving point is found

**Specification**

Alias: none
  **Argument(s):** none

**Description**

In the *nonblocking* case, all points in the pattern may not be evaluated. The first improving point found becomes the next iterate. Since the algorithm steps will be subject to parallel timing variabilities, these runs will not generally be repeatable.

merit\_function
  • Keywords Area
  • method
  • asynch_pattern_search
  • merit\_function

Balance goals of reducing objective function and satisfying constraints

**Specification**

Alias: none
  **Argument(s):** none
  **Default:** merit2\_squared

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Required</strong> (Choose One)</td>
<td>merit function (Group 1)</td>
<td>merit_max</td>
<td>Nonsmoothed merit function</td>
</tr>
<tr>
<td></td>
<td></td>
<td>merit_max_smooth</td>
<td>Smoothed merit function</td>
</tr>
</tbody>
</table>
6.2. METHOD

<table>
<thead>
<tr>
<th>merit1</th>
<th>Nonsmoothed merit function</th>
</tr>
</thead>
<tbody>
<tr>
<td>merit1_smooth</td>
<td>Smoothed merit function</td>
</tr>
<tr>
<td>merit2</td>
<td>Nonsmoothed merit function</td>
</tr>
<tr>
<td>merit2_smooth</td>
<td>Smoothed merit function</td>
</tr>
<tr>
<td>merit2_squared</td>
<td>Nonsmoothed merit function</td>
</tr>
</tbody>
</table>

**Description**

A merit_function is a function in constrained optimization that attempts to provide joint progress toward reducing the objective function and satisfying the constraints.

**merit_max**

- Keywords Area
- method
- asynch_pattern_search
- merit_function
- merit_max

Nonsmoothed merit function

**Specification**

Alias: none
Argument(s): none

**Description**

APPS solves nonlinearly constrained problems by solving a sequence of linearly constrained merit function-base subproblems. There are several exact and smoothed exact penalty functions.

merit_max: based on $\ell_\infty$ norm

**merit_max_smooth**

- Keywords Area
- method
- asynch_pattern_search
- merit_function
- merit_max_smooth

Smoothed merit function
KEYWORDS AREA

CHAPTER 6

Specification

Alias: none
Argument(s): none

Description

APPS solves nonlinearly constrained problems by solving a sequence of linearly constrained merit function-base subproblems. There are several exact and smoothed exact penalty functions.

\[ \text{merit}_{\text{max\_smooth}}: \text{based on smoothed } \ell_{\infty} \text{ norm} \]

merit1

- Keywords Area
- method
- asynch\_pattern\_search
- merit\_function
- merit1

Nonsmoothed merit function

Specification

Alias: none
Argument(s): none

Description

APPS solves nonlinearly constrained problems by solving a sequence of linearly constrained merit function-base subproblems. There are several exact and smoothed exact penalty functions.

- merit1: based on \( \ell_1 \) norm

merit1\_smooth

- Keywords Area
- method
- asynch\_pattern\_search
- merit\_function
- merit1\_smooth

Smoothed merit function

Specification

Alias: none
Argument(s): none
6.2. METHOD

Description
APPS solves nonlinearly constrained problems by solving a sequence of linearly constrained merit function-base subproblems. There are several exact and smoothed exact penalty functions.

\( \text{merit1\_smooth: based on smoothed } \ell_1 \text{ norm} \)

**merit2**
- Keywords Area
- method
- asynch\_pattern\_search
- merit\_function
- merit2

Nonsmoothed merit function

Specification
Alias: none
Argument(s): none

Description
APPS solves nonlinearly constrained problems by solving a sequence of linearly constrained merit function-base subproblems. There are several exact and smoothed exact penalty functions.

\( \text{merit2: based on } \ell_2 \text{ norm} \)

**merit2\_smooth**
- Keywords Area
- method
- asynch\_pattern\_search
- merit\_function
- merit2\_smooth

Smoothed merit function

Specification
Alias: none
Argument(s): none

Description
APPS solves nonlinearly constrained problems by solving a sequence of linearly constrained merit function-base subproblems. There are several exact and smoothed exact penalty functions.

\( \text{merit2\_smooth: based on smoothed } \ell_2 \text{ norm} \)
merit2.squared

- Keywords Area
- method
- asynch_pattern_search
- merit_function
- merit2.squared

Nonsmoothed merit function

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

APPS solves nonlinearly constrained problems by solving a sequence of linearly constrained merit function-base subproblems. There are several exact and smoothed exact penalty functions.

`merit2.squared`: based on $\ell_2^2$ norm

**constraint_penalty**

- Keywords Area
- method
- asynch_pattern_search
- constraint_penalty

Multiplier for the penalty function

**Specification**

**Alias:** none

**Argument(s):** REAL

**Default:** 1.0

**Description**

Most SCOLIB optimizers treat constraints with a simple penalty scheme that adds `constraint_penalty` times the sum of squares of the constraint violations to the objective function. The default value of `constraint_penalty` is 1000.0, except for methods that dynamically adapt their constraint penalty, for which the default value is 1.0.
6.2. METHOD

smoothing_factor

- Keywords Area
- method
- asynch_pattern_search
- smoothing_factor

Smoothing value for smoothed penalty functions

Specification

Alias: none

Argument(s): REAL
Default: 0.0

Description

- smoothing_parameter: initial smoothing value for smoothed penalty functions, must be between 0 and 1 (inclusive)

constraint_tolerance

- Keywords Area
- method
- asynch_pattern_search
- constraint_tolerance

The maximum allowable value of constraint violation still considered to be feasible

Topics

This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none

Argument(s): REAL
Default: Library default
CHAPTER 6. KEYWORDS AREA

Description

The constraint_tolerance specification determines the maximum allowable value of infeasibility that any constraint in an optimization problem may possess and still be considered to be satisfied.

If a constraint function is greater than this value then it is considered to be violated by the optimization algorithm. This specification gives some control over how tightly the constraints will be satisfied at convergence of the algorithm. However, if the value is set too small the algorithm may terminate with one or more constraints being violated.

This specification is currently meaningful for the NPSOL, NLSSOL, DOT and CONMIN constrained optimizers.

Defaults

Defaults can vary depending on the method.

- DOT constrained optimizers: 0.003
- NPSOL: dependent upon the machine precision, typically on the order of $1.e-8$ for double precision computations

max_function_evaluations

- Keywords Area
- method
- asynch_pattern_search
- max_function_evaluations

Number of function evaluations allowed for optimizers

Topics

This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none

Argument(s): INTEGER

Default: 1000

Description

The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed max_function_evaluations evaluations. See also max_iterations.

Default Behavior

Default value is 1000.
6.2. METHOD

scaling

- Keywords Area
- method
- asynch_pattern_search
- scaling

Turn on scaling for variables, responses, and constraints

Topics
This keyword is related to the topics:

- method_independent_controls

Specification
Alias: none
- Argument(s): none
- Default: no scaling

Description
Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by by providing the `scaling` keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the method, variables, and responses blocks. When the `scaling` keyword is omitted, all `_scale_types` and `*scales` specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.

- a `*scales` keyword, which gives characteristic values
- a `*scale_type` keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

Scale Types
There are four scale types:

1. none (default) - no scaling, value of `*scales` keyword is ignored
2. value - multiplicative scaling
3. **auto** - automatic scaling

First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:

- two-sided bounds scaled into the interval \([0,1]\);
- one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
- no bounds or targets: no automatic scaling possible, therefore no scaling for this component

Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into \([0,1]\).

4. **log** - logarithmic scaling

First, any characteristic values from the optional \(*_scales\) specification are applied. Then logarithm base 10 scaling is applied.

Logarithmic scaling is not available for linear constraints.

When continuous design variables are log scaled, linear constraints are not allowed.

**Scales**

The \(*_scales\) keywords are used to specify the characteristic values. These must be non-zero real numbers. The numbers are used according to the corresponding \(*scale_type\), as described above.

Depending on the scale type, the characteristic values may be required or optional.

- **none, auto, log** - optional
- **value** - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than \(1.0e10\*\text{DBL_MIN}\). User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.

**Examples**

The two examples below are equivalent:

```
responses
doctive_functions 3
  sense "maximize"
  primary_scale_types = "value"
  primary_scales = 1 1 100

responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value" "value" "value"
  primary_scales = 1 1 100
```
6.2. METHOD

model_pointer

- Keywords Area
- method
- asynch_pattern_search
- model_pointer

Identifier for model block to be used by a method

Topics

This keyword is related to the topics:

- block_pointer

Specification

Alias: none

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)

Description

The model_pointer is used to specify which model block will be used to perform the function evaluations
needed by the Dakota method.

Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model
block in the Dakota input file that has a corresponding id_model with the same name.

Usage Tips

When doing advanced analyses that involve using multiple methods and multiple models, defining a model_pointer for each method is imperative.

See block_pointer for details about pointers.

Examples

```plaintext
environment
tabular_graphics_data
method_pointer = 'UQ'

method
id_method = 'UQ'
model_pointer = 'SURR'
sampling,
samples = 10
seed = 98765 rng rnum2
response_levels = 0.1 0.2 0.6
                      0.1 0.2 0.6
                      0.1 0.2 0.6
sample_type lhs
distribution cumulative

model
id_model = 'SURR'
```
surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
id_method = 'DACE'
model_pointer = 'DACE_M'
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = 'DACE_M'
single
interface_pointer = 'I1'

variables
uniform_uncertain = 2
lower_bounds = 0. 0.
upper_bounds = 1. 1.
descriptors = 'x1' 'x2'

interface
id_interface = 'I1'
system asynch evaluation_concurrency = 5
analysis_driver = 'text_book'

responses
response_functions = 3
no_gradients
no_hessians

6.2.31 mesh_adaptive_search

- Keywords Area
- method
- mesh_adaptive_search

Finds optimal variable values using adaptive mesh-based search

Specification

Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>initial_delta</td>
<td></td>
<td>Initial step size for derivative-free optimizers</td>
</tr>
</tbody>
</table>
### Optional Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>threshold_delta</td>
<td>Optional</td>
<td>Step length-based stopping criteria for derivative-free optimizers</td>
</tr>
<tr>
<td>function_precision</td>
<td>Optional</td>
<td>Specify the maximum precision of the analysis code responses</td>
</tr>
<tr>
<td>seed</td>
<td>Optional</td>
<td>Seed of the random number generator</td>
</tr>
<tr>
<td>history_file</td>
<td>Optional</td>
<td>Name of file where mesh adaptive search records all evaluation points.</td>
</tr>
<tr>
<td>display_format</td>
<td>Optional</td>
<td>Information to be reported from mesh adaptive search’s internal records.</td>
</tr>
<tr>
<td>variable_neighborhood_search</td>
<td>Optional</td>
<td>Percentage of evaluations to do to escape local minima.</td>
</tr>
<tr>
<td>neighbor_order</td>
<td>Optional</td>
<td>Number of dimensions in which to perturb categorical variables.</td>
</tr>
<tr>
<td>display_all_evaluations</td>
<td>Optional</td>
<td>Shows mesh adaptive search’s internally held list of all evaluations.</td>
</tr>
</tbody>
</table>
### Description

The mesh adaptive direct search algorithm\cite{9} is a derivative-free generalized pattern search in which the set of points evaluated becomes increasingly dense, leading to good convergence properties. It can handle unconstrained problems as well as those with bound constraints and general nonlinear constraints. Furthermore, it can handle continuous, discrete, and categorical variables.

**Default Behavior**

By default, `mesh_adaptive_search` operates on design variables. The types of variables can be expanded through the use of the `active` keyword in the `variables` block in the Dakota input file. Categorical variables, however, must be limited to design variables.

**Expected Outputs**

The best objective function value achieved and associated parameter and constraint values can be found at the end of the Dakota output. The method’s internally summarized iteration history will appear in the screen output by default, with the option to control the method’s output through Dakota’s output level. It also generates a history file containing a list of all function evaluations done.

**Additional Discussion**

The mesh adaptive direct search method is made available in Dakota through the NOMAD software\cite{2}, available to the public under the GNU LGPL from [http://www.gerad.ca/nomad](http://www.gerad.ca/nomad).

**Examples**

The following is an example of a Dakota input file that makes use of `mesh_adaptive_search` to optimize the textbook function.

<table>
<thead>
<tr>
<th>Optional</th>
<th>use_surrogate</th>
<th>Surrogate model usage mode for mesh adaptive search</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>max_iterations</td>
<td>Number of iterations allowed for optimizers and adaptive UQ methods</td>
</tr>
<tr>
<td>Optional</td>
<td>max_function_evaluations</td>
<td>Number of function evaluations allowed for optimizers</td>
</tr>
<tr>
<td>Optional</td>
<td>scaling</td>
<td>Turn on scaling for variables, responses, and constraints</td>
</tr>
<tr>
<td>Optional</td>
<td>model_pointer</td>
<td>Identifier for model block to be used by a method</td>
</tr>
</tbody>
</table>
6.2. METHOD

method,
  mesh_adaptive_search
  seed = 1234

variables,
  continuous_design = 3
  initial_point -1.0  1.5  2.0
  upper_bounds  10.0  10.0  10.0
  lower_bounds -10.0 -10.0 -10.0
  descriptors  'x1'  'x2'  'x3'

interface,
  direct
  analysis_driver = 'text_book'

responses,
  objective_functions = 1
  no_gradients
  no_hessians

The best function value and associated parameters are found at the end of the Dakota output.

<<<< Function evaluation summary: 674 total (674 new, 0 duplicate)
<<<< Best parameters =
  1.0000000000e+00 x1
  1.0000000000e+00 x2
  1.0000000000e+00 x3
<<<< Best objective function =
  1.0735377280e-52
<<<< Best data captured at function evaluation 658

A NOMAD-generated iteration summary is also printed to the screen.

MADS run {
  BBE OBJ

  1  17.0625000000
  2  1.0625000000
  13  0.0625000000
  24  0.0002441406
  41  0.0000314713
  43  0.0000028610
  54  0.0000000037
  83  0.0000000000
  105  0.0000000000
  112  0.0000000000
  114  0.0000000000
  135  0.0000000000
  142  0.0000000000
  153  0.0000000000
  159  0.0000000000
  171  0.0000000000
  193  0.0000000000
  200  0.0000000000
  207  0.0000000000
  223  0.0000000000
  229  0.0000000000
  250  0.0000000000
  266  0.0000000000
  282  0.0000000000
  288  0.0000000000

}
CHAPTER 6. KEYWORDS AREA

314 0.0000000000
320 0.0000000000
321 0.0000000000
327 0.0000000000
354 0.0000000000
361 0.0000000000
372 0.0000000000
373 0.0000000000
389 0.0000000000
400 0.0000000000
417 0.0000000000
444 0.0000000000
459 0.0000000000
461 0.0000000000
488 0.0000000000
492 0.0000000000
494 0.0000000000
501 0.0000000000
518 0.0000000000
530 0.0000000000
537 0.0000000000
564 0.0000000000
566 0.0000000000
583 0.0000000000
590 0.0000000000
592 0.0000000000
604 0.0000000000
606 0.0000000000
629 0.0000000000
636 0.0000000000
658 0.0000000000
674 0.0000000000

) end of run (mesh size reached NOMAD precision)
blackbox evaluations : 674
best feasible solution : ( 1 1 1 ) h=0 f=1.073537728e-52

initial_delta

- Keywords Area

- method

- mesh_adaptive_search

- initial_delta

Initial step size for derivative-free optimizers

Specification

Alias: none
Argument(s): REAL
Default: 1.0
Description

The `initial_delta` keyword defines the size of the first search step in derivative-free optimization methods, specifically `asynch_pattern_search`, `coliny_cobyla`, `coliny_pattern_search`, `coliny_solis_wets`, and `mesh_adaptive_search`. It is applied in an absolute sense to all search directions.

**Default Behavior**

The default value is 1.0.

**Usage Tips**

It is recommended that `initial_delta` be the approximate distance from the initial point to the solution. If this distance is unknown, it is advisable to err on the side of choosing an `initial_delta` that is too large or to not specify it. Relative application of `initial_delta` is not available unless the user scales the problem accordingly.

Examples

Three example method input blocks appear below.

For `asynch_pattern_search`:

```plaintext
method
asynch_pattern_search
  initial_delta = .5
  contraction_factor = 0.25
  merit_function merit1_smooth
  smoothing_factor = 1.0
  constraint_tolerance = 1.e-6
```

For `coliny_pattern_search`:

```plaintext
method
coliny_pattern_search
  initial_delta = .2
  threshold_delta = 1.e-4
  max_iterations 100
  solution_accuracy = 1.e-6
  seed = 1234
  max_function_evaluations = 1000
```

For `mesh_adaptive_search`:

```plaintext
method
mesh_adaptive_search
  initial_delta = 2.0
  seed = 1234
```

**threshold_delta**

- **Keywords Area**

- **method**

- **mesh_adaptive_search**

- **threshold_delta**

Step length-based stopping criteria for derivative-free optimizers
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): REAL

Default: 1.0e-6

Description

The \texttt{threshold\_delta} keyword defines the minimum step length allowed by the optimizer and is used to determine convergence. It is applicable to \texttt{asynch\_pattern\_search}, \texttt{coliny\_cobyla}, \texttt{coliny\_pattern\_search}, \texttt{coliny\_solis\_wets}, and \texttt{mesh\_adaptive\_search}.

Default Behavior

The default value varies according to method as follows:

- \texttt{asynch\_pattern\_search}: 1.0e-2
- \texttt{coliny\_cobyla}: 1.0e-4
- \texttt{coliny\_pattern\_search}: 1.0e-5
- \texttt{coliny\_solis\_wets}: 1.0e-6
- \texttt{mesh\_adaptive\_search}: 1.0e-6

Usage Tips

It is recommended that \texttt{threshold\_delta} be set to a value for which changes of that scale in parameter values cause negligible changes in the objective function.

Examples

Three example method input blocks appear below.

For \texttt{asynch\_pattern\_search}:

\begin{verbatim}
method
  asynch_pattern_search
  contraction_factor = 0.25
  threshold_delta = 1.e-4
  solution_target = 1.e-6
  max_function_evaluations 500
  constraint_tolerance 1.e-6
\end{verbatim}

For \texttt{coliny\_pattern\_search}:

\begin{verbatim}
method
  coliny_pattern_search
  initial_delta = .2
  threshold_delta = 1.e-4
  max_iterations 100
  solution_accuracy = 1.e-6
  seed = 1234
  max_function_evaluations = 1000
\end{verbatim}

For \texttt{mesh\_adaptive\_search}:

\begin{verbatim}
method
  mesh_adaptive_search
  threshold_delta = 0.01
  seed = 1234
\end{verbatim}
6.2. METHOD

function_precision
- Keywords Area
- method
- mesh_adaptive_search
- function_precision

Specify the maximum precision of the analysis code responses.

Specification
Alias: none
- Argument(s): REAL
- Default: 1.0e-10

Description
The function_precision control provides the algorithm with an estimate of the accuracy to which the problem functions can be computed. This is used to prevent the algorithm from trying to distinguish between function values that differ by less than the inherent error in the calculation.

seed
- Keywords Area
- method
- mesh_adaptive_search
- seed

Seed of the random number generator.

Specification
Alias: none
- Argument(s): INTEGER
- Default: system-generated (non-repeatable)

Description
The random seed control provides a mechanism for making a stochastic method repeatable. That is, the use of the same random seed in identical studies will generate identical results.

Default Behavior
If not specified, the seed is randomly generated.

Expected Output
If seed is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

Usage Tips
If a stochastic study was run without seed specified, and the user later wishes to repeat the study using the same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen. That value can then be added to the Dakota input file.
Examples

method
  sampling
    sample_type lhs
    samples = 10
    seed = 15347

history_file

- Keywords Area
- method
- mesh_adaptive_search
- history_file

Name of file where mesh adaptive search records all evaluation points.

Specification

Alias: none
  Argument(s): STRING
  Default: mads_history

Description

The history_file is used to specify the name of a file to which mesh adaptive direct search will write its own list of evaluated points.

  Default Behavior

  By default, mesh adaptive direct search will write the list of evaluation points in a file named mads_history.-xxxx, where xxxx corresponds to a randomly generated number. Dakota’s output level controls the method’s level of output to file.

Examples

The example below shows the syntax for specifying the name of the history file.

method
  mesh_adaptive_search
  history_file = ‘output.log’
  seed = 1234

display_format

- Keywords Area
- method
- mesh_adaptive_search
- display_format

  Information to be reported from mesh adaptive search’s internal records.
6.2. METHOD

Specification

Alias: none

Argument(s): STRING

Description

The `display_format` keyword is used to specify the set of information to be reported by the mesh adaptive direct search method. This is information mostly internal to the method and not reported via Dakota output.

Default Behavior

By default, only the number of function evaluations (bbe) and the objective function value (obj) are reported. The full list of options is as follows. Note that case does not matter.

- BBE: Blackbox evaluations.
- BBO: Blackbox outputs.
- EVAL: Evaluations (includes cache hits).
- MESH_INDEX: Mesh index.
- MESH_SIZE: Mesh size parameter.
- OBJ: Objective function value.
- POLL_SIZE: Poll size parameter.
- SOL: Solution, with format iSOLj where i and j are two (optional) strings: i will be displayed before each coordinate, and j after each coordinate (except the last).
- STAT_AVG: The AVG statistic.
- STAT_SUM: The SUM statistic defined by argument.
- TIME: Wall-clock time.
- VARi: Value of variable i. The index 0 corresponds to the first variable.

Expected Outputs

A list of the requested information will be printed to the screen.

Usage Tips

This will most likely only be useful for power users who want to understand and/or report more detailed information on method behavior.

Examples

The following example shows the syntax for specifying `display_format`. Note that all desired information options should be listed within a single string.

```
method
  mesh_adaptive_search
  display_format 'bbe obj poll_size'
  seed = 1234
```

Below is the output reported for the above example.
MADS run {
  BBE OBJ POLL_SIZE

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>17.0625000000</td>
<td>2.0000000000</td>
<td>2.0000000000</td>
<td>2.0000000000</td>
</tr>
<tr>
<td>2</td>
<td>1.0625000000</td>
<td>2.0000000000</td>
<td>2.0000000000</td>
<td>2.0000000000</td>
</tr>
<tr>
<td>3</td>
<td>0.0625000000</td>
<td>1.0000000000</td>
<td>1.0000000000</td>
<td>1.0000000000</td>
</tr>
<tr>
<td>24</td>
<td>0.0002441406</td>
<td>0.5000000000</td>
<td>0.5000000000</td>
<td>0.5000000000</td>
</tr>
<tr>
<td>41</td>
<td>0.0000314713</td>
<td>0.1250000000</td>
<td>0.1250000000</td>
<td>0.1250000000</td>
</tr>
<tr>
<td>43</td>
<td>0.0000028610</td>
<td>0.2500000000</td>
<td>0.2500000000</td>
<td>0.2500000000</td>
</tr>
<tr>
<td>83</td>
<td>0.0000000000</td>
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<td>0.0078125000</td>
<td>0.0078125000</td>
</tr>
<tr>
<td>105</td>
<td>0.0000000000</td>
<td>0.0009765625</td>
<td>0.0009765625</td>
<td>0.0009765625</td>
</tr>
<tr>
<td>112</td>
<td>0.0000000000</td>
<td>0.0009765625</td>
<td>0.0009765625</td>
<td>0.0009765625</td>
</tr>
<tr>
<td>114</td>
<td>0.0000000000</td>
<td>0.0019531250</td>
<td>0.0019531250</td>
<td>0.0019531250</td>
</tr>
<tr>
<td>135</td>
<td>0.0000000000</td>
<td>0.0000610352</td>
<td>0.0000610352</td>
<td>0.0000610352</td>
</tr>
<tr>
<td>207</td>
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<td>0.0000610352</td>
<td>0.0000610352</td>
<td>0.0000610352</td>
</tr>
<tr>
<td>223</td>
<td>0.0000000000</td>
<td>0.0000305176</td>
<td>0.0000305176</td>
<td>0.0000305176</td>
</tr>
<tr>
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<td>0.0000000000</td>
<td>0.0000076294</td>
<td>0.0000076294</td>
<td>0.0000076294</td>
</tr>
<tr>
<td>361</td>
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<td>0.0000038147</td>
<td>0.0000038147</td>
<td>0.0000038147</td>
</tr>
<tr>
<td>372</td>
<td>0.0000000000</td>
<td>0.0000009537</td>
<td>0.0000009537</td>
<td>0.0000009537</td>
</tr>
<tr>
<td>417</td>
<td>0.0000000000</td>
<td>0.0000019073</td>
<td>0.0000019073</td>
<td>0.0000019073</td>
</tr>
<tr>
<td>444</td>
<td>0.0000000000</td>
<td>0.0000000075</td>
<td>0.0000000075</td>
<td>0.0000000075</td>
</tr>
<tr>
<td>459</td>
<td>0.0000000000</td>
<td>0.0000000037</td>
<td>0.0000000037</td>
<td>0.0000000037</td>
</tr>
<tr>
<td>461</td>
<td>0.0000000000</td>
<td>0.0000000075</td>
<td>0.0000000075</td>
<td>0.0000000075</td>
</tr>
<tr>
<td>488</td>
<td>0.0000000000</td>
<td>0.0000000005</td>
<td>0.0000000005</td>
<td>0.0000000005</td>
</tr>
<tr>
<td>492</td>
<td>0.0000000000</td>
<td>0.0000000009</td>
<td>0.0000000009</td>
<td>0.0000000009</td>
</tr>
<tr>
<td>494</td>
<td>0.0000000000</td>
<td>0.0000000019</td>
<td>0.0000000019</td>
<td>0.0000000019</td>
</tr>
<tr>
<td>518</td>
<td>0.0000000000</td>
<td>0.0000000019</td>
<td>0.0000000019</td>
<td>0.0000000019</td>
</tr>
<tr>
<td>530</td>
<td>0.0000000000</td>
<td>0.0000000002</td>
<td>0.0000000002</td>
<td>0.0000000002</td>
</tr>
<tr>
<td>537</td>
<td>0.0000000000</td>
<td>0.0000000002</td>
<td>0.0000000002</td>
<td>0.0000000002</td>
</tr>
<tr>
<td>564</td>
<td>0.0000000000</td>
<td>0.0000000000</td>
<td>0.0000000000</td>
<td>0.0000000000</td>
</tr>
<tr>
<td>566</td>
<td>0.0000000000</td>
<td>0.0000000000</td>
<td>0.0000000000</td>
<td>0.0000000000</td>
</tr>
<tr>
<td>583</td>
<td>0.0000000000</td>
<td>0.0000000000</td>
<td>0.0000000000</td>
<td>0.0000000000</td>
</tr>
<tr>
<td>590</td>
<td>0.0000000000</td>
<td>0.0000000000</td>
<td>0.0000000000</td>
<td>0.0000000000</td>
</tr>
<tr>
<td>592</td>
<td>0.0000000000</td>
<td>0.0000000000</td>
<td>0.0000000000</td>
<td>0.0000000000</td>
</tr>
<tr>
<td>604</td>
<td>0.0000000000</td>
<td>0.0000000000</td>
<td>0.0000000000</td>
<td>0.0000000000</td>
</tr>
<tr>
<td>606</td>
<td>0.0000000000</td>
<td>0.0000000000</td>
<td>0.0000000000</td>
<td>0.0000000000</td>
</tr>
<tr>
<td>629</td>
<td>0.0000000000</td>
<td>0.0000000000</td>
<td>0.0000000000</td>
<td>0.0000000000</td>
</tr>
<tr>
<td>636</td>
<td>0.0000000000</td>
<td>0.0000000000</td>
<td>0.0000000000</td>
<td>0.0000000000</td>
</tr>
<tr>
<td>658</td>
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<td>0.0000000000</td>
<td>0.0000000000</td>
<td>0.0000000000</td>
</tr>
<tr>
<td>674</td>
<td>0.0000000000</td>
<td>0.0000000000</td>
<td>0.0000000000</td>
<td>0.0000000000</td>
</tr>
</tbody>
</table>
6.2. METHOD

{ end of run (mesh size reached NOMAD precision)

blackbox evaluations : 674
best feasible solution : ( 1 1 1 ) h=0 f=1.073537728e-52

See Also

These keywords may also be of interest:

- **display_all_evaluations**

**variable_neighborhood_search**

- **Keywords Area**
- **method**
- **mesh_adaptive_search**
- **variable_neighborhood_search**

Percentage of evaluations to do to escape local minima.

**Specification**

**Alias:** none

**Argument(s):** REAL

**Default:** 0.0

**Description**

The **variable_neighborhood_search** keyword is used to set the percentage (in decimal form) of function evaluations used to escape local minima. The mesh adaptive direct search method will try to perform a maximum of that percentage of the function evaluations within this more extensive search.

**Default Behavior**

By default, **variable_neighborhood_search** is not used.

**Usage Tips**

Using **variable_neighborhood_search** results in an increased number of function evaluations. If the desired result is a local minimum, the added cost is of little or no value, so the recommendation is not to use it. If the desired result is the best local minimum possible within a computational budget, then there is value in setting this parameter. Note that the higher the value, the greater the computational cost. The value should be no greater than 1.0.

**Examples**

The following example shows the syntax used to set **variable_neighborhood_search**.

```plaintext
method
   mesh_adaptive_search
      seed = 1234
      variable_neighborhood_search = 0.1
```
neighbor\_order

- Keywords Area
- method
- mesh\_adaptive\_search
- neighbor\_order

Number of dimensions in which to perturb categorical variables.

**Specification**

**Alias:** none  
**Argument(s):** INTEGER

**Description**

The `neighbor\_order` keyword allows the user to specify the number of categorical dimensions to perturb when determining neighboring points that will be used by the mesh adaptive direct search method to augment its search. When greater than 1, the neighbors are defined from the tensor product of the admissible 1-dimensional perturbations.

**Default Behavior**

By default, the categorical neighbors will be defined by perturbing only one categorical variable at a time (according to the corresponding adjacency matrix; see `adjacency\_matrix`) while leaving the others fixed at their current values.

**Usage Tips**

The maximum meaningful value `neighbor\_order` can take on is the number of categorical variables.

**Examples**

In this example, suppose we have the following categorical variables and associated adjacency matrices.

```plaintext
variables
discrete\_design\_set
    real = 2
    categorical yes yes
    num\_set\_values = 3 5
    set\_values = 1.2 2.3 3.4 4.4 5.5 7.7
    adjacency\_matrix =
        1 1 0
        1 1 0
        1 0 1 0 1
        1 0 1 0
        1 0 1 0
        1 0 1 0
```

Also suppose that we have the following method specification.

```plaintext
method
    mesh\_adaptive\_search
    seed = 1234
```
If the mesh adaptive direct search is at the point (1.2, 1.2), then the neighbors will be defined by the default 1-dimensional perturbations and would be the following:

(2.3, 1.2)
(1.2, 4.4)
(1.2, 7.7)

If, instead, the method specification is the following:

```
method
  mesh_adaptive_search
  seed = 1234
  neighbor_order = 2
```

The neighbors will be defined by 2-dimensional perturbations defined from the tensor product of the 1-dimensional perturbation and would be the following:

(2.3, 1.2)
(2.3, 4.4)
(2.3, 7.7)
(1.2, 4.4)
(1.2, 7.7)

**See Also**

These keywords may also be of interest:

- `adjacency_matrix`

**display_all_evaluations**

- `Keywords Area`
- `method`
- `mesh_adaptive_search`
- `display_all_evaluations`

Shows mesh adaptive search’s internally held list of all evaluations

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** false

**Description**

If `set.display_all_evaluations` will instruct the mesh adaptive direct search method to print out its own record of all evaluations. The information reported may be controlled using `display_format`.

**Default Behavior**

By default, mesh adaptive direct search does not report information on all evaluations, only on those for which an improvement in the objective function is found.

**Expected Outputs**
The information specified by `display_format` will be reported to the screen for every function evaluation.

**Usage Tips**

This will most likely only be useful for power users who want to understand and/or report more detailed information on method behavior.

**Examples**

The following example shows the syntax for specifying `display_all_evaluations`.

```plaintext
method
  mesh_adaptive_search
  display_all_evaluations
  max_function_evaluations=20
  seed = 1234
```

Note that the output below reports information (default for `display_format`) for all function evaluations.

```plaintext
MADS run {

BBE OBJ
1 17.0625000000
2 1.0625000000
3 1297.0625000000
4 257.0625000000
5 81.0625000000
6 151.0625000000
7 1051.0625000000
8 40.0625000000
9 17.0625000000
10 40.0625000000
11 1.0625000000
12 102.0625000000
13 0.0625000000
14 231.0625000000
15 16.0625000000
16 5.0625000000
17 16.0625000000
18 71.0625000000
19 0.0625000000
20 1.0625000000
}

) end of run (max number of blackbox evaluations)

blackbox evaluations : 20
best feasible solution : ( 1 0.5 1 ) h=0 f=0.0625
```

That is in contrast with what would be reported by default.

```plaintext
MADS run {

BBE OBJ
1 17.0625000000
2 1.0625000000
13 0.0625000000
20 0.0625000000
}

) end of run (max number of blackbox evaluations)

blackbox evaluations : 20
best feasible solution : ( 1 0.5 1 ) h=0 f=0.0625
```
See Also

These keywords may also be of interest:

- display_format

use_surrogate

- Keywords Area
- method
- mesh_adaptive_search
- use_surrogate

Surrogate model usage mode for mesh adaptive search

Specification

Alias: none
Argument(s): none
Default: optimize

<table>
<thead>
<tr>
<th>Required/-Optional (Choose One)</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>inform_search</td>
<td>optimize</td>
<td>Surrogate is used in lieu of true model for mesh adaptive search</td>
</tr>
</tbody>
</table>

Description

The use_surrogate keyword is used to define how a surrogate model (if one is provided) is to be used by mesh_adaptive_search. There are two approaches available: inform_search uses the surrogate to sort list of trial points and subsequently the true function is evaluated on the most promising points first. Both true function and surrogate are used interchangeably within the method. optimize forces the use of a surrogate in lieu of the true model and thus the true function is never invoked except to construct the surrogate.

Known Issue: When using discrete variables, there have been sometimes significant differences in surrogate behavior observed across computing platforms in some cases. The cause has not yet been fully diagnosed and is currently under investigation. In addition, guidance on appropriate construction and use of surrogates with discrete variables is under development. In the meantime, users should therefore be aware that there is a risk of inaccurate results when using surrogates with discrete variables.

Default Behavior

By default, mesh_adaptive_search follows behaviour provided by optimize option.
Examples

The following example shows the syntax used to set `use_surrogate`.

```
method,
    mesh_adaptive_search
    model_pointer = 'SURROGATE'
    use_surrogate inform_search

model,
    id_model = 'SURROGATE'
    surrogate global
    polynomial quadratic
    dace_method_pointer = 'SAMPLING'

variables,
    continuous_design = 3
        initial_point  -1.0  1.5  2.0
        upper_bounds  10.0  10.0  10.0
        lower_bounds  -10.0 -10.0 -10.0
        descriptors 'x1' 'x2' 'x3'
    discrete_design_range = 2
        initial_point  2  2
        lower_bounds  1  1
        upper_bounds  4  9
        descriptors 'y1' 'y2'
    discrete_design_set
        real = 2
            elements_per_variable = 4 5
            elements = 1.2 2.3 3.4 4.5
            descriptors 'y3' 'y4'
        integer = 2
            elements_per_variable = 2 2
            elements = 4 7 8 9
            descriptors 'z1' 'z2'

method,
    id_method = 'SAMPLING'
    model_pointer = 'TRUTH'
    sampling
        samples = 55

model,
    id_model = 'TRUTH'
    single
        interface_pointer = 'TRUE_FN'

interface,
    id_interface = 'TRUE_FN'
    direct
        analysis_driver = 'text_book'

responses,
    objective_functions = 1
    no_gradients
    no_hessians
```

**inform_search**

- Keywords Area
- method
6.2. METHOD

- mesh_adaptive_search
- use_surrogate
- inform_search

Surrogate informs evaluation order in mesh adaptive search

Specification

Alias: none

Argument(s): none

Description

When inform_search is specified with use_surrogate, mesh_adaptive_search uses the surrogate to sort list of trial points and subsequently the true function is evaluated on the most promising points first. Both true function and surrogate are used interchangeably within the method.

Default Behavior

inform_search is not the default surrogate usage mode.

Expected Output

The user can expect to see both the number of true model evaluations and the number of approximation (i.e., surrogate) evaluations reported in the Dakota screen output. The former captures the sum of truth evaluations done for the surrogate construction and for the optimization.

Usage Tips

When inform_search is specified, the maximum_function_evaluations keyword applies to only the optimization method and does not account for evaluations needed to construct the surrogate. If the user has a strict evaluation budget, they should set maximum_function_evaluations such that evaluation budget = number of evaluations to construct surrogate + maximum_function_evaluations.

Examples

The following example shows the syntax used to set use_surrogate to optimize.

```dakota
method,
  mesh_adaptive_search
  model_pointer = 'SURROGATE'
  use_surrogate inform_search

model,
  id_model = 'SURROGATE'
  surrogate global
  polynomial quadratic
  dace_method_pointer = 'SAMPLING'

variables,
  continuous_design = 3
  initial_point  -1.0  1.5  2.0
  upper_bounds  10.0  10.0  10.0
  lower_bounds  -10.0 -10.0 -10.0
  descriptors  'x1' 'x2' 'x3'
  discrete_design_range = 2
  initial_point  2  2
  lower_bounds  1  1
  upper_bounds  4  9
```
```
descriptors 'y1' 'y2'
discrete_design_set
    real = 2
    elements_per_variable = 4 5
    elements = 1.2 2.3 3.4 4.5 1.2 3.3 4.4 5.5 7.7
    descriptors 'y3' 'y4'
integer = 2
    elements_per_variable = 2 2
    elements = 4 7 8 9
    descriptors 'z1' 'z2'

method,
    id_method = 'SAMPLING'
    model_pointer = 'TRUTH'
sampling
    samples = 55

model,
    id_model = 'TRUTH'
    single
        interface_pointer = 'TRUE_FN'

interface,
    id_interface = 'TRUE_FN'
    direct
        analysis_driver = 'text_book'

responses,
    objective_functions = 1
    no_gradients
    no_hessians

The following will appear toward the end of the screen output when Dakota is run on this example. The number of true function evaluations includes the 55 evaluations that were done to construct the surrogate (as specified in the SAMPLING method block) plus the number of truth evaluations done by meshadaptive.search.

<<<<<< Function evaluation summary (APPROX_INTERFACE): 1660 total (1660 new, 0 duplicate)
<<<<<< Function evaluation summary (TRUE_FN): 795 total (795 new, 0 duplicate)

optimize
  • Keywords Area
  • method
  • meshadaptive_search
  • use_surrogate
  • optimize

Surrogate is used in lieu of true model for mesh adaptive search

Specification
Alias: none
  Argument(s): none
6.2. METHOD

Description

When optimize is specified with use_surrogate, mesh_adaptive_search will use the surrogate in lieu of the true model and thus the true function is never invoked except to construct the surrogate.

Default Behavior

optimize is the default surrogate usage mode.

Expected Output

The user can expect to see both the number of true model evaluations and the number of approximation (i.e., surrogate) evaluations reported in the Dakota screen output. The former should equal the number of truth evaluations done for the surrogate construction.

Examples

The following example shows the syntax used to set use_surrogate to optimize.

```
method, 
    mesh_adaptive_search 
    model_pointer = 'SURROGATE' 
    use_surrogate optimize

model, 
    id_model = 'SURROGATE' 
    surrogate global 
    polynomial quadratic 
    dace_method_pointer = 'SAMPLING'

variables, 
    continuous_design = 3 
    initial_point  -1.0  1.5  2.0 
    upper_bounds  10.0  10.0  10.0 
    lower_bounds  -10.0 -10.0 -10.0 
    descriptors   'x1'  'x2'  'x3'
    discrete_design_range = 2 
    initial_point  2   2 
    lower_bounds   1   1 
    upper_bounds   4   9 
    descriptors    'y1'  'y2'
    discrete_design_set 
      real = 2 
      elements_per_variable = 4 5 
      elements = 1.2 2.3 3.4 4.5 1.2 3.3 4.4 4.5 5.5 7.7 
      descriptors 'y3' 'y4'
      integer = 2 
      elements_per_variable = 2 2 
      elements = 4 7 8 9 
      descriptors 'z1' 'z2'

method, 
    id_method = 'SAMPLING' 
    model_pointer = 'TRUTH' 
    sampling 
      samples = 55 

model, 
    id_model = 'TRUTH' 
    single 
      interface_pointer = 'TRUE_FN'

interface, 
    id_interface = 'TRUE_FN'
```
direct
analysis_driver = 'text_book'

responses,
objective_functions = 1
no_gradients
no_hessians

The following will appear toward the end of the screen output when Dakota is run on this example. The number of true function evaluations includes only the 55 evaluations that were done to construct the surrogate (as specified in the SAMPLING method block).

<<<<<< Function evaluation summary (APPROX_INTERFACE): 221 total (221 new, 0 duplicate)
<<<<<< Function evaluation summary (TRUE_FN): 55 total (55 new, 0 duplicate)

max_iterations

- Keywords Area
- method
- mesh_adaptive_search
- max_iterations

Number of iterations allowed for optimizers and adaptive UQ methods

Topics

This keyword is related to the topics:
- method_independent_controls

Specification

Alias: none
Argument(s): INTEGER
Default: 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence} / efficient_global: 25*n)

Description

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed max_iterations iterations. See also max_function_evaluations.

Default Behavior
Default value is 100.
6.2. METHOD

max_function_evaluations

- Keywords Area
- method
- mesh_adaptive_search
- max_function_evaluations

Number of function evaluations allowed for optimizers

Topics

This keyword is related to the topics:
- method_independent_controls

Specification

Alias: none
Argument(s): INTEGER
Default: 1000

Description

The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed max_function_evaluations evaluations. See also max_iterations.

Default Behavior

Default value is 1000.

scaling

- Keywords Area
- method
- mesh_adaptive_search
- scaling

Turn on scaling for variables, responses, and constraints

Topics

This keyword is related to the topics:
- method_independent_controls

Specification

Alias: none
Argument(s): none
Default: no scaling
CHAPTER 6. KEYWORDS AREA

Description

Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by by providing the scaling keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the method, variables, and responses blocks. When the scaling keyword is omitted, all _scale_types and *scales specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.

• a *scales keyword, which gives characteristic values

• a *scale_type keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

Scale Types

There are four scale types:

1. none (default) - no scaling, value of *scales keyword is ignored

2. value - multiplicative scaling

3. auto - automatic scaling

First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:

• two-sided bounds scaled into the interval [0,1];
• one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
• no bounds or targets: no automatic scaling possible, therefore no scaling for this component

Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into [0,1].

4. log - logarithmic scaling

First, any characteristic values from the optional _scales specification are applied. Then logarithm base 10 scaling is applied.

Logarithmic scaling is not available for linear constraints.

When continuous design variables are log scaled, linear constraints are not allowed.

Scales

The _scales keywords are used to specify the characteristic values. These must be non-zero real numbers. The numbers are used according to the corresponding _scale_type, as described above.

Depending on the scale type, the characteristic values may be required or optional.
6.2. METHOD

- none, auto, log - optional
- value - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than $1.0\times10^{-10}$ DBL_MIN. User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.

Examples

The two examples below are equivalent:

```plaintext
responses
 objective_functions 3
   sense "maximize"
   primary_scale_types = "value"
   primary_scales = 1 1 100

responses
 objective_functions 3
   sense "maximize"
   primary_scale_types = "value" "value" "value"
   primary_scales = 1 1 100
```

model_pointer

- Keywords Area
- method
- mesh_adaptive_search
- model_pointer

Identifier for model block to be used by a method

Topics

This keyword is related to the topics:

- block_pointer

Specification

Alias: none

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)

Description

The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.
Usage Tips
When doing advanced analyses that involve using multiple methods and multiple models, defining a `model-pointer` for each method is imperative.
See `block_pointer` for details about pointers.

Examples

```plaintext
environment
tabular_graphics_data
method_pointer = 'UQ'

method
id_method = 'UQ'
model_pointer = 'SURR'
sampling,
samples = 10
seed = 98765 rng rnum2
response_levels = 0.1 0.2 0.6
0.1 0.2 0.6
0.1 0.2 0.6
sample_type lhs
distribution cumulative

model
id_model = 'SURR'
surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
id_method = 'DACE'
model_pointer = 'DACE_M'
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = 'DACE_M'
single
interface_pointer = 'I1'

variables
uniform_uncertain = 2
lower_bounds = 0. 0.
upper_bounds = 1. 1.
descriptors = 'x1' 'x2'

interface
id_interface = 'I1'
system asynch evaluation_concurrency = 5
analysis_driver = 'text_book'

responses
response_functions = 3
no_gradients
no_hessians

6.2.32 nowpac

- Keywords Area
6.2. METHOD

- method
- nowpac

Gradient-free inequality-constrained optimization using Nonlinear Optimization With Path Augmented Constraints (NOWPAC).

Specification

Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>trust_region</td>
<td>Use trust region as the globalization strategy. Number of iterations allowed for optimizers and adaptive UQ methods</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>max_iterations</td>
<td>Number of function evaluations allowed for optimizers</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>max_function_evaluations</td>
<td>Turn on scaling for variables, responses, and constraints</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>scaling</td>
<td>Identifier for model block to be used by a method</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>model_pointer</td>
<td></td>
</tr>
</tbody>
</table>

Description

NOWPAC is a provably-convergent gradient-free optimization method from MIT that solves a series of trust region surrogate-based subproblems to generate improving steps. Due to its use of an interior penalty scheme and enforcement of strict feasibility, it does not support linear or nonlinear equality constraints. As opposed to the stochastic version (SNOWPAC), NOWPAC does not currently support a feasibility restoration mode, so it is necessary to start from a feasible design.

Note: (S)NOWPAC is not configured with Dakota by default and requires a separate installation of the NOWPAC distribution from MIT, combined with its TPLs of Eigen and NLOPT.

Examples

```
method
nowpac
```
max_function_evaluations = 1000
convergence_tolerance = 1e-4
trust_region
  initial_size = 0.10
  minimum_size = 1.0e-6
  contract_threshold = 0.25
  expand_threshold = 0.75
  contraction_factor = 0.50
  expansion_factor = 1.50

trust_region

- Keywords Area
- method
- nowpac
- trust_region

Use trust region as the globalization strategy.

**Specification**

**Alias:** none

**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>initial_size</td>
<td>initial_size</td>
<td>Trust region initial size (relative to bounds)</td>
</tr>
<tr>
<td>Optional</td>
<td>minimum_size</td>
<td>minimum_size</td>
<td>Trust region minimum size</td>
</tr>
<tr>
<td>Optional</td>
<td>contract_threshold</td>
<td>contract_threshold</td>
<td>Shrink trust region if trust region ratio is below this value</td>
</tr>
<tr>
<td>Optional</td>
<td>expand_threshold</td>
<td>expand_threshold</td>
<td>Expand trust region if trust region ratio is above this value</td>
</tr>
<tr>
<td>Optional</td>
<td>contraction_factor</td>
<td>contraction_factor</td>
<td>Amount by which step length is rescaled</td>
</tr>
<tr>
<td>Optional</td>
<td>expansion_factor</td>
<td>expansion_factor</td>
<td>Trust region expansion factor</td>
</tr>
</tbody>
</table>

**Description**

The `trust_region` optional group specification can be used to specify the initial size of the trust region (using `initial_size`) relative to the total variable bounds, the minimum size of the trust region (using `minimum_size`), the contraction factor for the trust region size (using `contraction_factor`) used when the surrogate model is performing poorly, and the expansion factor for the trust region size (using `expansion_factor`) used
when the the surrogate model is performing well. Two additional commands are the trust region size contraction threshold (using `contract_threshold`) and the trust region size expansion threshold (using `expand_threshold`). These two commands are related to what is called the trust region ratio, which is the actual decrease in the truth model divided by the predicted decrease in the truth model in the current trust region. The command `contract_threshold` sets the minimum acceptable value for the trust region ratio, i.e., values below this threshold cause the trust region to shrink for the next SBL iteration. The command `expand_threshold` determines the trust region value above which the trust region will expand for the next SBL iteration.

`initial_size`

- Keywords Area
- method
- nowpac
- trust_region
- initial_size

Trust region initial size (relative to bounds)

**Specification**

**Alias:** none

**Argument(s):** REALLIST

**Description**

The `trust_region` optional group specification can be used to specify the initial size of the trust region (using `initial_size`) relative to the total variable bounds, the minimum size of the trust region (using `minimum_size`), the contraction factor for the trust region size (using `contraction_factor`) used when the surrogate model is performing poorly, and the expansion factor for the trust region size (using `expansion_factor`) used when the the surrogate model is performing well. Two additional commands are the trust region size contraction threshold (using `contract_threshold`) and the trust region size expansion threshold (using `expand_threshold`). These two commands are related to what is called the trust region ratio, which is the actual decrease in the truth model divided by the predicted decrease in the truth model in the current trust region. The command `contract_threshold` sets the minimum acceptable value for the trust region ratio, i.e., values below this threshold cause the trust region to shrink for the next SBL iteration. The command `expand_threshold` determines the trust region value above which the trust region will expand for the next SBL iteration.

All of these specifications are REAL scalars, with the exception of the specification of `initial_size`, which is a REALLIST. This array corresponds to the case when there are more than 2 model forms or discretizations within a model hierarchy. The default `initial_size` involves a recursive halving of the global bounds for each trust region in the hierarchy: e.g., a scalar value of .5 for a single trust region managing two model forms/discretizations, or an array of (.125, .25, .5) for four model forms/discretizations (three trust regions ordered from the lowest to highest fidelity surrogate, with model four as truth).

`minimum_size`

- Keywords Area
- method
CHAPTER 6. KEYWORDS AREA

- nowpac
- trust_region
- minimum_size

Trust region minimum size

**Specification**

*Alias:* none

*Argument(s):* REAL

*Default:* 1.e-6

**Description**

The `trust_region` optional group specification can be used to specify the initial size of the trust region (using `initial_size`) relative to the total variable bounds, the minimum size of the trust region (using `minimum_size`), the contraction factor for the trust region size (using `contraction_factor`) used when the surrogate model is performing poorly, and the expansion factor for the trust region size (using `expansion_factor`) used when the surrogate model is performing well. Two additional commands are the trust region size contraction threshold (using `contract_threshold`) and the trust region size expansion threshold (using `expand_threshold`). These two commands are related to what is called the trust region ratio, which is the actual decrease in the truth model divided by the predicted decrease in the truth model in the current trust region. The command `contract_threshold` sets the minimum acceptable value for the trust region ratio, i.e., values below this threshold cause the trust region to shrink for the next SBL iteration. The command `expand_threshold` determines the trust region value above which the trust region will expand for the next SBL iteration.

**contract_threshold**

- Keywords Area
- method
- nowpac
- trust_region
- contract_threshold

Shrink trust region if trust region ratio is below this value

**Specification**

*Alias:* none

*Argument(s):* REAL

*Default:* 0.25
6.2. METHOD

Description

The trust_region optional group specification can be used to specify the initial size of the trust region (using initial_size) relative to the total variable bounds, the minimum size of the trust region (using minimum_size), the contraction factor for the trust region size (using contraction_factor) used when the surrogate model is performing poorly, and the expansion factor for the trust region size (using expansion_factor) used when the surrogate model is performing well. Two additional commands are the trust region size contraction threshold (using contract_threshold) and the trust region size expansion threshold (using expand_threshold). These two commands are related to what is called the trust region ratio, which is the actual decrease in the truth model divided by the predicted decrease in the truth model in the current trust region. The command contract_threshold sets the minimum acceptable value for the trust region ratio, i.e., values below this threshold cause the trust region to shrink for the next SBL iteration. The command expand_threshold determines the trust region value above which the trust region will expand for the next SBL iteration.

expand_threshold

- Keywords Area
- method
- nowpac
- trust_region
- expand_threshold

Expand trust region if trust region ratio is above this value

Specification

Alias: none
Argument(s): REAL
Default: 0.75

Description

The trust_region optional group specification can be used to specify the initial size of the trust region (using initial_size) relative to the total variable bounds, the minimum size of the trust region (using minimum_size), the contraction factor for the trust region size (using contraction_factor) used when the surrogate model is performing poorly, and the expansion factor for the trust region size (using expansion_factor) used when the surrogate model is performing well. Two additional commands are the trust region size contraction threshold (using contract_threshold) and the trust region size expansion threshold (using expand_threshold). These two commands are related to what is called the trust region ratio, which is the actual decrease in the truth model divided by the predicted decrease in the truth model in the current trust region. The command contract_threshold sets the minimum acceptable value for the trust region ratio, i.e., values below this threshold cause the trust region to shrink for the next SBL iteration. The command expand_threshold determines the trust region value above which the trust region will expand for the next SBL iteration.
contraction_factor

- Keywords Area
- method
- nowpac
- trust_region
- contraction_factor

Amount by which step length is rescaled

**Specification**

Alias: none  
Argument(s): REAL  
Default: 0.25

**Description**

For pattern search methods, `contraction_factor` specifies the amount by which step length is rescaled after unsuccessful iterates, must be strictly between 0 and 1.

For methods that can expand the step length, the expansion is $1/\text{contraction\_factor}$

expansion_factor

- Keywords Area
- method
- nowpac
- trust_region
- expansion_factor

Trust region expansion factor

**Specification**

Alias: none  
Argument(s): REAL  
Default: 2.0
6.2. METHOD

Description

The trust_region optional group specification can be used to specify the initial size of the trust region (using initial_size) relative to the total variable bounds, the minimum size of the trust region (using minimum_size), the contraction factor for the trust region size (using contraction_factor) used when the surrogate model is performing poorly, and the expansion factor for the trust region size (using expansion_factor) used when the surrogate model is performing well. Two additional commands are the trust region size contraction threshold (using contract_threshold) and the trust region size expansion threshold (using expand_threshold). These two commands are related to what is called the trust region ratio, which is the actual decrease in the truth model divided by the predicted decrease in the truth model in the current trust region. The command contract_threshold sets the minimum acceptable value for the trust region ratio, i.e., values below this threshold cause the trust region to shrink for the next SBL iteration. The command expand_threshold determines the trust region value above which the trust region will expand for the next SBL iteration.

max_iterations

- Keywords Area
  - method
  - nowpac
  - max_iterations

Number of iterations allowed for optimizers and adaptive UQ methods

Topics

This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none

Argument(s): INTEGER

Default: 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence}/efficient_global: 25*n)

Description

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed max_iterations iterations. See also max_function_evaluations.

Default Behavior

Default value is 100.

max_function_evaluations

- Keywords Area
  - method
• nowpac

• max_function_evaluations

Number of function evaluations allowed for optimizers

Topics
This keyword is related to the topics:

• method_independent_controls

Specification
Alias: none

Argument(s): INTEGER
Default: 1000

Description
The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed max_function_evaluations evaluations. See also max_iterations.

Default Behavior
Default value is 1000.

scaling

• Keywords Area

• method

• nowpac

• scaling

Turn on scaling for variables, responses, and constraints

Topics
This keyword is related to the topics:

• method_independent_controls

Specification
Alias: none

Argument(s): none
Default: no scaling
6.2. METHOD

Description

Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by providing the `scaling` keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the `method`, `variables`, and `responses` blocks. When the `scaling` keyword is omitted, all `_scale_types` and `*_scales` specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.

- `a _scales` keyword, which gives characteristic values
- `a _scale_type` keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

Scale Types

There are four scale types:

1. none (default) - no scaling, value of `*_scales` keyword is ignored
2. value - multiplicative scaling
3. auto - automatic scaling
4. log - logarithmic scaling

First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:

- two-sided bounds scaled into the interval [0,1];
- one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
- no bounds or targets: no automatic scaling possible, therefore no scaling for this component

Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into [0,1].

4. log - logarithmic scaling

First, any characteristic values from the optional `*_scales` specification are applied. Then logarithm base 10 scaling is applied.

Logarithmic scaling is not available for linear constraints.

When continuous design variables are log scaled, linear constraints are not allowed.

Scales

The `*_scales` keywords are used to specify the characteristic values. These must be non-zero real numbers. The numbers are used according to the corresponding `*_scale_type`, as described above.

Depending on the scale type, the characteristic values may be required or optional.
• none, auto, log - optional

• value - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than 1.0e10*DBL_MIN. User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.

Examples

The two examples below are equivalent:

```
responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value"
  primary_scales = 1 1 100

responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value" "value" "value"
  primary_scales = 1 1 100
```

**model_pointer**

• Keywords Area

• method

• nowpac

• model_pointer

Identifier for model block to be used by a method

Topics

This keyword is related to the topics:

• block_pointer

Specification

Alias: none

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)

Description

The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.
6.2. METHOD

Usage Tips
When doing advanced analyses that involve using multiple methods and multiple models, defining a `model_pointer` for each method is imperative.
See `block_pointer` for details about pointers.

Examples

evironment
    tabular_graphics_data
    method_pointer = 'UQ'

method
    id_method = 'UQ'
    model_pointer = 'SURR'
    sampling,
        samples = 10
        seed = 98765 rng rnum2
        response_levels = 0.1 0.2 0.6
            0.1 0.2 0.6
            0.1 0.2 0.6
    sample_type lhs
distribution cumulative

model
    id_model = 'SURR'
surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
    id_method = 'DACE'
    model_pointer = 'DACE_M'
    sampling sample_type lhs
        samples = 121 seed = 5034 rng rnum2

model
    id_model = 'DACE_M'
single
    interface_pointer = 'I1'

variables
    uniform_uncertain = 2
    lower_bounds = 0. 0.
    upper_bounds = 1. 1.
    descriptors = 'x1' 'x2'

interface
    id_interface = 'I1'
system asynch evaluation_concurrency = 5
    analysis_driver = 'text_book'

responses
    response_functions = 3
    no_gradients
    no_hessians

6.2.33 snowpac

- Keywords Area
• method

• snowpac

Stochastic version of NOWPAC that incorporates error estimates and noise mitigation.

**Specification**

**Alias:** none

**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>seed</td>
<td>Seed of the random number generator</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>trust_region</td>
<td>Use trust region as the globalization strategy</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>max_iterations</td>
<td>Number of iterations allowed for optimizers and adaptive UQ methods</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>max_function_evaluations</td>
<td>Number of function evaluations allowed for optimizers</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>scaling</td>
<td>Turn on scaling for variables, responses, and constraints</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>model_pointer</td>
<td>Identifier for model block to be used by a method</td>
</tr>
</tbody>
</table>

**Description**

NOWPAC is a provably-convergent gradient-free optimization method from MIT that solves a series of trust region surrogate-based subproblems to generate improving steps. The stochastic version is SNOWPAC, which incorporates noise estimates in its objective and inequality constraints. SNOWPAC modifies its trust region controls and adds smoothing from a Gaussian process surrogate in order to mitigate noise. SNOWPAC also supports a feasibility restoration mode, so it is not necessary to start from a feasible design.

Note: (S)NOWPAC is not configured with Dakota by default and requires a separate installation of the NOWPAC distribution from MIT, combined with its TPLs of Eigen and NLOPT.
Examples

Relative to the NOWPAC specification, SNOWPAC supports a seed control for repeatability of runs and also requires the return of error estimates from the underlying evaluator (e.g., UQ method such as Monte Carlo sampling).

```
method,
  snowpac
  seed = 2504
  max_function_evaluations = 1000
  convergence_tolerance = 1e-4
  trust_region
    initial_size = 0.10
    minimum_size = 1.0e-6
    contract_threshold = 0.25
    expand_threshold = 0.75
    contraction_factor = 0.50
    expansion_factor = 1.50

seed

  • Keywords Area
  • method
  • snowpac
  • seed

Seed of the random number generator

Specification

Alias: none
  Argument(s): INTEGER
  Default: system-generated (non-repeatable)

Description

The random seed control provides a mechanism for making a stochastic method repeatable. That is, the use of the same random seed in identical studies will generate identical results.

Default Behavior
  If not specified, the seed is randomly generated.

Expected Output
  If seed is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

Usage Tips
  If a stochastic study was run without seed specified, and the user later wishes to repeat the study using the same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen. That value can then be added to the Dakota input file.
Examples

```plaintext
method
  sampling
    sample_type lhs
    samples = 10
    seed = 15347
```

trust_region

- Keywords Area
- method
- snowpac
- trust_region

Use trust region as the globalization strategy.

Specification

**Alias:** none

**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>initial_size</td>
<td></td>
<td>Trust region initial size (relative to bounds)</td>
</tr>
<tr>
<td>Optional</td>
<td>minimum_size</td>
<td></td>
<td>Trust region minimum size</td>
</tr>
<tr>
<td>Optional</td>
<td>contract_threshold</td>
<td></td>
<td>Shrink trust region if trust region ratio is below this value</td>
</tr>
<tr>
<td>Optional</td>
<td>expand_threshold</td>
<td></td>
<td>Expand trust region if trust region ratio is above this value</td>
</tr>
<tr>
<td>Optional</td>
<td>contraction_factor</td>
<td></td>
<td>Amount by which step length is rescaled</td>
</tr>
<tr>
<td>Optional</td>
<td>expansion_factor</td>
<td></td>
<td>Trust region expansion factor</td>
</tr>
</tbody>
</table>

Description

The `trust_region` optional group specification can be used to specify the initial size of the trust region (using `initial_size`) relative to the total variable bounds, the minimum size of the trust region (using `minimum_size`), the contraction factor for the trust region size (using `contraction_factor`) used when the surrogate model is performing poorly, and the expansion factor for the trust region size (using `expansion_factor`) used...
when the surrogate model is performing well. Two additional commands are the trust region size contraction threshold (using \texttt{contract\_threshold}) and the trust region size expansion threshold (using \texttt{expand\_threshold}). These two commands are related to what is called the trust region ratio, which is the actual decrease in the truth model divided by the predicted decrease in the truth model in the current trust region. The command \texttt{contract\_threshold} sets the minimum acceptable value for the trust region ratio, i.e., values below this threshold cause the trust region to shrink for the next SBL iteration. The command \texttt{expand\_threshold} determines the trust region value above which the trust region will expand for the next SBL iteration.

\begin{itemize}
\item \textbf{initial\_size}
\end{itemize}

- \textbf{Keywords Area}
- \textbf{method}
- \textbf{snowpac}
- \textbf{trust\_region}
- \textbf{initial\_size}

Trust region initial size (relative to bounds)

**Specification**

**Alias:** none

**Argument(s):** \texttt{REALLIST}

**Description**

The \texttt{trust\_region} optional group specification can be used to specify the initial size of the trust region (using \texttt{initial\_size}) relative to the total variable bounds, the minimum size of the trust region (using \texttt{minimum\_size}), the contraction factor for the trust region size (using \texttt{contraction\_factor}) used when the surrogate model is performing poorly, and the expansion factor for the trust region size (using \texttt{expansion\_factor}) used when the surrogate model is performing well. Two additional commands are the trust region size contraction threshold (using \texttt{contract\_threshold}) and the trust region size expansion threshold (using \texttt{expand\_threshold}). These two commands are related to what is called the trust region ratio, i.e., values below this threshold cause the trust region to shrink for the next SBL iteration. The command \texttt{expand\_threshold} determines the trust region value above which the trust region will expand for the next SBL iteration.

All of these specifications are \texttt{REAL} scalars, with the exception of the specification of \texttt{initial\_size}, which is a \texttt{REALLIST}. This array corresponds to the case when there are more than 2 model forms or discretizations within a model hierarchy. The default \texttt{initial\_size} involves a recursive halving of the global bounds for each trust region in the hierarchy: e.g., a scalar value of .5 for a single trust region managing two model forms/discretizations, or an array of (.125, .25, .5) for four model forms/discretizations (three trust regions ordered from the lowest to highest fidelity surrogate, with model four as truth).

\begin{itemize}
\item \textbf{minimum\_size}
\end{itemize}

- \textbf{Keywords Area}
- \textbf{method}
CHAPTER 6. KEYWORDS AREA

- snowpac
- trust_region
- minimum_size

Trust region minimum size

**Specification**

**Alias:** none

**Argument(s):** REAL

**Default:** 1.e-6

**Description**

The trust_region optional group specification can be used to specify the initial size of the trust region (using initial_size) relative to the total variable bounds, the minimum size of the trust region (using minimum_size), the contraction factor for the trust region size (using contraction_factor) used when the surrogate model is performing poorly, and the expansion factor for the trust region size (using expansion_factor) used when the surrogate model is performing well. Two additional commands are the trust region size contraction threshold (using contract_threshold) and the trust region size expansion threshold (using expand_threshold). These two commands are related to what is called the trust region ratio, which is the actual decrease in the truth model divided by the predicted decrease in the truth model in the current trust region. The command contract_threshold sets the minimum acceptable value for the trust region ratio, i.e., values below this threshold cause the trust region to shrink for the next SBL iteration. The command expand_threshold determines the trust region value above which the trust region will expand for the next SBL iteration.

**contract_threshold**

- Keywords Area
- method
- snowpac
- trust_region
- contract_threshold

Shrink trust region if trust region ratio is below this value

**Specification**

**Alias:** none

**Argument(s):** REAL

**Default:** 0.25
6.2. METHOD

Description

The `trust_region` optional group specification can be used to specify the initial size of the trust region (using `initial_size`) relative to the total variable bounds, the minimum size of the trust region (using `minimum_size`), the contraction factor for the trust region size (using `contraction_factor`) used when the surrogate model is performing poorly, and the expansion factor for the trust region size (using `expansion_factor`) used when the surrogate model is performing well. Two additional commands are the trust region size contraction threshold (using `contract_threshold`) and the trust region size expansion threshold (using `expand_threshold`). These two commands are related to what is called the trust region ratio, which is the actual decrease in the truth model divided by the predicted decrease in the truth model in the current trust region. The command `contract_threshold` sets the minimum acceptable value for the trust region ratio, i.e., values below this threshold cause the trust region to shrink for the next SBL iteration. The command `expand_threshold` determines the trust region value above which the trust region will expand for the next SBL iteration.

`expand_threshold`

- Keywords Area
- method
- snowpac
- trust_region
- expand_threshold

Expand trust region if trust region ratio is above this value

Specification

**Alias:** none

**Argument(s):** REAL

**Default:** 0.75

**Description**

The `trust_region` optional group specification can be used to specify the initial size of the trust region (using `initial_size`) relative to the total variable bounds, the minimum size of the trust region (using `minimum_size`), the contraction factor for the trust region size (using `contraction_factor`) used when the surrogate model is performing poorly, and the expansion factor for the trust region size (using `expansion_factor`) used when the surrogate model is performing well. Two additional commands are the trust region size contraction threshold (using `contract_threshold`) and the trust region size expansion threshold (using `expand_threshold`). These two commands are related to what is called the trust region ratio, which is the actual decrease in the truth model divided by the predicted decrease in the truth model in the current trust region. The command `contract_threshold` sets the minimum acceptable value for the trust region ratio, i.e., values below this threshold cause the trust region to shrink for the next SBL iteration. The command `expand_threshold` determines the trust region value above which the trust region will expand for the next SBL iteration.
**contraction_factor**

- **Keywords Area**
- **method**
- **snowpac**
- **trust_region**
- **contraction_factor**

Amount by which step length is rescaled

**Specification**

Alias: none

- **Argument(s):** REAL
- **Default:** 0.25

**Description**

For pattern search methods, `contraction_factor` specifies the amount by which step length is rescaled after unsuccessful iterates, must be strictly between 0 and 1.

For methods that can expand the step length, the expansion is $1/\text{contraction\_factor}$

**expansion_factor**

- **Keywords Area**
- **method**
- **snowpac**
- **trust_region**
- **expansion_factor**

Trust region expansion factor

**Specification**

Alias: none

- **Argument(s):** REAL
- **Default:** 2.0
6.2. METHOD

Description

The `trust_region` optional group specification can be used to specify the initial size of the trust region (using `initial_size`) relative to the total variable bounds, the minimum size of the trust region (using `minimum_size`), the contraction factor for the trust region size (using `contraction_factor`) used when the surrogate model is performing poorly, and the expansion factor for the trust region size (using `expansion_factor`) used when the surrogate model is performing well. Two additional commands are the trust region size contraction threshold (using `contract_threshold`) and the trust region size expansion threshold (using `expand_threshold`). These two commands are related to what is called the trust region ratio, which is the actual decrease in the truth model divided by the predicted decrease in the truth model in the current trust region. The command `contract_threshold` sets the minimum acceptable value for the trust region ratio, i.e., values below this threshold cause the trust region to shrink for the next SBL iteration. The command `expand_threshold` determines the trust region value above which the trust region will expand for the next SBL iteration.

**max_iterations**

- Keywords Area
- method
- snowpac
- `max_iterations`

Number of iterations allowed for optimizers and adaptive UQ methods

Topics

This keyword is related to the topics:

- `method_independent_controls`

Specification

**Alias:** none

**Argument(s):** INTEGER

**Default:** 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence} / efficient_global: 25*n)

Description

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed `max_iterations` iterations. See also `max_function_evaluations`.

**Default Behavior**

Default value is 100.

**max_function_evaluations**

- Keywords Area
- method
• snowpac

• max_function_evaluations

Number of function evaluations allowed for optimizers

Topics
This keyword is related to the topics:

• method_independent_controls

Specification
Alias: none
Argument(s): INTEGER
Default: 1000

Description
The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed max_function_evaluations evaluations. See also max_iterations.

Default Behavior
Default value is 1000.

scaling

• Keywords Area

• method

• snowpac

• scaling

Turn on scaling for variables, responses, and constraints

Topics
This keyword is related to the topics:

• method_independent_controls

Specification
Alias: none
Argument(s): none
Default: no scaling
6.2. **METHOD**

**Description**

Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by providing the `scaling` keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the `method`, `variables`, and `responses` blocks. When the `scaling` keyword is omitted, all `scale_types` and `∗_scales` specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.

- a `∗_scales` keyword, which gives characteristic values
- a `∗_scale_type` keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

**Scale Types**

There are four scale types:

1. `none` (default) - no scaling, value of `∗_scales` keyword is ignored
2. `value` - multiplicative scaling
3. `auto` - automatic scaling
   - First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:
     - two-sided bounds scaled into the interval [0,1];
     - one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
     - no bounds or targets: no automatic scaling possible, therefore no scaling for this component
   - Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into [0,1].
4. `log` - logarithmic scaling
   - First, any characteristic values from the optional `∗_scales` specification are applied. Then logarithm base 10 scaling is applied.
   - Logarithmic scaling is not available for linear constraints.

   When continuous design variables are log scaled, linear constraints are not allowed.

**Scales**

The `∗_scales` keywords are used to specify the characteristic values. These must be non-zero real numbers. The numbers are used according to the corresponding `∗_scale_type`, as described above.

Depending on the scale type, the characteristic values may be required or optional.
• none, auto, log - optional
• value - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than $1.0 \cdot 10^{-10} \cdot \text{DBL_MIN}$. User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.

Examples

The two examples below are equivalent:

```
responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value"
  primary_scales = 1 1 100

responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value" "value" "value"
  primary_scales = 1 1 100
```

model_pointer

• Keywords Area
• method
• snowpac
• model_pointer

Identifier for model block to be used by a method

Topics

This keyword is related to the topics:

• block_pointer

Specification

Alias: none
Argument(s): STRING
Default: method use of last model parsed (or use of default model if none parsed)

Description

The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.
6.2. METHOD

Usage Tips
When doing advanced analyses that involve using multiple methods and multiple models, defining a model-pointer for each method is imperative.
See block_pointer for details about pointers.

Examples

environment
tabular_graphics_data
method_pointer = 'UQ'

method
id_method = 'UQ'
model_pointer = 'SURR'
sampling,
samples = 10
seed = 98765 rng rnum2
response_levels = 0.1 0.2 0.6
0.1 0.2 0.6
0.1 0.2 0.6
sample_type lhs
distribution cumulative

model
id_model = 'SURR'
surrogate global,
daice_method_pointer = 'DACE'
polynomial quadratic

method
id_method = 'DACE'
model_pointer = 'DACE_M'
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = 'DACE_M'
single
interface_pointer = 'I1'

variables
uniform_uncertain = 2
lower_bounds = 0. 0.
upper_bounds = 1. 1.
descriptors = 'x1' 'x2'

interface
id_interface = 'I1'
system asynch evaluation_concurrency = 5
analysis_driver = 'text_book'

responses
response_functions = 3
no_gradients
no_hessians

6.2.34 moga

• Keywords Area
Multi-objective Genetic Algorithm (a.k.a Evolutionary Algorithm)

**Topics**
This keyword is related to the topics:
- package_jega

**Specification**

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of Group</th>
<th>Dakota Keyword Group</th>
<th>Dakota Keyword Description</th>
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<td>postprocessor_type</td>
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<td>Post process the final solution from moga</td>
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<td>Optional</td>
<td>max_iterations</td>
<td>max_iterations</td>
<td>Number of iterations allowed for optimizers and adaptive UQ methods</td>
</tr>
<tr>
<td>Optional</td>
<td>max_function_evaluations</td>
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<td>Number of function evaluations allowed for optimizers</td>
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6.2. METHOD

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<th>Turn on scaling for variables, responses, and constraints</th>
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<td>population_size</td>
<td>Set the initial population size in JEGA methods</td>
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<td>log_file</td>
<td>Specify the name of a log file</td>
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<td>Optional</td>
<td>print_each_pop</td>
<td>Print every population to a population file</td>
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<td>Optional</td>
<td>initialization_type</td>
<td>Specify how to initialize the population</td>
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<td>Select a crossover type for JEGA methods</td>
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<td>Optional</td>
<td>mutation_type</td>
<td>Select a mutation type for JEGA methods</td>
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<tr>
<td>Optional</td>
<td>seed</td>
<td>Seed of the random number generator</td>
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<td>convergence_tolerance</td>
<td>Stopping criterion based on convergence of the objective function or statistics</td>
</tr>
<tr>
<td>Optional</td>
<td>model_pointer</td>
<td>Identifier for model block to be used by a method</td>
</tr>
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</table>

Description

moga stands for Multi-objective Genetic Algorithm, which is a global optimization method that does Pareto optimization for multiple objectives. It supports general constraints and a mixture of real and discrete variables.

Constraints
moga can utilize linear constraints using the keywords:

- linear_inequality_constraint_matrix
- linear_inequality_lower_bounds
- linear_inequality_upper_bounds
- linear_inequality_scale_types
- linear_inequality_scales
- linear_equality_constraint_matrix
- linear_equality_targets
- linear_equality_scale_types
- linear_equality_scales

Configuration
The genetic algorithm configurations are:

1. fitness
2. replacement
3. niching
4. convergence
5. postprocessor
6. initialization
7. crossover
8. mutation
9. population size

The steps followed by the algorithm are listed below. The configurations will effect how the algorithm completes each step.

**Stopping Criteria**
The moga method respects the `max_iterations` and `max_function_evaluations` method independent controls to provide integer limits for the maximum number of generations and function evaluations, respectively.

The algorithm also stops when convergence is reached. This involves repeated assessment of the algorithm’s progress in solving the problem, until some criterion is met.

The specification for convergence in a moga can either be `metric_tracker` or can be omitted all together. If omitted, no convergence algorithm will be used and the algorithm will rely on stopping criteria only.

**Outputs**
The moga method respects the `output` method independent control to vary the amount of information presented to the user during execution.

The final results are written to the Dakota tabular output. Additional information is also available - see the `log_file` and `print_each_pop` keywords.

Note that moga and SOGA create additional output files during execution. “finaldata.dat” is a file that holds the final set of Pareto optimal solutions after any post-processing is complete. “discards.dat” holds solutions that were discarded from the population during the course of evolution.

It can often be useful to plot objective function values from these files to visually see the Pareto front and ensure that finaldata.dat solutions dominate discards.dat solutions. The solutions are written to these output files in the format “Input1...InputN..Output1...OutputM”.

**Important Notes**
The pool of potential members is the current population and the current set of offspring.

Choice of fitness assessors is strongly related to the type of replacement algorithm being used and can have a profound effect on the solutions selected for the next generation.

If using the fitness types `layer_rank` or `domination_count`, it is strongly recommended that you use the `replacement_type below_limit` (although the roulette wheel selectors can also be used).

The functionality of the domination_count selector of JEGA v1.0 can now be achieved using the domination_count fitness type and `below_limit` replacement type.

**Theory**
The basic steps of the moga algorithm are as follows:

1. Initialize the population
2. Evaluate the population (calculate the values of the objective function and constraints for each population member)
3. Loop until converged, or stopping criteria reached
   (a) Perform crossover
   (b) Perform mutation
   (c) Evaluate the new population
   (d) Assess the fitness of each member in the population
   (e) Replace the population with members selected to continue in the next generation
   (f) Apply niche pressure to the population
   (g) Test for convergence

4. Perform post processing

If moga is used in a hybrid optimization method (which requires one optimal solution from each individual optimization method to be passed to the subsequent optimization method as its starting point), the solution in the Pareto set closest to the "utopia" point is given as the best solution. This solution is also reported in the Dakota output.

This "best" solution in the Pareto set has minimum distance from the utopia point. The utopia point is defined as the point of extreme (best) values for each objective function. For example, if the Pareto front is bounded by (1,100) and (90,2), then (1,2) is the utopia point. There will be a point in the Pareto set that has minimum L2-norm distance to this point, for example (10,10) may be such a point.

If moga is used in a method which may require passing multiple solutions to the next level (such as the surrogate based global method or hybrid methods), the orthogonal_distance postprocessor type may be used to specify the distances between each solution value to winnow down the solutions in the full Pareto front to a subset which will be passed to the next iteration.

See Also
These keywords may also be of interest:

- soga

fitness_type

- Keywords Area
- method
- moga
- fitness_type

Select the fitness type for JEGA methods

Specification

Alias: none
Argument(s): none
Default: domination_count
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<tr>
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<th>Description of</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<td>Assign each member to a layer, based on domination the rank based on layers</td>
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<tr>
<td>Required/</td>
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<td>domination_count</td>
<td>Rank each member by the number of members that dominate it</td>
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</table>

**Description**

The two JEGA methods use different fitness types, which are described on their respective pages.

**layer_rank**

- Keywords Area
- method
- moga
- fitness_type
- layer_rank

Assign each member to a layer, based on domination the rank based on layers

**Specification**

Alias: none

**Argument(s):** none

**Description**

The fitness_type: layer_rank has been specifically designed to avoid problems with aggregating and scaling objective function values and transforming them into a single objective.

The layer_rank fitness assessor works by assigning all non-dominated designs a layer of 0, then from what remains, assigning all the non-dominated a layer of 1, and so on until all designs have been assigned a layer. The values are negated to follow the higher-is-better fitness convention.

Use of the below_limit selector with the layer_rank fitness assessor has the effect of keeping all those designs whose layer is below a certain threshold again subject to the shrinkage limit.

**domination_count**

- Keywords Area
- method
- moga
6.2. METHOD

- fitness_type
- domination_count

Rank each member by the number of members that dominate it

**Specification**

**Alias:** none  
**Argument(s):** none

**Description**

The fitness type: domination count has been specifically designed to avoid problems with aggregating and scaling objective function values and transforming them into a single objective.

Instead, the domination count fitness assessor works by ordering population members by the negative of the number of designs that dominate them. The values are negated in keeping with the convention that higher fitness is better.

The layer rank fitness assessor works by assigning all non-dominated designs a layer of 0, then from what remains, assigning all the non-dominated a layer of 1, and so on until all designs have been assigned a layer. Again, the values are negated for the higher-is-better fitness convention.

Use of the below limit selector with the domination count fitness assessor has the effect of keeping all designs that are dominated by fewer then a limiting number of other designs subject to the shrinkage limit.

Using it with the layer rank fitness assessor has the effect of keeping all those designs whose layer is below a certain threshold again subject to the shrinkage limit.

**replacement_type**

- Keywords Area
- method
- moga
- replacement_type

Select a replacement type for JEGA methods

**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** below_limit

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<td>Use the best designs to form a new population</td>
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CHAPTER 6. KEYWORDS AREA

<table>
<thead>
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<th>roulette_wheel</th>
<th>Replace population</th>
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<tr>
<td>unique_roulette_wheel</td>
<td>Replace population</td>
</tr>
<tr>
<td>below_limit</td>
<td>Limit number of designs dominating those kept</td>
</tr>
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</table>

Description

Replace the population with members selected to continue in the next generation. The pool of potential members is the current population and the current set of offspring. The replacement_type of roulette_wheel or unique_roulette_wheel may be used either with MOGA or SOGA problems however they are not recommended for use with MOGA. Given that the only two fitness assessors for MOGA are the layer_rank and domination_count, the recommended selector is the below_limit selector. The below_limit replacement will only keep designs that are dominated by fewer than a limiting number of other designs.

In roulette_wheel replacement, each design is conceptually allotted a portion of a wheel proportional to its fitness relative to the fitnesses of the other Designs. Then, portions of the wheel are chosen at random and the design occupying those portions are duplicated into the next population. Those Designs allotted larger portions of the wheel are more likely to be selected (potentially many times). unique_roulette_wheel replacement is the same as roulette_wheel replacement, with the exception that a design may only be selected once. The below_limit selector attempts to keep all designs for which the negated fitness is below a certain limit. The values are negated to keep with the convention that higher fitness is better. The inputs to the below_limit selector are the limit as a real value, and a shrinkage_percentage as a real value. The shrinkage_percentage defines the minimum amount of selections that will take place if enough designs are available. It is interpreted as a percentage of the population size that must go on to the subsequent generation. To enforce this, below_limit makes all the selections it would make anyway and if that is not enough, it takes the remaining that it needs from the best of what is left (effectively raising its limit as far as it must to get the minimum number of selections). It continues until it has made enough selections. The shrinkage_percentage is designed to prevent extreme decreases in the population size at any given generation, and thus prevent a big loss of genetic diversity in a very short time. Without a shrinkage limit, a small group of “super” designs may appear and quickly cull the population down to a size on the order of the limiting value. In this case, all the diversity of the population is lost and it is expensive to re-diversify and spread the population. The

The replacement_type for a SOGA may be roulette_wheel, unique_roulette_wheel, elitist, or favor_feasible. The elitist selector simply chooses the required number of designs taking the most fit. For example, if 100 selections are requested, then the top 100 designs as ranked by fitness will be selected and the remaining will be discarded. The favor_feasible replacement type first considers feasibility as a selection criteria. If that does not produce a “winner” then it moves on to considering fitness value. Because of this, any fitness assessor used with the favor_feasible selector must only account objectives in the creation of fitness. Therefore, there is such a fitness assessor and it’s use is enforced when the favor_feasible selector is chosen. In that case, and if the output level is set high enough, a message will be presented indicating that the weighted_sumonly fitness assessor will be used.

**elitist**

- Keywords Area
- method
- moga
- replacement_type
6.2. METHOD

- elitist

Use the best designs to form a new population

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

The elitist (default) setting creates a new population using (a) the replacement size best individuals from the current population, (b) and population size - replacement size individuals randomly selected from the newly generated individuals. It is possible in this case to lose a good solution from the newly generated individuals if it is not randomly selected for replacement; however, the default new_solutions_generated value is set such that the entire set of newly generated individuals will be selected for replacement.

**roulette_wheel**

- Keywords Area
- method
- moga
- replacement_type
- roulette_wheel

Replace population

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

Replace the population with members selected to continue in the next generation. The pool of potential members is the current population and the current set of offspring. The replacement_type of roulette_wheel or unique_roulette_wheel may be used either with MOGA or SOGA problems however they are not recommended for use with MOGA. Given that the only two fitness assessors for MOGA are the layer_rank and domination_count, the recommended selector is the below_limit selector. The below_limit replacement will only keep designs that are dominated by fewer than a limiting number of other designs. The replacement_type of favor_feasible is specific to a SOGA. This replacement operator will always prefer a more feasible design to a less feasible one. Beyond that, it favors solutions based on an assigned fitness value which must have been installed by the weighted sum only fitness assessor (see the discussion below).
unique_roulette_wheel

- Keywords Area
- method
- moga
- replacement_type
- unique_roulette_wheel

Replace population

**Specification**

**Alias:** none  
**Argument(s):** none

**Description**

Replace the population with members selected to continue in the next generation. The pool of potential members is the current population and the current set of offspring. The `replacement_type` of `roulette_wheel` or `unique_roulette_wheel` may be used either with MOGA or SOGA problems however they are not recommended for use with MOGA. Given that the only two fitness assessors for MOGA are the `layer_rank` and `domination_count`, the recommended selector is the `below_limit` selector. The `below_limit` replacement will only keep designs that are dominated by fewer than a limiting number of other designs. The `replacement_type` of `favor_feasible` is specific to a SOGA. This replacement operator will always prefer a more feasible design to a less feasible one. Beyond that, it favors solutions based on an assigned fitness value which must have been installed by the weighted sum only fitness assessor (see the discussion below).

**below_limit**

- Keywords Area
- method
- moga
- replacement_type
- below_limit

Limit number of designs dominating those kept

**Specification**

**Alias:** none  
**Argument(s):** REAL  
**Default:** 6
Description

The below_limit replacement will only keep designs that are dominated by fewer than a limiting number of other designs.

shrinkage_fraction

- Keywords Area
- method
- moga
- replacement_type
- below_limit
- shrinkage_fraction

Decrease the population size by a percentage

Specification

Alias: shrinkage_percentage
Argument(s): REAL
Default: 0.9

Description

As of JEGA v2.0, all replacement types are common to both MOGA and SOGA. They include the roulette_wheel, unique_roulette_wheel, elitist, and below_limit selectors. In roulette_wheel replacement, each design is conceptually allotted a portion of a wheel proportional to its fitness relative to the fitnesses of the other Designs. Then, portions of the wheel are chosen at random and the design occupying those portions are duplicated into the next population. Those Designs allotted larger portions of the wheel are more likely to be selected (potentially many times). unique_roulette_wheel replacement is the same as roulette_wheel replacement, with the exception that a design may only be selected once. The below_limit selector attempts to keep all designs for which the negated fitness is below a certain limit. The values are negated to keep with the convention that higher fitness is better. The inputs to the below_limit selector are the limit as a real value, and a shrinkage_percentage as a real value. The shrinkage_percentage defines the minimum amount of selections that will take place if enough designs are available. It is interpreted as a percentage of the population size that must go on to the subsequent generation. To enforce this, below_limit makes all the selections it would make anyway and if that is not enough, it takes the remaining that it needs from the best of what is left (effectively raising its limit as far as it must to get the minimum number of selections). It continues until it has made enough selections. The shrinkage_percentage is designed to prevent extreme decreases in the population size at any given generation, and thus prevent a big loss of genetic diversity in a very short time. Without a shrinkage limit, a small group of ”super” designs may appear and quickly cull the population down to
a size on the order of the limiting value. In this case, all the diversity of the population is lost and it is expensive to re-diversify and spread the population. The elitist selector simply chooses the required number of designs taking the most fit. For example, if 100 selections are requested, then the top 100 designs as ranked by fitness will be selected and the remaining will be discarded.

**niche_type**
- Keywords Area
- method
- moga
- niche_type

Specify the type of niching pressure

**Specification**

**Alias:** none
**Argument(s):** none
**Default:** No niche pressure

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<th>Description of Group</th>
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<th>Dakota Keyword Description</th>
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<td>radial</td>
<td>Set niching distance to percentage of non-dominated range</td>
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<tr>
<td></td>
<td>distance</td>
<td></td>
<td>Enforce minimum Euclidean distance between designs</td>
</tr>
<tr>
<td></td>
<td>max_designs</td>
<td></td>
<td>Limit number of solutions to remain in the population</td>
</tr>
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</table>

**Description**

The purpose of niching is to encourage differentiation along the Pareto frontier and thus a more even and uniform sampling.

This is typically accomplished by discouraging clustering of design points in the performance space. In JEGA, the application of niche pressure occurs as a secondary selection operation. The nicher is given a chance to perform a pre-selection operation prior to the operation of the selection (replacement) operator, and is then called to perform niching on the set of designs that were selected by the selection operator.

The radial nicher takes information input from the user to compute a minimum allowable distance between designs in the performance space and acts as a secondary selection operator whereby it enforces this minimum distance. The distance nicher requires that solutions must be separated from other solutions by a minimum distance in each dimension (vs. Euclidean distance for the radial niching). After niching is complete, all designs in the population will be at least the minimum distance from one another in all directions.

The radial niche pressure applicator works by enforcing a minimum Euclidean distance between designs in the performance space at each generation. The algorithm proceeds by starting at the (or one of the) extreme
designs along objective dimension 0 and marching through the population removing all designs that are too close to the current design. One exception to the rule is that the algorithm will never remove an extreme design which is defined as a design that is maximal or minimal in all but 1 objective dimension (for a classical 2 objective problem, the extreme designs are those at the tips of the non-dominated frontier). The distance nicher enforces a minimum distance in each dimension.

The designs that are removed by the nicher are not discarded. They are buffered and re-inserted into the population during the next pre-selection operation. This way, the selector is still the only operator that discards designs and the algorithm will not waste time "re-filling" gaps created by the nicher.

The radial nicher requires as input a vector of fractions with length equal to the number of objectives. The elements of the vector are interpreted as percentages of the non-dominated range for each objective defining a minimum distance to all other designs. All values should be in the range (0, 1). The minimum allowable distance between any two designs in the performance space is the Euclidian (simple square-root-sum-of-squares calculation) distance defined by these percentages. The distance nicher has a similar input vector requirement, only the distance is the minimum distance in each dimension.

The max_designs niche pressure applicator is designed to choose a limited number of solutions to remain in the population. That number is specified by num_designs. It does so in order to balance the tendency for populations to grow very large and thus consuming too many computer resources. It operates by ranking designs according to their fitness standing and a computed count of how many other designs are too close to them. Too close is a function of the supplied niche_vector, which specifies the minimum distance between any two points in the performance space along each dimension individually. Once the designs are all ranked, the top \( c \) \( \frac{1}{\text{num的设计}} \) designs are kept in the population and the remaining ones are buffered or discarded. Note that like other niching operators, this one will not discard an extreme design.

radial

- Keywords Area
- method
- moga
- niching_type
- radial

Set niching distance to percentage of non-dominated range

**Specification**

**Alias:** none

- **Argument(s):** REALLIST
- **Default:** 0.01 for all objectives

**Description**

The radial nicher requires as input a vector of fractions with length equal to the number of objectives. The elements of the vector are interpreted as percentages of the non-dominated range for each objective defining a minimum distance to all other designs. All values should be in the range (0, 1). The minimum allowable distance between any two designs in the performance space is the Euclidian (simple square-root-sum-of-squares calculation) distance defined by these percentages. The distance nicher has a similar input vector requirement, only the distance is the minimum distance in each dimension.
distance

- Keywords Area
- method
- moga
- niching_type
- distance

Enforce minimum Euclidean distance between designs

**Specification**

**Alias:** none

**Argument(s):** REALLIST

**Description**

Currently, the only niche pressure operators available are the radial nicher, the distance nicher, and the max_designs nicher. The radial niche pressure applicator works by enforcing a minimum Euclidean distance between designs in the performance space at each generation. The algorithm proceeds by starting at the (or one of the) extreme designs along objective dimension 0 and marching through the population removing all designs that are too close to the current design. One exception to the rule is that the algorithm will never remove an extreme design which is defined as a design that is maximal or minimal in all but 1 objective dimension (for a classical 2 objective problem, the extreme designs are those at the tips of the non-dominated frontier). The distance nicher enforces a minimum distance in each dimension.

The designs that are removed by the nicher are not discarded. They are buffered and re-inserted into the population during the next pre-selection operation. This way, the selector is still the only operator that discards designs and the algorithm will not waste time “re-filling” gaps created by the nicher.

max_designs

- Keywords Area
- method
- moga
- niching_type
- max_designs

Limit number of solutions to remain in the population

**Specification**

**Alias:** none

**Argument(s):** REALLIST
The \texttt{max\_designs} niche pressure applicator is designed to choose a limited number of solutions to remain in the population. That number is specified by \texttt{num\_designs}. It does so in order to balance the tendency for populations to grow very large and thus consuming too many computer resources. It operates by ranking designs according to their fitness standing and a computed count of how many other designs are too close to them. Too close is a function of the supplied niche\_vector, which specifies the minimum distance between any two points in the performance space along each dimension individually. Once the designs are all ranked, the top $c \cdot \texttt{num\_designs}$ designs designs are kept in the population and the remaining ones are buffered or discarded. Note that like other niching operators, this one will not discard an extreme design.

\begin{itemize}
  \item \texttt{num\_designs}
  \item Keywords Area
  \item method
  \item moga
  \item niching\_type
  \item max\_designs
  \item num\_designs
\end{itemize}

\textbf{Specification}

\textbf{Alias:} none
\begin{itemize}
  \item \textbf{Argument(s):} INTEGER
  \item \textbf{Default:} 100
\end{itemize}

\begin{itemize}
  \item \texttt{num\_designs}
  \item Keywords Area
  \item method
  \item moga
  \item niching\_type
  \item max\_designs
  \item num\_designs
\end{itemize}

Limit the number of solutions
convergence_type

- Keywords Area
- method
- moga
- convergence_type

Select the convergence type for JEGA methods

**Specification**

*Alias: none*

*Argument(s): none*

*Default: average_fitness_tracker*

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<th>Required/Optional</th>
<th>Description of Group</th>
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<th>Dakota Keyword Description</th>
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<td>Track changes in the non-dominated frontier</td>
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<tr>
<td>Optional</td>
<td>percent_change</td>
<td></td>
<td>Define the convergence criterion for JEGA methods</td>
</tr>
<tr>
<td>Optional</td>
<td>num_generations</td>
<td></td>
<td>Define the convergence criterion for JEGA methods</td>
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</table>

**Description**

The two JEGA methods use different convergence types, which are described on their respective pages.

All the convergence types are modified by the optional keywords `percent_change` and `num_generations`.

**metric_tracker**

- Keywords Area
- method
- moga
- convergence_type
- metric_tracker

Track changes in the non-dominated frontier
6.2. **METHOD**

**Specification**

*Alias:* none

*Argument(s):* none

*Default:* metric_tracker

**Description**

The moga converger (metric_tracker) operates by tracking various changes in the non-dominated frontier from generation to generation. When the changes occurring over a user specified number of generations fall below a user specified threshold, the algorithm stops.

If `metric_tracker` is specified, then a `percent_change` and `num_generations` must be supplied as well. These are listed as optional keywords in the input spec.

**Theory**

The `metric_tracker` converger tracks 3 metrics specific to the non-dominated frontier from generation to generation. All 3 of these metrics are computed as percent changes between the generations. In order to compute these metrics, the converger stores a duplicate of the non-dominated frontier at each generation for comparison to the non-dominated frontier of the next generation.

The first metric is one that indicates how the expanse of the frontier is changing. The expanse along a given objective is defined by the range of values existing within the non-dominated set. The expansion metric is computed by tracking the extremes of the non-dominated frontier from one generation to the next. Any movement of the extreme values is noticed and the maximum percentage movement is computed as:

\[
Em = \text{max over } j \text{ of } \frac{\text{abs}((\text{range}(j, i) - \text{range}(j, i-1))/\text{range}(j, i-1))}{j=1,\text{nof}}
\]

where `Em` is the max expansion metric, `j` is the objective function index, `i` is the current generation number, and `nof` is the total number of objectives. The range is the difference between the largest value along an objective and the smallest when considering only non-dominated designs.

The second metric monitors changes in the density of the non-dominated set. The density metric is computed as the number of non-dominated points divided by the hypervolume of the non-dominated region of space. Therefore, changes in the density can be caused by changes in the number of non-dominated points or by changes in size of the non-dominated space or both. The size of the non-dominated space is computed as:

\[
V_{ps}(i) = \text{product over } j \text{ of } \text{range}(j, i) \quad j=1,\text{nof}
\]

where `V_{ps}(i)` is the hypervolume of the non-dominated space at generation `i` and all other terms have the same meanings as above.

The density of a given non-dominated space is then:

\[
D_{ps}(i) = \frac{\text{Pct}(i)}{V_{ps}(i)}
\]

where `Pct(i)` is the number of points on the non-dominated frontier at generation `i`.

The percentage increase in density of the frontier is then calculated as

\[
Cd = \text{abs}((D_{ps}(i) - D_{ps}(i-1))/D_{ps}(i-1))
\]

where `Cd` is the change in density metric.

The final metric is one that monitors the ”goodness” of the non-dominated frontier. This metric is computed by considering each design in the previous population and determining if it is dominated by any designs in the current population. All that are determined to be dominated are counted. The metric is the ratio of the number that are dominated to the total number that exist in the previous population.

As mentioned above, each of these metrics is a percentage. The tracker records the largest of these three at each generation. Once the recorded percentage is below the supplied percent change for the supplied number of generations consecutively, the algorithm is converged.
percent_change

- Keywords Area
- method
- moga
- convergence_type
- percent_change

Define the convergence criterion for JEGA methods

**Specification**

*Alias:* none

*Argument(s):* REAL

*Default:* 0.1

**Description**

The `percent_change` is the threshold beneath which convergence is attained whereby it is compared to the metric value computed.

**num_generations**

- Keywords Area
- method
- moga
- convergence_type
- num_generations

Define the convergence criterion for JEGA methods

**Specification**

*Alias:* none

*Argument(s):* INTEGER

*Default:* 10

**Description**

The `num_generations` is the number of generations over which the metric value should be tracked. Convergence will be attained if the recorded metric is below `percent_change` for `num_generations` consecutive generations.
6.2. METHOD

**postprocessor_type**
- Keywords Area
- method
- moga
- postprocessor_type

Post process the final solution from moga

**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** No post-processing of solutions

<p>| Required/- | Description of | Dakota Keyword | Dakota Keyword |</p>
<table>
<thead>
<tr>
<th>Optional Required</th>
<th>Group</th>
<th>orthogonal_distance</th>
<th>Description</th>
</tr>
</thead>
</table>

**Description**

The purpose of this operation is to perform any needed data manipulations on the final solution deemed necessary. Currently the **orthogonal_distance** is the only one. It reduces the final solution set size such that a minimum distance in each direction exists between any two designs.

**orthogonal_distance**
- Keywords Area
- method
- moga
- postprocessor_type
- orthogonal_distance

Get subset of Pareto front based on distance

**Specification**

**Alias:** none  
**Argument(s):** REALLIST  
**Default:** 0.01 for all objectives
CHAPTER 6. KEYWORDS AREA

Description

Note that MOGA and SOGA create additional output files during execution. "finaldata.dat" is a file that holds the final set of Pareto optimal solutions after any post-processing is complete. "discards.dat" holds solutions that were discarded from the population during the course of evolution. It can often be useful to plot objective function values from these files to visually see the Pareto front and ensure that finaldata.dat solutions dominate discards.dat solutions. The solutions are written to these output files in the format "Input1...InputN..Output1...OutputM". If MOGA is used in a hybrid optimization meta-iteration (which requires one optimal solution from each individual optimization method to be passed to the subsequent optimization method as its starting point), the solution in the Pareto set closest to the "utopia" point is given as the best solution. This solution is also reported in the Dakota output. This "best" solution in the Pareto set has minimum distance from the utopia point. The utopia point is defined as the point of extreme (best) values for each objective function. For example, if the Pareto front is bounded by (1,100) and (90,2), then (1,2) is the utopia point. There will be a point in the Pareto set that has minimum L2-norm distance to this point, for example (10,10) may be such a point. In SOGA, the solution that minimizes the single objective function is returned as the best solution. If moga is used in meta-iteration which may require passing multiple solutions to the next level (such as the surrogate_based_global or hybrid methods), the orthogonal_distance postprocessor type may be used to specify the distances between each solution value to winnow down the solutions in the full Pareto front to a subset which will be passed to the next iteration.

max_iterations

- Keywords Area
- method
- moga
- max_iterations

Number of iterations allowed for optimizers and adaptive UQ methods

Topics

This keyword is related to the topics:
- method_independent_controls

Specification

Alias: none
Argument(s): INTEGER
Default: 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence} / efficient_global: 25*n)

Description

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed max_iterations iterations. See also max_function_evaluations.

Default Behavior
Default value is 100.
6.2. METHOD

max_function_evaluations

- Keywords Area
- method
- moga
- max_function_evaluations

Number of function evaluations allowed for optimizers

Topics

This keyword is related to the topics:
- method_independent_controls

Specification

Alias: none

Argument(s): INTEGER

Default: 1000

Description

The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed max_function_evaluations evaluations. See also max_iterations.

Default Behavior

Default value is 1000.

scaling

- Keywords Area
- method
- moga
- scaling

Turn on scaling for variables, responses, and constraints

Topics

This keyword is related to the topics:
- method_independent_controls

Specification

Alias: none

Argument(s): none

Default: no scaling
### Description

Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by providing the `scaling` keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the method, variables, and responses blocks. When the `scaling` keyword is omitted, all `_scale_types` and `∗_scales` specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.

- a `∗_scales` keyword, which gives characteristic values
- a `∗_scale_type` keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

### Scale Types

There are four scale types:

1. **none** (default) - no scaling, value of `∗_scales` keyword is ignored
2. **value** - multiplicative scaling
3. **auto** - automatic scaling
   
   First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:
   
   - two-sided bounds scaled into the interval [0,1];
   - one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
   - no bounds or targets: no automatic scaling possible, therefore no scaling for this component
   
   Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into [0,1].
4. **log** - logarithmic scaling
   
   First, any characteristic values from the optional `∗_scales` specification are applied. Then logarithm base 10 scaling is applied.

   Logarithmic scaling is not available for linear constraints.

   When continuous design variables are log scaled, linear constraints are not allowed.

### Scales

The `∗_scales` keywords are used to specify the characteristic values. These must be non-zero real numbers. The numbers are used according to the corresponding `∗_scale_type`, as described above.

Depending on the scale type, the characteristic values may be required or optional.
6.2. METHOD

- none, auto, log - optional
- value - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than $1.0 \times 10^{-10}$. User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.

Examples

The two examples below are equivalent:

```plaintext
responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value"
  primary_scales = 1 1 100

responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value" "value" "value"
  primary_scales = 1 1 100
```

population_size

- Keywords Area
- method
- moga
- population_size

Set the initial population size in JEGA methods

Specification

Alias: none

Argument(s): INTEGER

Default: 50

Description

The number of designs in the initial population is specified by the population_size. Note that the population_size only sets the size of the initial population. The population size may vary in the JEGA methods according to the type of operators chosen for a particular optimization run.

log_file

- Keywords Area
- method
- moga
- log_file

Specify the name of a log file
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none
  Argument(s): STRING
  Default: JEGAGlobal.log

Description

New as of JEGA v2.0 is the introduction of the log_file specification. JEGA now uses a logging library to output messages and status to the user. JEGA can be configured at build time to log to both the console window and a text file, one or the other, or neither. The log_file input is a string name of a file into which to log. If the build was configured without file logging in JEGA, this input is ignored. If file logging is enabled and no log_file is specified, the default file name of JEGAGlobal.log is used.

print_each_pop

  • Keywords Area
  • method
  • moga
  • print_each_pop

  Print every population to a population file

Specification

Alias: none
  Argument(s): none
  Default: No printing

Description

New to JEGA v2.0 is the introduction of the print_each_pop specification. It serves as a flag and if supplied, the population at each generation will be printed to a file named "population<GEN#>.dat" where <GEN#> is the number of the current generation.

initialization_type

  • Keywords Area
  • method
  • moga
  • initialization_type

  Specify how to initialize the population

Specification

Alias: none
  Argument(s): none
  Default: unique_random
### Description

The `initialization_type` defines how the initial population is created for the GA. There are three types:

1. `simple_random`
2. `unique_random` (default)
3. `flat_file`

Setting the size for the `flat_file` initializer has the effect of requiring a minimum number of designs to create. If this minimum number has not been created once the files are all read, the rest are created using the `unique_random` initializer and then the `simple_random` initializer if necessary.

#### `simple_random`

- **Keywords Area**
  - `method`
  - `moga`
  - `initialization_type`
  - `simple_random`

Create random initial solutions

#### Specification

**Alias:** none

**Argument(s):** none

#### Description

`simple_random` creates initial solutions with random variable values according to a uniform random number distribution. It gives no consideration to any previously generated designs.
**unique_random**

- **Keywords Area**
- **method**
- **moga**
- **initialization_type**
- **unique_random**

Create random initial solutions, but enforce uniqueness (default)

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

`unique_random` is the same as `simple_random`, except that when a new solution is generated, it is checked against the rest of the solutions. If it duplicates any of them, it is rejected.

**flat_file**

- **Keywords Area**
- **method**
- **moga**
- **initialization_type**
- **flat_file**

Read initial solutions from file

**Specification**

**Alias:** none

**Argument(s):** STRING

**Description**

`flat_file` allows the initial population to be read from a flat file. If `flat_file` is specified, a file name must be given.

Variables can be delimited in the flat file in any way you see fit with a few exceptions. The delimiter must be the same on any given line of input with the exception of leading and trailing whitespace. So a line could look like: 1.1, 2.2, 3.3 for example but could not look like: 1.1, 2.2 3.3. The delimiter can vary from line to line within the file which can be useful if data from multiple sources is pasted into the same input file. The delimiter can be any string that does not contain any of the characters .+-dDeE or any of the digits 0-9. The input will be read until the end of the file. The algorithm will discard any configurations for which it was unable to retrieve at least the
6.2. METHOD

number of design variables. The objective and constraint entries are not required but if ALL are present, they will be recorded and the design will be tagged as evaluated so that evaluators may choose not to re-evaluate them.

Setting the size for this initializer has the effect of requiring a minimum number of designs to create. If this minimum number has not been created once the files are all read, the rest are created using the unique_random initializer and then the simple_random initializer if necessary.

crossover_type

- Keywords Area
- method
- moga
- crossover_type

Select a crossover type for JEGA methods

Specification

Alias: none
Argument(s): none
Default: shuffle_random

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dako...</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required</td>
<td>Group 1</td>
<td>Dako...</td>
</tr>
<tr>
<td>multi_point_binary</td>
<td>Use bit switching for crossover events</td>
<td></td>
</tr>
<tr>
<td>multi_point_parameterized_binary</td>
<td>Use bit switching to crossover each design variable</td>
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<tr>
<td>multi_point_real</td>
<td>Perform crossover in real valued genome</td>
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</tr>
<tr>
<td>shuffle_random</td>
<td>Perform crossover by choosing design variable(s)</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td></td>
</tr>
<tr>
<td>crossover_rate</td>
<td>Specify the probability of a crossover event</td>
<td></td>
</tr>
</tbody>
</table>

Description

There are many crossover types available. multi_point_binary crossover requires an integer number, N, of crossover points. This crossover type performs a bit switching crossover at N crossover points in the binary encoded genome of two designs. Thus, crossover may occur at any point along a solution chromosome (in the middle of a gene representing a design variable, for example). multi_point_parameterized_binary crossover is similar in that it performs a bit switching crossover routine at N crossover points. However, this crossover type performs crossover on each design variable individually. So the individual chromosomes are crossed at N locations. multi_point_real crossover performs a variable switching crossover routine at N crossover points in the real real valued genome of two designs. In this scheme, crossover only occurs between design variables.
(chromosomes). Note that the standard solution chromosome representation in the JEGA algorithm is real encoded and can handle integer or real design variables. For any crossover types that use a binary representation, real variables are converted to long integers by multiplying the real number by $10^6$ and then truncating. Note that this assumes a precision of only six decimal places. Discrete variables are represented as integers (indices within a list of possible values) within the algorithm and thus require no special treatment by the binary operators.

The final crossover type is shuffle_random. This crossover type performs crossover by choosing design variables at random from a specified number of parents enough times that the requested number of children are produced. For example, consider the case of 3 parents producing 2 children. This operator would go through and for each design variable, select one of the parents as the donor for the child. So it creates a random shuffle of the parent design variable values. The relative numbers of children and parents are controllable to allow for as much mixing as desired. The more parents involved, the less likely that the children will wind up exact duplicates of the parents.

All crossover types take a crossover_rate. The crossover rate is used to calculate the number of crossover operations that take place. The number of crossovers is equal to the rate $\times$ population_size.

**multi_point_binary**

- Keywords Area
- method
- moga
- crossover_type
- multi_point_binary

Use bit switching for crossover events

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Description**

There are many crossover types available. multi_point_binary crossover requires an integer number, N, of crossover points. This crossover type performs a bit switching crossover at N crossover points in the binary encoded genome of two designs. Thus, crossover may occur at any point along a solution chromosome (in the middle of a gene representing a design variable, for example). multi_point_parameterized_binary crossover is similar in that it performs a bit switching crossover routine at N crossover points. However, this crossover type performs crossover on each design variable individually. So the individual chromosomes are crossed at N locations. multi_point_real crossover performs a variable switching crossover routing at N crossover points in the real real valued genome of two designs. In this scheme, crossover only occurs between design variables (chromosomes). Note that the standard solution chromosome representation in the JEGA algorithm is real encoded and can handle integer or real design variables. For any crossover types that use a binary representation, real variables are converted to long integers by multiplying the real number by $10^6$ and then truncating. Note that this assumes a precision of only six decimal places. Discrete variables are represented as integers (indices within a list of possible values) within the algorithm and thus require no special treatment by the binary operators.
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**multi_point_parameterized_binary**

- **Keywords Area**
- **method**
- **moga**
- **crossover_type**
- **multi_point_parameterized_binary**

Use bit switching to crossover each design variable

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Description**

There are many crossover types available. **multi_point_binary** crossover requires an integer number, N, of crossover points. This crossover type performs a bit switching crossover at N crossover points in the binary encoded genome of two designs. Thus, crossover may occur at any point along a solution chromosome (in the middle of a gene representing a design variable, for example). **multi_point_parameterized_binary** crossover is similar in that it performs a bit switching crossover routine at N crossover points. However, this crossover type performs crossover on each design variable individually. So the individual chromosomes are crossed at N locations. **multi_point_real** crossover performs a variable switching crossover routing at N crossover points in the real real valued genome of two designs. In this scheme, crossover only occurs between design variables (chromosomes). Note that the standard solution chromosome representation in the JEGA algorithm is real encoded and can handle integer or real design variables. For any crossover types that use a binary representation, real variables are converted to long integers by multiplying the real number by $10^6$ and then truncating. Note that this assumes a precision of only six decimal places. Discrete variables are represented as integers (indices within a list of possible values) within the algorithm and thus require no special treatment by the binary operators.

**multi_point_real**

- **Keywords Area**
- **method**
- **moga**
- **crossover_type**
- **multi_point_real**

Perform crossover in real valued genome

**Specification**

**Alias:** none

**Argument(s):** INTEGER
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**Description**

There are many crossover types available. `multi_point_binary` crossover requires an integer number, N, of crossover points. This crossover type performs a bit switching crossover at N crossover points in the binary encoded genome of two designs. Thus, crossover may occur at any point along a solution chromosome (in the middle of a gene representing a design variable, for example). `multi_point_parameterized_binary` crossover is similar in that it performs a bit switching crossover routine at N crossover points. However, this crossover type performs crossover on each design variable individually. So the individual chromosomes are crossed at N locations. `multi_point_real` crossover performs a variable switching crossover routing at N crossover points in the real real valued genome of two designs. In this scheme, crossover only occurs between design variables (chromosomes). Note that the standard solution chromosome representation in the JEGA algorithm is real encoded and can handle integer or real design variables. For any crossover types that use a binary representation, real variables are converted to long integers by multiplying the real number by $10^6$ and then truncating. Note that this assumes a precision of only six decimal places. Discrete variables are represented as integers (indices within a list of possible values) within the algorithm and thus require no special treatment by the binary operators.

**shuffle_random**

- **Keywords Area**
- **method**
- **moga**
- **crossover_type**
- **shuffle_random**

Perform crossover by choosing design variable(s)

**Specification**

**Alias:** none

**Argument(s):** none

| Required/-  | Description of Group | Dakota Keyword | Dakota Keyword Description |
| Optinal     |                      |                |                           |
| num_parents |                      |                | Number of parents in random shuffle crossover |
| num_offspring |                   |                | Number of offspring in random shuffle crossover |

**Description**

The final crossover type is `shuffle_random`. This crossover type performs crossover by choosing design variables at random from a specified number of parents enough times that the requested number of children are produced. For example, consider the case of 3 parents producing 2 children. This operator would go through and for each design variable, select one of the parents as the donor for the child. So it creates a random shuffle of the parent design variable values. The relative numbers of children and parents are controllable to allow for as much mixing as desired. The more parents involved, the less likely that the children will wind up exact duplicates of the parents.
6.2. METHOD

num_parents

- Keywords Area
- method
- moga
- crossover_type
- shuffle_random
- num_parents

Number of parents in random shuffle crossover

**Specification**

**Alias:** none

- **Argument(s):** INTEGER
- **Default:** 2

**Description**

Number of parents in random shuffle crossover

num_offspring

- Keywords Area
- method
- moga
- crossover_type
- shuffle_random
- num_offspring

Number of offspring in random shuffle crossover

**Specification**

**Alias:** none

- **Argument(s):** INTEGER
- **Default:** 2

**Description**

Number of offspring in random shuffle crossover
crossover_rate

- Keywords Area
- method
- moga
- crossover_type
- crossover_rate

Specify the probability of a crossover event

**Specification**

Alias: none

- **Argument(s):** REAL
- **Default:** 0.8

**Description**

The `crossover_type` controls what approach is employed for combining parent genetic information to create offspring, and the `crossover_rate` specifies the probability of a crossover operation being performed to generate a new offspring. The SCOLIB EA method supports three forms of crossover, two_point, blend, and uniform, which generate a new individual through combinations of two parent individuals. Two-point crossover divides each parent into three regions, where offspring are created from the combination of the middle region from one parent and the end regions from the other parent. Since the SCOLIB EA does not utilize bit representations of variable values, the crossover points only occur on coordinate boundaries, never within the bits of a particular coordinate. Uniform crossover creates offspring through random combination of coordinates from the two parents. Blend crossover generates a new individual randomly along the multidimensional vector connecting the two parents.

mutation_type

- Keywords Area
- method
- moga
- mutation_type

Select a mutation type for JEGA methods

**Specification**

Alias: none

- **Argument(s):** none
- **Default:** replace_uniform
## Description

Five mutation types are available for selection by keyword: `replace_uniform`, `bit_random`, `offset_cauchy`, `offset_normal`, and `offset_uniform`. They are described in greater detail on their respective keyword pages.

The `offset_*` mutators all act by adding a random "offset" to a variable value. The random amount has a mean of zero in all cases. The size of the offset is controlled using the `mutation_scale` keyword, which is interpreted differently for each `offset_*` type.

The rate of mutations for all types is controlled using the `mutation_rate`. The rate is applied differently in each `mutation_type`.

### bit_random

- **Keywords Area**
- **method**
- **moga**
- **mutation_type**
- **bit_random**

Mutate by flipping a random bit

### Specification

**Alias:** none

**Argument(s):** none
Description

The `bit_random` mutator introduces random variation by first converting a randomly chosen variable of a randomly chosen design into a binary string. It then flips a randomly chosen bit in the string from a 1 to a 0 or visa versa. In this mutation scheme, the resulting value has more probability of being similar to the original value.

`replace_uniform`

- **Keywords Area**
- **method**
- **moga**
- **mutation_type**
- **replace_uniform**

Use uniformly distributed value over range of parameter

Specification

**Alias:** none

**Argument(s):** none

Description

`replace_uniform` introduces random variation by first randomly choosing a design variable of a randomly selected design and reassigning it to a random valid value for that variable. No consideration of the current value is given when determining the new value.

`offset_normal`

- **Keywords Area**
- **method**
- **moga**
- **mutation_type**
- **offset_normal**

Set mutation offset to use a normal distribution

Specification

**Alias:** none

**Argument(s):** none
Description

The offset_normal mutator introduces random variation by adding a Gaussian random amount to a variable value. The random amount has a standard deviation dependent on the mutation_scale.

<table>
<thead>
<tr>
<th>Optional</th>
<th>mutation_scale</th>
<th>Scales mutation across range of parameter</th>
</tr>
</thead>
</table>

**mutation_scale**
- Keywords Area
- method
- moga
- mutation_type
- offset_normal
- mutation_scale
  Scales mutation across range of parameter

**Specification**

*Alias:* none

*Argument(s):* REAL

*Default:* 0.15

**Description**

The mutation_scale is a fraction in the range [0, 1] and is meant to help control the amount of variation that takes place when a variable is mutated. Its behavior depends on the selected mutation_type. For offset_normal and offset_cauchy, mutation_scale is multiplied by the range of the variable being mutated to obtain the standard deviation of the offset. For offset_uniform, the range of possible deviation amounts is +/- 1/2 * (mutation_scale * variable range).

**offset_cauchy**
- Keywords Area
- method
- moga
- mutation_type
- offset_cauchy
  Use a Cauchy distribution for the mutation offset

**Specification**

*Alias:* none

*Argument(s):* none
### Description

The *offset_cauchy* mutator introduces random variation by adding a Cauchy random amount to a variable value. The random amount has a standard deviation dependent on the *mutation_scale*.

- **mutation_scale**
  - Keywords Area
  - method
  - moga
  - mutation_type
  - offset_cauchy
  - mutation_scale

  Scales mutation across range of parameter

### Specification

- **Alias**: none
- **Argument(s)**: REAL
- **Default**: 0.15

### Description

The *mutation_scale* is a fraction in the range [0, 1] and is meant to help control the amount of variation that takes place when a variable is mutated. Its behavior depends on the selected *mutation_type*. For *offset_normal* and *offset_cauchy*, *mutation_scale* is multiplied by the range of the variable being mutated to obtain the standard deviation of the offset. For *offset_uniform*, the range of possible deviation amounts is +/- 1/2 * (mutation_scale * variable range).

- **offset_uniform**
  - Keywords Area
  - method
  - moga
  - mutation_type
  - offset_uniform

  Set mutation offset to use a uniform distribution
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Specification

Alias: none

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>mutation_scale</td>
<td>Scales mutation across range of parameter</td>
</tr>
</tbody>
</table>

Description

The `offset_uniform` mutator introduces random variation by adding a uniform random amount to a variable value. The random amount depends on the `mutation_scale`.

- **mutation_scale**
  - Keywords Area
  - method
  - moga
  - mutation_type
  - offset_uniform
  - mutation_scale

  Scales mutation across range of parameter

Specification

Alias: none

Argument(s): REAL

Default: 0.15

Description

The `mutation_scale` is a fraction in the range [0, 1] and is meant to help control the amount of variation that takes place when a variable is mutated. Its behavior depends on the selected `mutation_type`. For `offset_normal` and `offset_cauchy`, `mutation_scale` is multiplied by the range of the variable being mutated to obtain the standard deviation of the offset. For `offset_uniform`, the range of possible deviation amounts is +/- 1/2 * (mutation_scale * variable range).

- **mutation_rate**
  - Keywords Area
  - method
  - moga
  - mutation_type
• **mutation_rate**

Set probability of a mutation

### Specification

**Alias:** none  
**Argument(s):** REAL  
**Default:** 0.08

### Description

All mutation types have a `mutation_rate`, which controls the number of mutations performed. For `replace-uniform` and all the `offset_*` types, the number of mutations performed is the product of `mutation_rate` and `population_size`. For `bit_random`, it's the product of the `mutation_rate`, number of design variables, and `population_size`.

**seed**

• **Keywords Area**

• **method**

• **moga**

• **seed**

Seed of the random number generator

### Specification

**Alias:** none  
**Argument(s):** INTEGER  
**Default:** system-generated (non-repeatable)

### Description

The random `seed` control provides a mechanism for making a stochastic method repeatable. That is, the use of the same random seed in identical studies will generate identical results.

**Default Behavior**

If not specified, the seed is randomly generated.

**Expected Output**

If `seed` is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

**Usage Tips**

If a stochastic study was run without `seed` specified, and the user later wishes to repeat the study using the same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen. That value can then be added to the Dakota input file.
6.2. METHOD

Examples

method
   sampling
      sample_type lhs
      samples = 10
      seed = 15347

convergence_tolerance

- Keywords Area
- method
- moga
- convergence_tolerance

Stopping criterion based on convergence of the objective function or statistics

Topics

This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none

Argument(s): REAL

Default: \[1.e^{-4}\]

Description

The convergence_tolerance specification provides a real value for controlling the termination of iteration. For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by convergence_tolerance, then this convergence criterion is satisfied on the current iteration. Therefore, permissible values are between 0 and 1, non-inclusive.

Behavior Varies by Package/Library

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- DOT: must be satisfied for two consecutive iterations
• NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of convergence_tolerance approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., convergence_tolerance = 1.e-6 will result in approximately six digits of accuracy in the final objective function).

• NL2SOL: See nl2sol

model_pointer

- Keywords Area
- method
- moga
- model_pointer

Identifier for model block to be used by a method

Topics

This keyword is related to the topics:

- block_pointer

Specification

Alias: none

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)

Description

The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.

Usage Tips

When doing advanced analyses that involve using multiple methods and multiple models, defining a model_pointer for each method is imperative.

See block_pointer for details about pointers.

Examples

```plaintext
environment
tabular_graphics_data
method_pointer = 'UQ'

method
id_method = 'UQ'
model_pointer = 'SURR'
sampling,
```
6.2. METHOD

samples = 10
seed = 98765 rng rnum2
response_levels = 0.1 0.2 0.6 0.1 0.2 0.6
sample_type lhs
distribution cumulative

model
id_model = 'SURR'
surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
id_method = 'DACE'
model_pointer = 'DACE_M'
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = 'DACE_M'
single
interface_pointer = 'I1'

variables
uniform_uncertain = 2
lower_bounds = 0. 0.
upper_bounds = 1. 1.
descriptors = 'x1' 'x2'

interface
id_interface = 'I1'
system asynch evaluation_concurrency = 5
analysis_driver = 'text_book'

responses
response_functions = 3
no_gradients
no_hessians

6.2.35 soga

- Keywords Area
- method
- soga

Single-objective Genetic Algorithm (a.k.a Evolutionary Algorithm)

Topics
This keyword is related to the topics:

- package_jega
- global_optimization_methods
## Specification

**Alias:** none  
**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>fitness_type</td>
<td></td>
<td>Select the fitness type for JEGA methods</td>
</tr>
<tr>
<td>Optional</td>
<td>replacement_type</td>
<td></td>
<td>Select a replacement type for JEGA methods</td>
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<tr>
<td>Optional</td>
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<td></td>
<td>Select the convergence type for JEGA methods</td>
</tr>
<tr>
<td>Optional</td>
<td>max_iterations</td>
<td></td>
<td>Number of iterations allowed for optimizers and adaptive UQ methods</td>
</tr>
<tr>
<td>Optional</td>
<td>max_function_evaluations</td>
<td></td>
<td>Number of function evaluations allowed for optimizers</td>
</tr>
<tr>
<td>Optional</td>
<td>scaling</td>
<td></td>
<td>Turn on scaling for variables, responses, and constraints</td>
</tr>
<tr>
<td>Optional</td>
<td>population_size</td>
<td></td>
<td>Set the initial population size in JEGA methods</td>
</tr>
<tr>
<td>Optional</td>
<td>log_file</td>
<td></td>
<td>Specify the name of a log file</td>
</tr>
<tr>
<td>Optional</td>
<td>print_each_pop</td>
<td></td>
<td>Print every population to a population file</td>
</tr>
<tr>
<td>Optional</td>
<td>initialization_type</td>
<td></td>
<td>Specify how to initialize the population</td>
</tr>
</tbody>
</table>
### Description

**soga** stands for Single-objective Genetic Algorithm, which is a global optimization method that supports general constraints and a mixture of real and discrete variables. **soga** is part of the JEGA library.

**Constraints** **soga** can utilize linear constraints.

**Configuration**

The genetic algorithm configurations are:

1. fitness
2. replacement
3. convergence
4. initialization
5. crossover
6. mutation
7. population size

The pool of potential members is the current population and the current set of offspring. Choice of fitness assessors is strongly related to the type of replacement algorithm being used and can have a profound effect on the solutions selected for the next generation.

**Stopping Criteria**

The **soga** method respects the **max_iterations** and **max_function_evaluations** method independent controls to provide integer limits for the maximum number of generations and function evaluations, respectively.

The algorithm also stops when convergence is reached. This involves repeated assessment of the algorithm’s progress in solving the problem, until some criterion is met.

**Outputs** The **soga** method respects the **output** method independent control to vary the amount of information presented to the user during execution.
The final results are written to the Dakota tabular output. Additional information is also available - see the `log_file` and `print_each_pop` keywords.

**Theory**

The basic steps of the `soga` algorithm are as follows:

1. Initialize the population
2. Evaluate the population (calculate the values of the objective function and constraints for each population member)
3. Loop until converged, or stopping criteria reached
   (a) Perform crossover
   (b) Perform mutation
   (c) Evaluate the new population
   (d) Assess the fitness of each member in the population
   (e) Replace the population with members selected to continue in the next generation
   (f) Test for convergence

**See Also**

These keywords may also be of interest:

- moga

**fitness_type**

- Keywords Area
- method
- soga
- fitness_type

Select the fitness type for JEGA methods

**Specification**

Alias: none

Argument(s): none

Default: `merit_function`

<table>
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<tr>
<th>Required/-</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<tr>
<td>Optional</td>
<td></td>
<td>merit_function</td>
<td>Balance goals of reducing objective function and satisfying constraints</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>constraint_penalty</td>
<td>Multiplier for the penalty function</td>
</tr>
</tbody>
</table>
6.2. METHOD

Description
The two JEGA methods use different fitness types, which are described on their respective pages.

merit_function

- Keywords Area
- method
- soga
- fitness_type
- merit_function

Balance goals of reducing objective function and satisfying constraints

Specification
Alias: none
Argument(s): none

Description
A merit_function is a function in constrained optimization that attempts to provide joint progress toward reducing the objective function and satisfying the constraints.

constraint_penalty

- Keywords Area
- method
- soga
- fitness_type
- constraint_penalty

Multiplier for the penalty function

Specification
Alias: none
Argument(s): REAL
Default: 1.0

Description
The merit_function fitness assessor uses an exterior penalty function formulation to penalize infeasible designs. The specification allows the input of a constraint_penalty which is the multiplier to use on the constraint violations.
replacement_type
  • Keywords Area
  • method
  • soga
  • replacement_type

Select a replacement type for JEGA methods

Specification
Alias: none
Argument(s): none
Default: elitist

<table>
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<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<td>elitist</td>
<td>Use the best designs to form a new population</td>
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</thead>
<tbody>
<tr>
<td>favor_feasible</td>
<td>Prioritize feasible designs</td>
<td></td>
<td></td>
</tr>
<tr>
<td>roulette_wheel</td>
<td>Replace population</td>
<td></td>
<td></td>
</tr>
<tr>
<td>unique_roulette_wheel</td>
<td>Replace population</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Description
Replace the population with members selected to continue in the next generation. The pool of potential members is the current population and the current set of offspring. The replacement_type of roulette_wheel or unique_roulette_wheel may be used either with MOGA or SOGA problems however they are not recommended for use with MOGA. Given that the only two fitness assessors for MOGA are the layer_rank and domination_count, the recommended selector is the below_limit selector. The below_limit replacement will only keep designs that are dominated by fewer than a limiting number of other designs.

In roulette_wheel replacement, each design is conceptually allotted a portion of a wheel proportional to its fitness relative to the fitnesses of the other Designs. Then, portions of the wheel are chosen at random and the design occupying those portions are duplicated into the next population. Those Designs allotted larger portions of the wheel are more likely to be selected (potentially many times). unique_roulette_wheel replacement is the same as roulette_wheel replacement, with the exception that a design may only be selected once. The below_limit selector attempts to keep all designs for which the negated fitness is below a certain limit. The values are negated to keep with the convention that higher fitness is better. The inputs to the below_limit selector are the limit as a real value, and a shrinkage_percentage as a real value. The shrinkage_percentage defines the minimum amount of selections that will take place if enough designs are available. It is interpreted as a percentage of the population size that must go on to the subsequent generation. To enforce this, below_limit makes all the selections it would make anyway and if that is not enough, it takes the remaining that it needs from the best of what is left (effectively raising its limit as far as it must to get the minimum number of selections). It continues until it has made enough selections. The shrinkage_percentage is designed to prevent extreme decreases in the population size at any given generation, and thus prevent a big loss of genetic diversity in a very short time. Without a shrinkage limit, a small group of ”super” designs may appear and quickly
cull the population down to a size on the order of the limiting value. In this case, all the diversity of the population is lost and it is expensive to re-diversify and spread the population. The replacement_type for a SOGA may be roulette_wheel, unique_roulette_wheel, elitist, or favor_feasible. The elitist selector simply chooses the required number of designs taking the most fit. For example, if 100 selections are requested, then the top 100 designs as ranked by fitness will be selected and the remaining will be discarded. The favor_feasible replacement type first considers feasibility as a selection criteria. If that does not produce a “winner” then it moves on to considering fitness value. Because of this, any fitness assessor used with the favor_feasible selector must only account objectives in the creation of fitness. Therefore, there is such a fitness assessor and it’s use is enforced when the favor_feasible selector is chosen. In that case, and if the output level is set high enough, a message will be presented indicating that the weighted_sum_only fitness assessor will be used.

elitist

- Keywords Area
- method
- soga
- replacement_type
- elitist

Use the best designs to form a new population

Description

The elitist (default) setting creates a new population using (a) the replacement_size best individuals from the current population, (b) and population_size - replacement_size individuals randomly selected from the newly generated individuals. It is possible in this case to lose a good solution from the newly generated individuals if it is not randomly selected for replacement; however, the default new_solutions_generated value is set such that the entire set of newly generated individuals will be selected for replacement.

favor_feasible

- Keywords Area
- method
- soga
- replacement_type
- favor_feasible

Prioritize feasible designs
CHAPTER 6. KEYWORDS AREA

Specifying

Alias: none

Argument(s): none

Description

This replacement operator will always prefer a more feasible design to a less feasible one. Beyond that, it favors solutions based on an assigned fitness value which must have been installed by the weighted sum only fitness assessor.

The favor_feasible replacement type first considers feasibility as a selection criteria. If that does not produce a “winner” then it moves on to considering fitness value. Because of this, any fitness assessor used with the favor_feasible selector must only account objectives in the creation of fitness. Therefore, there is such a fitness assessor and it’s use is enforced when the favor_feasible selector is chosen. In that case, and if the output level is set high enough, a message will be presented indicating that the weighted_sum_only fitness assessor will be used.

roulette_wheel

- Keywords Area
- method
- soga
- replacement_type
- roulette_wheel

Replace population

Specifying

Alias: none

Argument(s): none

Description

Replace the population with members selected to continue in the next generation. The pool of potential members is the current population and the current set of offspring. The replacement_type of roulette_wheel or unique_roulette_wheel may be used either with MOGA or SOGA problems however they are not recommended for use with MOGA. Given that the only two fitness assessors for MOGA are the layer_rank and domination_count, the recommended selector is the below_limit selector. The below_limit replacement will only keep designs that are dominated by fewer than a limiting number of other designs. The replacement_type of favor_feasible is specific to a SOGA. This replacement operator will always prefer a more feasible design to a less feasible one. Beyond that, it favors solutions based on an assigned fitness value which must have been installed by the weighted sum only fitness assessor (see the discussion below).
6.2. METHOD

unique_roulette_wheel

- Keywords Area
- method
- soga
- replacement_type
- unique_roulette_wheel

Replace population

Specification

Alias: none
Argument(s): none

Description

Replace the population with members selected to continue in the next generation. The pool of potential members is the current population and the current set of offspring. The replacement_type of roulette_wheel or unique_roulette_wheel may be used either with MOGA or SOGA problems however they are not recommended for use with MOGA. Given that the only two fitness assessors for MOGA are the layer_rank and domination_count, the recommended selector is the below_limit selector. The below_limit replacement will only keep designs that are dominated by fewer than a limiting number of other designs. The replacement_type of favor_feasible is specific to a SOGA. This replacement operator will always prefer a more feasible design to a less feasible one. Beyond that, it favors solutions based on an assigned fitness value which must have been installed by the weighted sum only fitness assessor (see the discussion below).

convergence_type

- Keywords Area
- method
- soga
- convergence_type

Select the convergence type for JEGA methods

Specification

Alias: none
Argument(s): none
Default: average_fitness_tracker

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<tbody>
<tr>
<td>Required</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### Description

The two JEGA methods use different convergence types, which are described on their respective pages. All the convergence types are modified by the optional keywords `percent_change` and `num_generations`.

#### best_fitness_tracker

- **Keywords Area**
- **method**
- **soga**
- **convergence_type**
- **best_fitness_tracker**

Tracks the best fitness of the population

#### Specification

**Alias:** none  
**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td><code>percent_change</code></td>
<td>Define the convergence criterion for JEGA methods</td>
</tr>
<tr>
<td></td>
<td></td>
<td><code>num_generations</code></td>
<td>Define the convergence criterion for JEGA methods</td>
</tr>
</tbody>
</table>

**Description**

The `best_fitness_tracker` tracks the best fitness in the population. Convergence occurs after `num_generations` has passed and there has been less than `percent_change` in the best fitness value. The percent change can be as low as 0% in which case there must be no change at all over the number of generations.

**See Also**

These keywords may also be of interest:

- `average_fitness_tracker`
6.2. METHOD

percent_change

- Keywords Area
- method
- soga
- convergence_type
- best_fitness_tracker
- percent_change

Define the convergence criterion for JEGA methods

Specification

Alias: none

Argument(s): REAL
Default: 0.1

Description

The percent_change is the threshold beneath which convergence is attained whereby it is compared to the metric value computed.

num_generations

- Keywords Area
- method
- soga
- convergence_type
- best_fitness_tracker
- num_generations

Define the convergence criterion for JEGA methods

Specification

Alias: none

Argument(s): INTEGER
Default: 10

Description

The num Generations is the number of generations over which the metric value should be tracked. Convergence will be attained if the recorded metric is below percent_change for num_generations consecutive generations.
average_fitness_tracker

- Keywords Area
- method
- soga
- convergence_type
- average_fitness_tracker

Tracks the average fitness of the population

**Specification**

**Alias:** none

**Argument(s): none**

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>percent_change</td>
<td>Define the convergence criterion for JEGA methods</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>num_generations</td>
<td>Define the convergence criterion for JEGA methods</td>
</tr>
</tbody>
</table>

**Description**

The `convergence_type` called `average_fitness_tracker` keeps track of the average fitness in a population. If this average fitness does not change more than `percent_change` over some number of generations, `num_generations`, then the solution is reported as converged and the algorithm terminates.

**See Also**

These keywords may also be of interest:

- best_fitness_tracker

**percent_change**

- Keywords Area
- method
- soga
- convergence_type
- average_fitness_tracker
- percent_change

Define the convergence criterion for JEGA methods
6.2. METHOD

Specification

Alias: none
  Argument(s): REAL
  Default: 0.1

Description

The percent_change is the threshold beneath which convergence is attained whereby it is compared to the metric value computed.

  num_generations
  • Keywords Area
  • method
  • soga
  • convergence_type
  • average_fitness_tracker
  • num_generations
  Define the convergence criterion for JEGA methods

Specification

Alias: none
  Argument(s): INTEGER
  Default: 10

Description

The num_generations is the number of generations over which the metric value should be tracked. Convergence will be attained if the recorded metric is below percent_change for num_generations consecutive generations.

max_iterations

  • Keywords Area
  • method
  • soga
  • max_iterations

  Number of iterations allowed for optimizers and adaptive UQ methods

Topics

This keyword is related to the topics:
  • method_independent_controls
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none
Argument(s): INTEGER
Default: 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence} / efficient_global: 25*n)

Description

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed \( \text{max}\_\text{iterations} \) iterations. See also \text{max}\_\text{function_evaluations}.

Default Behavior
Default value is 100.

\text{max}\_\text{function_evaluations}

- Keywords Area
- method
- soga
- \text{max}\_\text{function_evaluations}

Number of function evaluations allowed for optimizers

Topics

This keyword is related to the topics:

- \text{method_independent_controls}

Specification

Alias: none
Argument(s): INTEGER
Default: 1000

Description

The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed \text{max}\_\text{function_evaluations} evaluations. See also \text{max}\_\text{iterations}.

Default Behavior
Default value is 1000.
6.2. METHOD

scaling

- Keywords Area
- method
- soga
- scaling

Turn on scaling for variables, responses, and constraints

Topics

This keyword is related to the topics:

- method, independent, controls

Specification

Alias: none

Argument(s): none

Default: no scaling

Description

Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by by providing the scaling keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the method, variables, and responses blocks. When the scaling keyword is omitted, all _scale_types and * scales specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.

- a *scales keyword, which gives characteristic values
- a *scale_type keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

Scale Types

There are four scale types:

1. none (default) - no scaling, value of *scales keyword is ignored
2. value - multiplicative scaling
3. **auto** - automatic scaling

First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:

- two-sided bounds scaled into the interval [0,1];
- one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
- no bounds or targets: no automatic scaling possible, therefore no scaling for this component

Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into [0,1].

4. **log** - logarithmic scaling

First, any characteristic values from the optional \(*_\text{scales}\) specification are applied. Then logarithm base 10 scaling is applied.

Logarithmic scaling is not available for linear constraints.

When continuous design variables are log scaled, linear constraints are not allowed.

**Scales**

The \(*_\text{scales}\) keywords are used to specify the characteristic values. These must be non-zero real numbers. The numbers are used according to the corresponding \(*\text{scale\_type}\), as described above.

Depending on the scale type, the characteristic values may be required or optional.

- none, auto, log - optional
- value - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than 1.0e10*DBL_MIN. User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.

**Examples**

The two examples below are equivalent:

```plaintext
responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value"
  primary_scales = 1 1 100

responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value" "value" "value"
  primary_scales = 1 1 100
```
6.2. METHOD

population_size

- Keywords Area
- method
- soga
- population_size

Set the initial population size in JEGA methods

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** 50

**Description**

The number of designs in the initial population is specified by the `population_size`. Note that the `population_size` only sets the size of the initial population. The population size may vary in the JEGA methods according to the type of operators chosen for a particular optimization run.

log_file

- Keywords Area
- method
- soga
- log_file

Specify the name of a log file

**Specification**

**Alias:** none

**Argument(s):** STRING

**Default:** JEGAGlobal.log

**Description**

New as of JEGA v2.0 is the introduction of the `log_file` specification. JEGA now uses a logging library to output messages and status to the user. JEGA can be configured at build time to log to both the console window and a text file, one or the other, or neither. The `log_file` input is a string name of a file into which to log. If the build was configured without file logging in JEGA, this input is ignored. If file logging is enabled and no `log_file` is specified, the default file name of JEGAGlobal.log is used.
print_each_pop

- Keywords Area
- method
- soga
- print_each_pop

Print every population to a population file

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** No printing

**Description**

New to JEGA v2.0 is the introduction of the `print_each_pop` specification. It serves as a flag and if supplied, the population at each generation will be printed to a file named “population<GEN#>.dat” where <GEN#> is the number of the current generation.

`initialization_type`

- Keywords Area
- method
- soga
- `initialization_type`

Specify how to initialize the population

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** `unique_random`

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Required</strong> (Choose One)</td>
<td><strong>Group 1</strong></td>
<td><code>simple_random</code></td>
<td>Create random initial solutions</td>
</tr>
<tr>
<td></td>
<td></td>
<td><code>unique_random</code></td>
<td>Create random initial solutions, but enforce uniqueness (default)</td>
</tr>
</tbody>
</table>
6.2. METHOD

| flat_file | Read initial solutions from file |

Description

The `initialization_type` defines how the initial population is created for the GA. There are three types:

1. `simple_random`
2. `unique_random` (default)
3. `flat_file`

Setting the size for the `flat_file` initializer has the effect of requiring a minimum number of designs to create. If this minimum number has not been created once the files are all read, the rest are created using the `unique_random` initializer and then the `simple_random` initializer if necessary.

**simple_random**

- **Keywords Area**
- **method**
- **soga**
- **initialization_type**
- **simple_random**

Create random initial solutions

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

`simple_random` creates initial solutions with random variable values according to a uniform random number distribution. It gives no consideration to any previously generated designs.

**unique_random**

- **Keywords Area**
- **method**
- **soga**
- **initialization_type**
- **unique_random**

Create random initial solutions, but enforce uniqueness (default)
**Keywords Area**

**Specification**

*Alias:* none  
*Argument(s):* none

**Description**

`unique_random` is the same as `simple_random`, except that when a new solution is generated, it is checked against the rest of the solutions. If it duplicates any of them, it is rejected.

**flat_file**

- **Keywords Area**
- **method**
- **soga**
- **initialization_type**
- **flat_file**

  Read initial solutions from file

**Specification**

*Alias:* none  
*Argument(s):* STRING

**Description**

`flat_file` allows the initial population to be read from a flat file. If `flat_file` is specified, a file name must be given.

Variables can be delimited in the flat file in any way you see fit with a few exceptions. The delimiter must be the same on any given line of input with the exception of leading and trailing whitespace. So a line could look like: 1.1, 2.2, 3.3 for example but could not look like: 1.1, 2.2 3.3. The delimiter can vary from line to line within the file which can be useful if data from multiple sources is pasted into the same input file. The delimiter can be any string that does not contain any of the characters .+-dDeE or any of the digits 0-9. The input will be read until the end of the file. The algorithm will discard any configurations for which it was unable to retrieve at least the number of design variables. The objective and constraint entries are not required but if ALL are present, they will be recorded and the design will be tagged as evaluated so that evaluators may choose not to re-evaluate them.

Setting the size for this initializer has the effect of requiring a minimum number of designs to create. If this minimum number has not been created once the files are all read, the rest are created using the `unique_random` initializer and then the `simple_random` initializer if necessary.

**crossover_type**

- **Keywords Area**
- **method**
- **soga**
- **crossover_type**

  Select a crossover type for JEGA methods
6.2. **METHOD**

### Specification

**Alias:** none  
**Argument(s):** none  
**Default:** shuffle_random

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required (Choose One)</td>
<td>Group 1</td>
<td>multi_point_binary</td>
<td>Use bit switching for crossover events</td>
</tr>
<tr>
<td></td>
<td></td>
<td>multi_point_parameterized_binary</td>
<td>Use bit switching to crossover each design variable</td>
</tr>
<tr>
<td></td>
<td></td>
<td>multi_point_real</td>
<td>Perform crossover in real valued genome</td>
</tr>
<tr>
<td></td>
<td></td>
<td>shuffle_random</td>
<td>Perform crossover by choosing design variable(s)</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>crossover_rate</td>
<td>Specify the probability of a crossover event</td>
</tr>
</tbody>
</table>

### Description

There are many crossover types available. `multi_point_binary` crossover requires an integer number, N, of crossover points. This crossover type performs a bit switching crossover at N crossover points in the binary encoded genome of two designs. Thus, crossover may occur at any point along a solution chromosome (in the middle of a gene representing a design variable, for example). `multi_point_parameterized_binary` crossover is similar in that it performs a bit switching crossover routine at N crossover points. However, this crossover type performs crossover on each design variable individually. So the individual chromosomes are crossed at N locations. `multi_point_real` crossover performs a variable switching crossover routing at N crossover points in the real valued genome of two designs. In this scheme, crossover only occurs between design variables (chromosomes). Note that the standard solution chromosome representation in the JEGA algorithm is real encoded and can handle integer or real design variables. For any crossover types that use a binary representation, real variables are converted to long integers by multiplying the real number by $10^6$ and then truncating. Note that this assumes a precision of only six decimal places. Discrete variables are represented as integers (indices within a list of possible values) within the algorithm and thus require no special treatment by the binary operators.

The final crossover type is `shuffle_random`. This crossover type performs crossover by choosing design variables at random from a specified number of parents enough times that the requested number of children are produced. For example, consider the case of 3 parents producing 2 children. This operator would go through and for each design variable, select one of the parents as the donor for the child. So it creates a random shuffle of the parent design variable values. The relative numbers of children and parents are controllable to allow for as much mixing as desired. The more parents involved, the less likely that the children will wind up exact duplicates of the parents.

All crossover types take a `crossover_rate`. The crossover rate is used to calculate the number of crossover operations that take place. The number of crossovers is equal to the rate * population_size.

**multi_point_binary**

- Keywords Area
Use bit switching for crossover events

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Description**

There are many crossover types available. *multi_point_binary* crossover requires an integer number, N, of crossover points. This crossover type performs a bit switching crossover at N crossover points in the binary encoded genome of two designs. Thus, crossover may occur at any point along a solution chromosome (in the middle of a gene representing a design variable, for example). *multi_point_parameterized_binary* crossover is similar in that it performs a bit switching crossover routine at N crossover points. However, this crossover type operates on each design variable individually. So the individual chromosomes are crossed at N locations. *multi_point_real* crossover performs a variable switching crossover routing at N crossover points in the real real valued genome of two designs. In this scheme, crossover only occurs between design variables (chromosomes). Note that the standard solution chromosome representation in the JEGA algorithm is real encoded and can handle integer or real design variables. For any crossover types that use a binary representation, real variables are converted to long integers by multiplying the real number by $10^6$ and then truncating. Note that this assumes a precision of only six decimal places. Discrete variables are represented as integers (indices within a list of possible values) within the algorithm and thus require no special treatment by the binary operators.

**multi_point_parameterized_binary**

- **Keywords Area**
- **method**
- **soga**
- **crossover_type**
- **multi_point_binary**

Use bit switching to crossover each design variable

**Specification**

**Alias:** none

**Argument(s):** INTEGER
6.2. **METHOD**

**Description**

There are many crossover types available. `multi_point_binary` crossover requires an integer number, N, of crossover points. This crossover type performs a bit switching crossover at N crossover points in the binary encoded genome of two designs. Thus, crossover may occur at any point along a solution chromosome (in the middle of a gene representing a design variable, for example). `multi_point_parameterized_binary` crossover is similar in that it performs a bit switching crossover routine at N crossover points. However, this crossover type performs crossover on each design variable individually. So the individual chromosomes are crossed at N locations. `multi_point_real` crossover performs a variable switching crossover routine at N crossover points in the real valued genome of two designs. In this scheme, crossover only occurs between design variables (chromosomes). Note that the standard solution chromosome representation in the JEGA algorithm is real encoded and can handle integer or real design variables. For any crossover types that use a binary representation, real variables are converted to long integers by multiplying the real number by $10^6$ and then truncating. Note that this assumes a precision of only six decimal places. Discrete variables are represented as integers (indices within a list of possible values) within the algorithm and thus require no special treatment by the binary operators.

**multi_point_real**

- **Keywords** Area
- method
- soga
- crossover_type
- multi_point_real

Perform crossover in real valued genome

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Description**

There are many crossover types available. `multi_point_binary` crossover requires an integer number, N, of crossover points. This crossover type performs a bit switching crossover at N crossover points in the binary encoded genome of two designs. Thus, crossover may occur at any point along a solution chromosome (in the middle of a gene representing a design variable, for example). `multi_point_parameterized_binary` crossover is similar in that it performs a bit switching crossover routine at N crossover points. However, this crossover type performs crossover on each design variable individually. So the individual chromosomes are crossed at N locations. `multi_point_real` crossover performs a variable switching crossover routine at N crossover points in the real valued genome of two designs. In this scheme, crossover only occurs between design variables (chromosomes). Note that the standard solution chromosome representation in the JEGA algorithm is real encoded and can handle integer or real design variables. For any crossover types that use a binary representation, real variables are converted to long integers by multiplying the real number by $10^6$ and then truncating. Note that this assumes a precision of only six decimal places. Discrete variables are represented as integers (indices within a list of possible values) within the algorithm and thus require no special treatment by the binary operators.
shuffle_random

- Keywords Area
- method
- soga
- crossover_type
- shuffle_random

Perform crossover by choosing design variable(s)

**Specification**

**Alias:** none  
**Argument(s):** none

| Required/- | Description of Group | Dakota Keyword | Dakota Keyword Description |
| Optional/Optional | num_parents | num_offspring | Number of parents in random shuffle crossover  
Number of offspring in random shuffle crossover |

**Description**

The final crossover type is **shuffle_random**. This crossover type performs crossover by choosing design variables at random from a specified number of parents enough times that the requested number of children are produced. For example, consider the case of 3 parents producing 2 children. This operator would go through and for each design variable, select one of the parents as the donor for the child. So it creates a random shuffle of the parent design variable values. The relative numbers of children and parents are controllable to allow for as much mixing as desired. The more parents involved, the less likely that the children will wind up exact duplicates of the parents.

**num_parents**

- Keywords Area
- method
- soga
- crossover_type
- shuffle_random
- num_parents

Number of parents in random shuffle crossover
6.2. METHOD

Specification

Alias: none
  Argument(s): INTEGER
  Default: 2

Description

Number of parents in random shuffle crossover

  num_offspring
  • Keywords Area
  • method
  • soga
  • crossover_type
  • shuffle_random
  • num_offspring

Number of offspring in random shuffle crossover

Specification

Alias: none
  Argument(s): INTEGER
  Default: 2

Description

Number of offspring in random shuffle crossover

crossover_rate

  • Keywords Area
  • method
  • soga
  • crossover_type
  • crossover_rate

Specify the probability of a crossover event

Specification

Alias: none
  Argument(s): REAL
  Default: 0.8
CHAPTER 6. KEYWORDS AREA

Description

The crossover.type controls what approach is employed for combining parent genetic information to create offspring, and the crossover.rate specifies the probability of a crossover operation being performed to generate a new offspring. The SCOLIB EA method supports three forms of crossover, two_point, blend, and uniform, which generate a new individual through combinations of two parent individuals. Two-point crossover divides each parent into three regions, where offspring are created from the combination of the middle region from one parent and the end regions from the other parent. Since the SCOLIB EA does not utilize bit representations of variable values, the crossover points only occur on coordinate boundaries, never within the bits of a particular coordinate. Uniform crossover creates offspring through random combination of coordinates from the two parents. Blend crossover generates a new individual randomly along the multidimensional vector connecting the two parents.

mutation_type

- Keywords Area
- method
- soga
- mutation.type

Select a mutation type for JEGA methods

Specification

Alias: none

Argument(s): none

Default: replace_uniform

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required(Choose One)</td>
<td>Group 1</td>
<td>replace_uniform</td>
<td>Mutate by flipping a random bit</td>
</tr>
<tr>
<td></td>
<td></td>
<td>offset_normal</td>
<td>Set mutation offset to use a normal distribution</td>
</tr>
<tr>
<td></td>
<td></td>
<td>offset_cauchy</td>
<td>Use a Cauchy distribution for the mutation offset</td>
</tr>
<tr>
<td></td>
<td></td>
<td>offset_uniform</td>
<td>Set mutation offset to use a uniform distribution</td>
</tr>
</tbody>
</table>
6.2. METHOD

<table>
<thead>
<tr>
<th>Optional</th>
<th>mutation_rate</th>
<th>Set probability of a mutation</th>
</tr>
</thead>
</table>

**Description**

Five mutation types are available for selection by keyword: `replace_uniform`, `bit_random`, `offset_cauchy`, `offset_normal`, and `offset_uniform`. They are described in greater detail on their respective keyword pages.

The `offset_*` mutators all act by adding a random "offset" to a variable value. The random amount has a mean of zero in all cases. The size of the offset is controlled using the `mutation_scale` keyword, which is interpreted differently for each `offset_*` type.

The rate of mutations for all types is controlled using the `mutation_rate`. The rate is applied differently in each `mutation_type`.

**bit_random**

- **Keywords Area**
- **method**
- **soga**
- **mutation_type**
- **bit_random**

Mutate by flipping a random bit

**Specification**

*Alias*: none

*Argument(s)*: none

**Description**

The `bit_random` mutator introduces random variation by first converting a randomly chosen variable of a randomly chosen design into a binary string. It then flips a randomly chosen bit in the string from a 1 to a 0 or visa versa. In this mutation scheme, the resulting value has more probability of being similar to the original value.

**replace_uniform**

- **Keywords Area**
- **method**
- **soga**
- **mutation_type**
- **replace_uniform**

Use uniformly distributed value over range of parameter
CHAPTER 6. KEYWORDS AREA

### Specification

**Alias:** none  
**Argument(s):** none

### Description

*replace_uniform* introduces random variation by first randomly choosing a design variable of a randomly selected design and reassigning it to a random valid value for that variable. No consideration of the current value is given when determining the new value.

*offset_normal*

- **Keywords Area**
- **method**
- **soga**
- **mutation_type**
- **offset_normal**

Set mutation offset to use a normal distribution

### Specification

**Alias:** none  
**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>mutation_scale</td>
<td>Scales mutation across range of parameter</td>
</tr>
</tbody>
</table>

### Description

The *offset_normal* mutator introduces random variation by adding a Gaussian random amount to a variable value. The random amount has a standard deviation dependent on the *mutation_scale*.

*mutation_scale*

- **Keywords Area**
- **method**
- **soga**
- **mutation_type**
- **offset_normal**
- **mutation_scale**

Scales mutation across range of parameter
6.2. METHOD

Specification

Alias: none
Argument(s): REAL
Default: 0.15

Description

The mutation_scale is a fraction in the range [0, 1] and is meant to help control the amount of variation that takes place when a variable is mutated. Its behavior depends on the selected mutation_type. For offset_normal and offset_cauchy, mutation_scale is multiplied by the range of the variable being mutated to obtain the standard deviation of the offset. For offset_uniform, the range of possible deviation amounts is +/- 1/2 * (mutation_scale * variable range).

offset_cauchy

- Keywords Area
- method
- soga
- mutation_type
- offset_cauchy

Use a Cauchy distribution for the mutation offset

Specification

Alias: none
Argument(s): none

| Required/- | Description of Group | Dakota Keyword | Dakota Keyword Description |
| Optional | | mutation_scale | Scales mutation across range of parameter |

Description

The offset_cauchy mutator introduces random variation by adding a Cauchy random amount to a variable value. The random amount has a standard deviation dependent on the mutation_scale.

mutation_scale

- Keywords Area
- method
- soga
- mutation_type
- offset_cauchy
• **mutation_scale**

Scales mutation across range of parameter

**Specification**

Alias: none

  Argument(s): REAL
  Default: 0.15

**Description**

The mutation_scale is a fraction in the range [0, 1] and is meant to help control the amount of variation that takes place when a variable is mutated. Its behavior depends on the selected mutation_type. For offset_normal and offset_cauchy, mutation_scale is multiplied by the range of the variable being mutated to obtain the standard deviation of the offset. For offset_uniform, the range of possible deviation amounts is +/- 1/2 * (mutation_scale * variable range).

**offset_uniform**

- Keywords Area
- method
- soga
- mutation_type
- offset_uniform

Set mutation offset to use a uniform distribution

**Specification**

Alias: none

  Argument(s): none

| Required/- | Description of | Dakota Keyword | Dakota Keyword |
| Optional Optional Group mutation_scale | Description | |

| Required/- | Description of | Dakota Keyword | Dakota Keyword |
| Optional Optional Group mutation_scale | Description | |

**Description**

The offset_uniform mutator introduces random variation by adding a uniform random amount to a variable value. The random amount depends on the mutation_scale.
6.2. METHOD

mutation_scale

- Keywords Area
- method
- soga
- mutation_type
- offset_uniform
- mutation_scale

Scales mutation across range of parameter

Specification

Alias: none
Argument(s): REAL
Default: 0.15

Description

The mutation_scale is a fraction in the range [0, 1] and is meant to help control the amount of variation that takes place when a variable is mutated. Its behavior depends on the selected mutation_type. For offset_normal and offset_cauchy, mutation_scale is multiplied by the range of the variable being mutated to obtain the standard deviation of the offset. For offset_uniform, the range of possible deviation amounts is +/- 1/2 * (mutation_scale * variable range).

mutation_rate

- Keywords Area
- method
- soga
- mutation_type
- mutation_rate

Set probability of a mutation

Specification

Alias: none
Argument(s): REAL
Default: 0.08

Description

All mutation types have a mutation_rate, which controls the number of mutations performed. For replace_uniform and all the offset_* types, the number of mutations performed is the product of mutation_rate and population_size. For bit_random, it’s the product of the mutation_rate, number of design variables, and population size.
seed

- **Keywords Area**
- **method**
- **soga**
- **seed**

Seed of the random number generator

**Specification**

**Alias:** none  
**Argument(s):** INTEGER  
**Default:** system-generated (non-repeatable)

**Description**

The random seed control provides a mechanism for making a stochastic method repeatable. That is, the use of the same random seed in identical studies will generate identical results.

**Default Behavior**

If not specified, the seed is randomly generated.

**Expected Output**

If `seed` is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

**Usage Tips**

If a stochastic study was run without `seed` specified, and the user later wishes to repeat the study using the same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen. That value can then be added to the Dakota input file.

**Examples**

```plaintext
method
  sampling
    sample_type lhs
    samples = 10
    seed = 15347
```

**convergence_tolerance**

- **Keywords Area**
- **method**
- **soga**
- **convergence_tolerance**

Stopping criterion based on convergence of the objective function or statistics
6.2. METHOD

Topics

This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none

Argument(s): REAL

Default: 1.e-4

Description

The convergence_tolerance specification provides a real value for controlling the termination of iteration. For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by convergence_tolerance, then this convergence criterion is satisfied on the current iteration.

Therefore, permissible values are between 0 and 1, non-inclusive.

Behavior Varies by Package/Library

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- DOT: must be satisfied for two consecutive iterations
- NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of convergence_tolerance approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., convergence_tolerance = 1.e-6 will result in approximately six digits of accuracy in the final objective function).
- NL2SOL: See nl2sol

model_pointer

- Keywords Area
- method
- soga
- model_pointer

Identifier for model block to be used by a method
CHAPTER 6. KEYWORDS AREA

Topics
This keyword is related to the topics:

- block_pointer

Specification
Alias: none

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)

Description
The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior
If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.

Usage Tips
When doing advanced analyses that involve using multiple methods and multiple models, defining a model_pointer for each method is imperative.

See block_pointer for details about pointers.

Examples

```
environment
  tabular_graphics_data
  method_pointer = 'UQ'

method
  id_method = 'UQ'
  model_pointer = 'SURR'
  sampling,
    samples = 10
    seed = 98765 rng rnum2
    response_levels = 0.1 0.2 0.6
    0.1 0.2 0.6
    0.1 0.2 0.6
  sample_type lhs
  distribution cumulative

model
  id_model = 'SURR'
  surrogate global,
  dace_method_pointer = 'DACE'
  polynomial quadratic

method
  id_method = 'DACE'
  model_pointer = 'DACE_M'
  sampling sample_type lhs
    samples = 121 seed = 5034 rng rnum2

model
  id_model = 'DACE_M'
  single
```
6.2. METHOD

interface_pointer = ‘I1’

variables
uniform_uncertain = 2
lower_bounds = 0.0
upper_bounds = 1.1
descriptors = ‘x1’ ‘x2’

interface
id_interface = ‘I1’
system asynch evaluation_concurrency = 5
analysis_driver = ‘text_book’

responses
response_functions = 3
no_gradients
no_hessians

6.2.36 coliny_pattern_search

- Keywords Area
- method
- coliny_pattern_search

Pattern search, derivative free optimization method

Topics
This keyword is related to the topics:

- package_scolib
- package_coliny
- global_optimization_methods

Specification

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>constant_penalty</td>
<td></td>
<td>Use a simple weighted penalty to manage feasibility</td>
</tr>
<tr>
<td>Keyword</td>
<td>Value</td>
<td>Description</td>
<td></td>
</tr>
<tr>
<td>-------------------------</td>
<td>----------------------------</td>
<td>--------------------------------------------------------------------------------------------------------------------------------------------</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>no expansion</td>
<td>Don’t allow expansion of the search pattern</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>expand_after_success</td>
<td>Set the factor by which a search pattern can be expanded</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>pattern_basis</td>
<td>Pattern basis selection</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>stochastic</td>
<td>Generate trial points in random order</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>total_pattern_size</td>
<td>Total number of points in search pattern</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>exploratory_moves</td>
<td>Exploratory moves selection</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>synchronization</td>
<td>Select how Dakota schedules function evaluations in a pattern search</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>contraction_factor</td>
<td>Amount by which step length is rescaled</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>constraint_penalty</td>
<td>Multiplier for the penalty function</td>
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</tr>
<tr>
<td>Optional</td>
<td>initial_delta</td>
<td>Initial step size for derivative-free optimizers</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>threshold_delta</td>
<td>Step length-based stopping criteria for derivative-free optimizers</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>solution_target</td>
<td>Stopping criteria based on objective function value</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>seed</td>
<td>Seed of the random number generator</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>show_misc_options</td>
<td>Show algorithm parameters not exposed in Dakota input</td>
<td></td>
</tr>
</tbody>
</table>
6.2. METHOD

| Optional | misc_options | Set method options not available through Dakota spec |
| Optional | max_iterations | Number of iterations allowed for optimizers and adaptive UQ methods |
| Optional | convergence_tolerance | Stopping criterion based on convergence of the objective function or statistics |
| Optional | max_function_evaluations | Number of function evaluations allowed for optimizers |
| Optional | scaling | Turn on scaling for variables, responses, and constraints |
| Optional | model_pointer | Identifier for model block to be used by a method |

**Description**

Pattern search techniques are nongradient-based optimization methods which use a set of offsets from the current iterate to locate improved points in the design space.

See the page package_scolib for important information regarding all SCOLIB methods.

Traditional pattern search methods search with a fixed pattern of search directions to try to find improvements to the current iterate. The SCOLIB pattern search methods generalize this simple algorithmic strategy to enable control of how the search pattern is adapted, as well as how each search pattern is evaluated. The **stochastic** and **synchronization** specifications denote how the the trial points are evaluated. The **stochastic** specification indicates that the trial points are considered in a random order. For parallel pattern search, **synchronization** dictates whether the evaluations are scheduled using a **blocking** or a **nonblocking** scheduler. In the **blocking** case, all points in the pattern are evaluated (in parallel), and if the best of these trial points is an improving point, then it becomes the next iterate. These runs are reproducible, assuming use of the same seed in the **stochastic** case. In the **nonblocking** case, all points in the pattern may not be evaluated, since the first improving point found becomes the next iterate. Since the algorithm steps will be subject to parallel timing variabilities, these runs will not generally be repeatable. The **synchronization** specification has similar connotations for sequential pattern search. If **blocking** is specified, then each sequential iteration terminates after all trial points have been considered, and if **nonblocking** is specified, then each
sequential iteration terminates after the first improving trial point is evaluated. In this release, both blocking and nonblocking specifications result in blocking behavior (except in the case where exploratory_moves below is set to adaptive_pattern). Nonblocking behavior will be re-enabled after some underlying technical issues have been resolved.

The particular form of the search pattern is controlled by the pattern_basis specification. If pattern_basis is coordinate basis, then the pattern search uses a plus and minus offset in each coordinate direction, for a total of $2n$ function evaluations in the pattern. This case is depicted in Figure 5.3 for three coordinate dimensions.

![Figure 6.1: Depiction of coordinate pattern search algorithm](image)

If pattern_basis is simplex, then pattern search uses a minimal positive basis simplex for the parameter space, for a total of $n+1$ function evaluations in the pattern. Note that the simplex pattern basis can be used for unbounded problems only. The total_pattern_size specification can be used to augment the basic coordinate and simplex patterns with additional function evaluations, and is particularly useful for parallel load balancing. For example, if some function evaluations in the pattern are dropped due to duplication or bound constraint interaction, then the total_pattern_size specification instructs the algorithm to generate new offsets to bring the total number of evaluations up to this consistent total.

The exploratory_moves specification controls how the search pattern is adapted. (The search pattern can be adapted after an improving trial point is found, or after all trial points in a search pattern have been found to be unimproving points.) The following exploratory_moves selections are supported by SCOLIB:

- The basic_pattern case is the simple pattern search approach, which uses the same pattern in each
6.2. **METHOD**

- The **multi_step** case examines each trial step in the pattern in turn. If a successful step is found, the pattern search continues examining trial steps about this new point. In this manner, the effects of multiple successful steps are cumulative within a single iteration. This option does not support any parallelism and will result in a serial pattern search.

- The **adaptive_pattern** case invokes a pattern search technique that adaptively rescales the different search directions to maximize the number of redundant function evaluations. See [45] for details of this method. In preliminary experiments, this method had more robust performance than the standard basic_pattern case in serial tests. This option supports a limited degree of parallelism. After successful iterations (where the step length is not contracted), a parallel search will be performed. After unsuccessful iterations (where the step length is contracted), only a single evaluation is performed.

The `initial_delta` and `threshold_delta` specifications provide the initial offset size and the threshold size at which to terminate the algorithm. For any dimension that has both upper and lower bounds, this step length will be internally rescaled to provide search steps of length `initial_delta * range * 0.1`. This rescaling does not occur for other dimensions, so search steps in those directions have length `initial_delta`. Note that the factor of 0.1 in the rescaling could result in an undesirably small initial step. This can be offset by providing a large `initial_delta`.

In general, pattern search methods can expand and contract their step lengths. SCOLIB pattern search methods contract the step length by the value `contraction_factor`, and they expand the step length by the value `(1/contraction_factor)`. The `expand_after_success` control specifies how many successful objective function improvements must occur with a specific step length prior to expansion of the step length, whereas the `no_expansion` flag instructs the algorithm to forgo pattern expansion altogether.

Finally, constraint infeasibility can be managed in a somewhat more sophisticated manner than the simple weighted penalty function. If the `constant_penalty` specification is used, then the simple weighted penalty scheme described above is used. Otherwise, the constraint penalty is adapted to the value `constraint_penalty/L`, where L is the the smallest step length used so far.

**See Also**

These keywords may also be of interest:

- `coliny_beta`
- `coliny_direct`
- `coliny_cobyla`
- `coliny_ea`
- `coliny_solis_wets`

**constant_penalty**

- **Keywords Area**
- **method**
- `coliny_pattern_search`
- `constant_penalty`

Use a simple weighted penalty to manage feasibility.
CHAPTER 6. KEYWORDS AREA

Specifi cation

Alias: none

Argument(s): none

Default: algorithm dynamically adapts the constraint penalty

Description

Finally, constraint infeasibility can be managed in a somewhat more sophisticated manner than the simple weighted penalty function. If the constant_penalty specification is used, then the simple weighted penalty scheme described above is used. Otherwise, the constraint penalty is adapted to the value constraint_penalty/L, where L is the smallest step length used so far.

no_expansion

• Keywords Area

• method

• coliny_pattern_search

• no_expansion

Don’t allow expansion of the search pattern

Specifi cation

Alias: none

Argument(s): none

Default: algorithm may expand pattern size

Description

In general, pattern search methods can expand and contract their step lengths. SCOLIB pattern search methods contract the step length by the value contraction_factor, and they expand the step length by the value (1/contraction_factor). The expand_after_success control specifies how many successful objective function improvements must occur with a specific step length prior to expansion of the step length, whereas the no_ expansion flag instructs the algorithm to forgo pattern expansion altogether.

expand_after_success

• Keywords Area

• method

• coliny_pattern_search

• expand_after_success

Set the factor by which a search pattern can be expanded
6.2. METHOD

Specification

Alias: none
Argument(s): INTEGER
Default: 5

Description

In general, pattern search methods can expand and contract their step lengths. SCOLIB pattern search methods contract the step length by the value contraction_factor, and they expand the step length by the value (1/contraction_factor). The expand_after_success control specifies how many successful objective function improvements must occur with a specific step length prior to expansion of the step length, whereas the no_expansion flag instructs the algorithm to forgo pattern expansion altogether.

pattern_basis

- Keywords Area
- method
- coliny_pattern_search
- pattern_basis

Pattern basis selection

Specification

Alias: none
Argument(s): none
Default: coordinate

<table>
<thead>
<tr>
<th>Required/-Optional Required (Choose One)</th>
<th>Description of Group</th>
<th>Dakota Keyword coordinate</th>
<th>Dakota Keyword Description</th>
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<tbody>
<tr>
<td>coordinate</td>
<td>simplex</td>
<td>Use coordinate directions as search pattern</td>
<td></td>
</tr>
</tbody>
</table>

Description

The particular form of the search pattern is controlled by the pattern_basis specification. If pattern_basis is coordinate basis, then the pattern search uses a plus and minus offset in each coordinate direction, for a total of 2n function evaluations in the pattern. This case is depicted in Figure 5.3 for three coordinate dimensions.

coordinate

- Keywords Area
- method
Use coordinate directions as search pattern

**Specification**

Alias: none

**Argument(s):** none

**Description**

The particular form of the search pattern is controlled by the **pattern_basis** specification. If **pattern_basis** is **coordinate** basis, then the pattern search uses a plus and minus offset in each coordinate direction, for a total of $2n$ function evaluations in the pattern. This case is depicted in Figure 5.3 for three coordinate dimensions.

**simplex**

- **Keywords Area**
- **method**
- **coliny_pattern_search**
- **pattern_basis**
- **simplex**

Use a minimal simplex for the search pattern

**Specification**

Alias: none

**Argument(s):** none

**Description**

If **pattern_basis** is **simplex**, then pattern search uses a minimal positive basis simplex for the parameter space, for a total of $n+1$ function evaluations in the pattern. Note that the **simplex** pattern basis can be used for unbounded problems only. The **total_pattern_size** specification can be used to augment the basic **coordinate** and **simplex** patterns with additional function evaluations, and is particularly useful for parallel load balancing. For example, if some function evaluations in the pattern are dropped due to duplication or bound constraint interaction, then the **total_pattern_size** specification instructs the algorithm to generate new offsets to bring the total number of evaluations up to this consistent total.
6.2. METHOD

stochastic

• Keywords Area
• method
• coliny_pattern_search
• stochastic

Generate trial points in random order

Specification

Alias: none
Argument(s): none

Description

Traditional pattern search methods search with a fixed pattern of search directions to try to find improvements to the current iterate. The SCOLIB pattern search methods generalize this simple algorithmic strategy to enable control of how the search pattern is adapted, as well as how each search pattern is evaluated. The stochastic and synchronization specifications denote how the trial points are evaluated. The stochastic specification indicates that the trial points are considered in a random order. For parallel pattern search, synchronization dictates whether the evaluations are scheduled using a blocking scheduler or a nonblocking scheduler (i.e.,

total_pattern_size

• Keywords Area
• method
• coliny_pattern_search
• total_pattern_size

Total number of points in search pattern

Specification

Alias: none
Argument(s): INTEGER
Default: no augmentation of basic pattern

Description

If pattern_basis is simplex, then pattern search uses a minimal positive basis simplex for the parameter space, for a total of $n+1$ function evaluations in the pattern. Note that the simplex pattern basis can be used for unbounded problems only. The total_pattern_size specification can be used to augment the basic coordinate and simplex patterns with additional function evaluations, and is particularly useful for parallel load balancing. For example, if some function evaluations in the pattern are dropped due to duplication or bound constraint interaction, then the total_pattern_size specification instructs the algorithm to generate new offsets to bring the total number of evaluations up to this consistent total.
The exploratory_moves specification controls how the search pattern is adapted. (The search pattern can be adapted after an improving trial point is found, or after all trial points in a search pattern have been found to be unimproving points.) The following exploratory_moves selections are supported by SCOLIB:

**multi_step**
- Keywords Area
- method
- coliny_pattern_search
- exploratory_moves
- multi_step

Examine trial step around successful new point

**Specification**

Alias: none

Argument(s): none

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<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<tbody>
<tr>
<td>Required <em>(Choose One)</em></td>
<td>multi_step</td>
<td>adaptive_pattern</td>
<td>Adaptively rescale search directions</td>
</tr>
<tr>
<td></td>
<td></td>
<td>basic_pattern</td>
<td>Use the same search pattern every iteration</td>
</tr>
</tbody>
</table>
6.2. METHOD

Description

The multi_step case examines each trial step in the pattern in turn. If a successful step is found, the pattern search continues examining trial steps about this new point. In this manner, the effects of multiple successful steps are cumulative within a single iteration. This option does not support any parallelism and will result in a serial pattern.

adaptive_pattern

- Keywords Area
- method
- coliny_pattern_search
- exploratory_moves
- adaptive_pattern

Adaptively rescale search directions

Specification

Alias: none
Argument(s): none

Description

The adaptive_pattern case invokes a pattern search technique that adaptively rescales the different search directions to maximize the number of redundant function evaluations. See [45] for details of this method. In preliminary experiments, this method had more robust performance than the standard basic_pattern case in serial tests. This option supports a limited degree of parallelism. After successful iterations (where the step length is not contracted), a parallel search will be performed. After unsuccessful iterations (where the step length is contracted), only a single evaluation is performed.

basic_pattern

- Keywords Area
- method
- coliny_pattern_search
- exploratory_moves
- basic_pattern

Use the same search pattern every iteration

Specification

Alias: none
Argument(s): none
CHAPTER 6. KEYWORDS AREA

Description
The basic_pattern case is the simple pattern search approach, which uses the same pattern in each iteration.

synchronization
- Keywords Area
- method
- coliny_pattern_search
- synchronization

Select how Dakota schedules function evaluations in a pattern search

Specification
Alias: none
Argument(s): none
Default: nonblocking

<table>
<thead>
<tr>
<th>Required/-Optional Required (Choose One)</th>
<th>Description of Group Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>nonblocking</td>
<td></td>
<td>Evaluate points in the pattern until an improving point is found</td>
</tr>
</tbody>
</table>

Description
The synchronization specification can be used to specify the use of either blocking or nonblocking schedulers.

blocking
- Keywords Area
- method
- coliny_pattern_search
- synchronization
- blocking

Evaluate all points in a pattern

Specification
Alias: none
Argument(s): none
6.2. METHOD

Description

In the blocking case, all points in the pattern are evaluated (in parallel), and if the best of these trial points is an improving point, then it becomes the next iterate. These runs are reproducible, assuming use of the same seed in the stochastic case.

nonblocking

- Keywords Area
- method
- coliny_pattern_search
- synchronization
- nonblocking

Evaluate points in the pattern until an improving point is found

Specification

Alias: none

Argument(s): none

Description

In the nonblocking case, all points in the pattern may not be evaluated. The first improving point found becomes the next iterate. Since the algorithm steps will be subject to parallel timing variabilities, these runs will not generally be repeatable.

contraction_factor

- Keywords Area
- method
- coliny_pattern_search
- contraction_factor

Amount by which step length is rescaled

Specification

Alias: none

Argument(s): REAL
Default: 0.5

Description

For pattern search methods, contraction_factor specifies the amount by which step length is rescaled after unsuccessful iterates, must be strictly between 0 and 1.

For methods that can expand the step length, the expansion is $1/\text{contraction\_factor}$
constraint_penalty

- Keywords Area
- method
- coliny_pattern_search
- constraint_penalty

Multiplier for the penalty function

**Specification**

*Alias:* none

*Argument(s):* REAL

*Default:* 1.0

**Description**

Most SCOLIB optimizers treat constraints with a simple penalty scheme that adds constraint_penalty times the sum of squares of the constraint violations to the objective function. The default value of constraint_penalty is 1000.0, except for methods that dynamically adapt their constraint penalty, for which the default value is 1.0.

**initial_delta**

- Keywords Area
- method
- coliny_pattern_search
- initial_delta

Initial step size for derivative-free optimizers

**Specification**

*Alias:* none

*Argument(s):* REAL

*Default:* 1.0 (COBYLA), 0.1*range (PS, SW)

**Description**

The initial_delta keyword defines the size of the first search step in derivative-free optimization methods, specifically asynch_pattern_search, coliny_cobyla, coliny_pattern_search, coliny_solis_wets, and mesh_adaptive_search. It is applied in an absolute sense to all search directions.

*Default Behavior*

The default value is 1.0.

*Usage Tips*

It is recommended that initial_delta be the approximate distance from the initial point to the solution. If this distance is unknown, it is advisable to err on the side of choosing an initial_delta that is too large or to not specify it. Relative application of initial_delta is not available unless the user scales the problem accordingly.
6.2. METHOD

Examples

Three example method input blocks appear below.

For **asynch_pattern_search**:

```plaintext
method
  asynch_pattern_search
  initial_delta = .5
  contraction_factor = 0.25
  merit_function merit1_smooth
  smoothing_factor = 1.0
  constraint_tolerance = 1.e-6
```

For **coliny_pattern_search**:

```plaintext
method
  coliny_pattern_search
  initial_delta = .2
  threshold_delta = 1.e-4
  max_iterations 100
  solution_accuracy = 1.e-6
  seed = 1234
  max_function_evaluations = 1000
```

For **mesh_adaptive_search**

```plaintext
method
  mesh_adaptive_search
  initial_delta = 2.0
  seed = 1234
```

**threshold_delta**

- **Keyword**: Area
- **Keyword**: method
- **Keyword**: coliny_pattern_search
- **Keyword**: threshold_delta

Step length-based stopping criteria for derivative-free optimizers

**Specification**

**Alias**: none

**Argument(s)**: REAL

**Default**: 1.0e-4 (COBYLA), 1.0e-5 (PS), 1.0e-6 (SW)

**Description**

The **threshold_delta** keyword defines the minimum step length allowed by the optimizer and is used to determine convergence. It is applicable to **asynch_pattern_search**, **coliny_cobyla**, **coliny_pattern_search**, **coliny_solis_wets**, and **mesh_adaptive_search**.

**Default Behavior**

The default value varies according to method as follows:

- **asynch_pattern_search**: 1.0e-2
Keywords Area

- `coliny_cobyla`: $1.0 \times 10^{-4}$
- `coliny_pattern_search`: $1.0 \times 10^{-5}$
- `coliny_solis_wets`: $1.0 \times 10^{-6}$
- `mesh_adaptive_search`: $1.0 \times 10^{-6}$

Usage Tips

It is recommended that `threshold_delta` be set to a value for which changes of that scale in parameter values cause negligible changes in the objective function.

Examples

Three example method input blocks appear below.

For `asynch_pattern_search`:

```hull
method
asynch_pattern_search
  contraction_factor = 0.25
  threshold_delta = 1.e-4
  solution_target = 1.e-6
  max_function_evaluations = 500
  constraint_tolerance = 1.e-6
```

For `coliny_pattern_search`:

```hull
method
coliny_pattern_search
  initial_delta = .2
  threshold_delta = 1.e-4
  max_iterations = 100
  solution_accuracy = 1.e-6
  seed = 1234
  max_function_evaluations = 1000
```

For `mesh_adaptive_search`:

```hull
method
mesh_adaptive_search
  threshold_delta = 0.01
  seed = 1234
```

solution_target

- **Keywords Area**
- **method**
- `coliny_pattern_search`
- `solution_target`

Stopping criteria based on objective function value

Specification

Alias: `solution_accuracy`

Argument(s): REAL

Default: -DBL_MAX
6.2. METHOD

Description

\texttt{solution_target} is a termination criterion. The algorithm will terminate when the function value falls below \texttt{solution_target}.

\texttt{seed}

- Keywords Area
- method
- \texttt{coliny_pattern_search}
- seed

Seed of the random number generator

Specification

Alias: none

Argument(s): INTEGER

Default: system-generated (non-repeable)

Description

The random seed control provides a mechanism for making a stochastic method repeatable. That is, the use of the same random seed in identical studies will generate identical results.

Default Behavior
If not specified, the seed is randomly generated.

Expected Output
If \texttt{seed} is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

Usage Tips
If a stochastic study was run without \texttt{seed} specified, and the user later wishes to repeat the study using the same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen. That value can then be added to the Dakota input file.

Examples

\begin{verbatim}
method
  sampling
    sample_type lhs
    samples = 10
    seed = 15347
\end{verbatim}

\texttt{show_misc_options}

- Keywords Area
- method
- \texttt{coliny_pattern_search}
- \texttt{show_misc_options}

Show algorithm parameters not exposed in Dakota input
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): none

Default: no dump of specification options

Description

All SCOLIB methods support the show Misc options optional specification which results in a dump of all the allowable method inputs. Note that the information provided by this command refers to optimizer parameters that are internal to SCOLIB, and which may differ from corresponding parameters used by the Dakota interface. The misc options optional specification provides a means for inputing additional settings supported by the SCOLIB methods but which are not currently mapped through the Dakota input specification. Care must be taken in using this specification; they should only be employed by users familiar with the full range of parameter specifications available directly from SCOLIB and understand any differences that exist between those specifications and the ones available through Dakota.

misc_options

- Keywords Area
- method
- coliny_pattern_search
- misc_options

Set method options not available through Dakota spec

Specification

Alias: none

Argument(s): STRINGLIST

Default: no misc options

Description

All SCOLIB methods support the show Misc options optional specification which results in a dump of all the allowable method inputs. Note that the information provided by this command refers to optimizer parameters that are internal to SCOLIB, and which may differ from corresponding parameters used by the Dakota interface. The misc options optional specification provides a means for inputing additional settings supported by the SCOLIB methods but which are not currently mapped through the Dakota input specification. Care must be taken in using this specification; they should only be employed by users familiar with the full range of parameter specifications available directly from SCOLIB and understand any differences that exist between those specifications and the ones available through Dakota.

max_iterations

- Keywords Area
- method
- coliny_pattern_search
6.2. METHOD

- **max_iterations**

  Number of iterations allowed for optimizers and adaptive UQ methods

**Topics**

This keyword is related to the topics:

- method_independent_controls

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence} / efficient-global: 25*n)

**Description**

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed max_iterations iterations. See also max_function_evaluations.

**Default Behavior**

Default value is 100.

**convergence_tolerance**

- **Keywords Area**

- method

- coliny_pattern_search

- convergence_tolerance

  Stopping criterion based on convergence of the objective function or statistics

**Topics**

This keyword is related to the topics:

- method_independent_controls

**Specification**

**Alias:** none

**Argument(s):** REAL

**Default:** 1.e-4
CHAPTER 6. KEYWORDS AREA

Description
The convergence_tolerance specification provides a real value for controlling the termination of iteration.

For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by convergence_tolerance, then this convergence criterion is satisfied on the current iteration.

Therefore, permissible values are between 0 and 1, non-inclusive.

Behavior Varies by Package/Library
This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

• DOT: must be satisfied for two consecutive iterations

• NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of convergence_tolerance approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., convergence_tolerance = 1.e-6 will result in approximately six digits of accuracy in the final objective function).

• NL2SOL: See nl2sol

max_function_evaluations

• Keywords Area

• method

• coliny_pattern_search

• max_function_evaluations

Number of function evaluations allowed for optimizers

Topics
This keyword is related to the topics:

• method_independent_controls

Specification
Alias: none
Argument(s): INTEGER
Default: 1000
6.2. METHOD

Description

The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed \texttt{max\_function\_evaluations} evaluations. See also \texttt{max\_iterations}.

Default Behavior

Default value is 1000.

scale

- Keywords Area
- method
- coliny\_pattern\_search
- scaling

Turn on scaling for variables, responses, and constraints

Topics

This keyword is related to the topics:

- method\_independent\_controls

Specification

Alias: none

Argument(s): none

Default: no scaling

Description

Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by by providing the scaling keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the method, variables, and responses blocks. When the scaling keyword is omitted, all _scale\_types and *scales specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.

- a *scales keyword, which gives characteristic values
- a *scale\_type keyword, which determines how to use the characteristic values
The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

**Scale Types**
There are four scale types:

1. **none** (default) - no scaling, value of *scales* keyword is ignored
2. **value** - multiplicative scaling
3. **auto** - automatic scaling
   First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:
   - two-sided bounds scaled into the interval [0,1];
   - one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
   - no bounds or targets: no automatic scaling possible, therefore no scaling for this component

Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into [0,1].

4. **log** - logarithmic scaling
   First, any characteristic values from the optional *scales* specification are applied. Then logarithm base 10 scaling is applied.
   Logarithmic scaling is not available for linear constraints.
   When continuous design variables are log scaled, linear constraints are not allowed.

**Scales**
The *scales* keywords are used to specify the characteristic values. These must be non-zero real numbers. The numbers are used according to the corresponding *scale_type*, as described above.

Depending on the scale type, the characteristic values may be required or optional.

- none, auto, log - optional
- value - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than \( 1.0e10 \times \text{DBL_MIN} \). User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.

**Examples**
The two examples below are equivalent:

```
responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value"
  primary_scales = 1 1 100
```

```
responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value" "value" "value"
  primary_scales = 1 1 100
```
6.2. METHOD

model_pointer

- Keywords Area
- method
- coliny_pattern_search
- model_pointer

Identifier for model block to be used by a method

Topics

This keyword is related to the topics:

- block_pointer

Specification

Alias: none

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)

Description

The `model_pointer` is used to specify which `model` block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a `model` block in the Dakota input file that has a corresponding `id_model` with the same name.

Usage Tips

When doing advanced analyses that involve using multiple methods and multiple models, defining a `model_pointer` for each method is imperative.

See `block_pointer` for details about pointers.

Examples

```
environment
tabular_graphics_data
method_pointer = 'UQ'

method
id_method = 'UQ'
model_pointer = 'SURR'
sampling,
samples = 10
seed = 98765 rng rnum2
response_levels = 0.1 0.2 0.6
0.1 0.2 0.6
0.1 0.2 0.6
sample_type lhs
distribution cumulative

model
id_model = 'SURR'
```
surrogate global,
 dace_method_pointer = 'DACE'
polynomial quadratic

method
 id_method = 'DACE'
 model_pointer = 'DACE_M'
 sampling sample_type lhs
 samples = 121 seed = 5034 rng rnum2

model
 id_model = 'DACE_M'
 single
 interface_pointer = 'I1'

variables
 uniform_uncertain = 2
 lower_bounds = 0. 0.
 upper_bounds = 1. 1.
 descriptors = 'x1' 'x2'

interface
 id_interface = 'I1'
 system asynch evaluation_concurrency = 5
 analysis_driver = 'text_book'

responses
 response_functions = 3
 no_gradients
 no_hessians

### 6.2.37 coliny_solis_wets

- **Keywords Area**

- **method**

- **coliny_solis_wets**

  Simple greedy local search method

**Topics**

This keyword is related to the topics:

- **package_scolib**

- **package_coliny**

**Specification**

**Alias:** none

**Argument(s):** none

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<thead>
<tr>
<th>Required/-</th>
<th>Description of</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>Group</td>
<td></td>
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</tr>
</tbody>
</table>


| Optional | contract_after_-failure | The number of unsuccessful cycles prior to contraction. |
| Optional | no_expansion | Don’t allow expansion of the search pattern. |
| Optional | expand_after_-success | Set the factor by which a search pattern can be expanded. |
| Optional | constant_penalty | Use a simple weighted penalty to manage feasibility. |
| Optional | contraction_factor | Amount by which step length is rescaled. |
| Optional | constraint_penalty | Multiplier for the penalty function. |
| Optional | initial_delta | Initial step size for derivative-free optimizers. |
| Optional | threshold_delta | Step length-based stopping criteria for derivative-free optimizers. |
| Optional | solution_target | Stopping criteria based on objective function value. |
| Optional | seed | Seed of the random number generator. |
| Optional | show_mis_options | Show algorithm parameters not exposed in Dakota input. |
| Optional | misc_options | Set method options not available through Dakota spec. |
### Description

The Solis-Wets method is a simple greedy local search heuristic for continuous parameter spaces. Solis-Wets generates trial points using a multivariate normal distribution, and unsuccessful trial points are reflected about the current point to find a descent direction.

**See the page `package_scolib` for important information regarding all SCOLIB methods**

*coliny.solis.wets* is inherently serial, no concurrency is used.

These specifications have the same meaning as corresponding specifications for *coliny_pattern_search*. Please see that page for specification details.

In particular, *coliny_solis.wets* supports dynamic rescaling of the step length, and dynamic rescaling of the constraint penalty. The only new specification is `contract_after_failure`, which specifies the number of unsuccessful cycles which must occur with a specific delta prior to contraction of the delta.

### See Also

These keywords may also be of interest:

- coliny_beta
- coliny_direct
- coliny_pattern_search
- coliny_cobyla
- coliny_ea
6.2. METHOD

contract_after_failure

- Keywords Area
- method
- coliny_solis_wets
- contract_after_failure

The number of unsuccessful cycles prior to contraction.

Specification

Alias: none

Argument(s): INTEGER

Default: 4+number of variables

Description

In particular, coliny_solis_wets supports dynamic rescaling of the step length, and dynamic rescaling of the constraint penalty. The only new specification is contract_after_failure, which specifies the number of unsuccessful cycles which must occur with a specific delta prior to contraction of the delta.

no_expansion

- Keywords Area
- method
- coliny_solis_wets
- no_expansion

Don’t allow expansion of the search pattern

Specification

Alias: none

Argument(s): none

Default: algorithm may expand pattern size

Description

In general, pattern search methods can expand and contract their step lengths. SCOLIB pattern search methods contract the step length by the value contraction_factor, and they expand the step length by the value (1/contraction_factor). The expand_after_success control specifies how many successful objective function improvements must occur with a specific step length prior to expansion of the step length, whereas the no_-expansion flag instructs the algorithm to forgo pattern expansion altogether.
expand_after_success

- Keywords Area
- method
- coliny_solis_wets
- expand_after_success

Set the factor by which a search pattern can be expanded

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** 5

**Description**

In general, pattern search methods can expand and contract their step lengths. SCOLIB pattern search methods contract the step length by the value contraction_factor, and they expand the step length by the value (1/contraction_factor). The expand_after_success control specifies how many successful objective function improvements must occur with a specific step length prior to expansion of the step length, whereas the no_expansion flag instructs the algorithm to forgo pattern expansion altogether.

constant_penalty

- Keywords Area
- method
- coliny_solis_wets
- constant_penalty

Use a simple weighted penalty to manage feasibility

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** algorithm dynamically adapts the constraint penalty

**Description**

Finally, constraint infeasibility can be managed in a somewhat more sophisticated manner than the simple weighted penalty function. If the constant_penalty specification is used, then the simple weighted penalty scheme described above is used. Otherwise, the constraint penalty is adapted to the value constraint_penalty/L, where L is the the smallest step length used so far.
6.2. METHOD

**contraction_factor**

- **Keywords Area**
- **method**
- **coliny_solis_wets**
- **contraction_factor**

Amount by which step length is rescaled

**Specification**

**Alias:** none

**Argument(s):** REAL

**Default:** 0.5

**Description**

For pattern search methods, **contraction_factor** specifies the amount by which step length is rescaled after unsuccessful iterates, must be strictly between 0 and 1.

For methods that can expand the step length, the expansion is $1/\text{contraction\_factor}$

**constraint\_penalty**

- **Keywords Area**
- **method**
- **coliny\_solis\_wets**
- **constraint\_penalty**

Multiplier for the penalty function

**Specification**

**Alias:** none

**Argument(s):** REAL

**Default:** 1.0

**Description**

Most SCOLIB optimizers treat constraints with a simple penalty scheme that adds **constraint\_penalty** times the sum of squares of the constraint violations to the objective function. The default value of **constraint\_penalty** is 1000.0, except for methods that dynamically adapt their constraint penalty, for which the default value is 1.0.
initial_delta

- Keywords Area
- method
- coliny_solis_wets
- initial_delta

Initial step size for derivative-free optimizers

**Specification**

*Alias:* none

**Argument(s):** REAL

**Default:** 1.0 (COBYLA), 0.1*range (PS, SW)

**Description**

The `initial_delta` keyword defines the size of the first search step in derivative-free optimization methods, specifically `asynch_pattern_search`, `coliny_cobyla`, `coliny_pattern_search`, `coliny_solis_wets`, and `mesh_adaptive_search`. It is applied in an absolute sense to all search directions.

**Default Behavior**

The default value is 1.0.

**Usage Tips**

It is recommended that `initial_delta` be the approximate distance from the initial point to the solution. If this distance is unknown, it is advisable to err on the side of choosing an `initial_delta` that is too large or to not specify it. Relative application of `initial_delta` is not available unless the user scales the problem accordingly.

**Examples**

Three example method input blocks appear below.

For `asynch_pattern_search`:

```
method
  asynch_pattern_search
  initial_delta = .5
  contraction_factor = 0.25
  merit_function merit1_smooth
  smoothing_factor = 1.0
  constraint_tolerance = 1.e-6
```

For `coliny_pattern_search`:

```
method
  coliny_pattern_search
  initial_delta = .2
  threshold_delta = 1.e-4
  max_iterations 100
  solution_accuracy = 1.e-6
  seed = 1234
  max_function_evaluations = 1000
```

For `mesh_adaptive_search`
6.2. METHOD

method
  mesh_adaptive_search
    initial_delta = 2.0
    seed = 1234

threshold_delta
  • Keywords Area
  • method
  • coliny_solis_wets
  • threshold_delta

Step length-based stopping criteria for derivative-free optimizers

Specification

Alias: none
  Argument(s): REAL
  Default: 1.0e-4 (COBYLA), 1.0e-5 (PS), 1.0e-6 (SW)

Description

The threshold_delta keyword defines the minimum step length allowed by the optimizer and is used to determine convergence. It is applicable to asynch_pattern_search, coliny_cobyla, coliny_pattern_search, coliny_solis_wets, and mesh_adaptive_search.

Default Behavior

The default value varies according to method as follows:

• asynch_pattern_search: 1.0e-2
• coliny_cobyla: 1.0e-4
• coliny_pattern_search: 1.0e-5
• coliny_solis_wets: 1.0e-6
• mesh_adaptive_search: 1.0e-6

Usage Tips

It is recommended that threshold_delta be set to a value for which changes of that scale in parameter values cause negligible changes in the objective function.

Examples

Three example method input blocks appear below.

For asynch_pattern_search:

method
  asynch_pattern_search
    contraction_factor = 0.25
    threshold_delta = 1.0e-4
    solution_target = 1.0e-6
    max_function_evaluations 500
    constraint_tolerance 1.0e-6
For *coliny_pattern_search*:

```python
method
coliny_pattern_search
  initial_delta = .2
  threshold_delta = 1.e-4
  max_iterations = 100
  solution_accuracy = 1.e-6
  seed = 1234
  max_function_evaluations = 1000
```

For *mesh_adaptive_search*:

```python
method
mesh_adaptive_search
  threshold_delta = 0.01
  seed = 1234
```

**solution_target**

- **Keywords Area**
- **method**
- **coliny_solis_wets**
- **solution_target**

Stopping criteria based on objective function value

**Specification**

**Alias:** solution_accuracy  
**Argument(s):** REAL  
**Default:** -DBL_MAX

**Description**

*solution_target* is a termination criterion. The algorithm will terminate when the function value falls below *solution_target*.

**seed**

- **Keywords Area**
- **method**
- **coliny_solis_wets**
- **seed**

Seed of the random number generator

**Specification**

**Alias:** none  
**Argument(s):** INTEGER  
**Default:** system-generated (non-repeatable)
6.2. METHOD

Description

The random seed control provides a mechanism for making a stochastic method repeatable. That is, the use of the same random seed in identical studies will generate identical results.

**Default Behavior**
If not specified, the seed is randomly generated.

**Expected Output**
If seed is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

**Usage Tips**
If a stochastic study was run without seed specified, and the user later wishes to repeat the study using the same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen. That value can then be added to the Dakota input file.

**Examples**

```
method
  sampling
    sample_type lhs
    samples = 10
    seed = 15347

show_misc_options
```

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no dump of specification options

**Description**

All SCOLIB methods support the `show_misc_options` optional specification which results in a dump of all the allowable method inputs. Note that the information provided by this command refers to optimizer parameters that are internal to SCOLIB, and which may differ from corresponding parameters used by the Dakota interface. The `misc_options` optional specification provides a means for inputting additional settings supported by the SCOLIB methods but which are not currently mapped through the Dakota input specification. Care must be taken in using this specification; they should only be employed by users familiar with the full range of parameter specifications available directly from SCOLIB and understand any differences that exist between those specifications and the ones available through Dakota.
misc_options

- Keywords Area
- method
- coliny_solis_wets
- misc_options

Set method options not available through Dakota spec

**Specification**

**Alias:** none

**Argument(s):** STRINGLIST  
**Default:** no misc options

**Description**

All SCOLIB methods support the `show_misc_options` optional specification which results in a dump of all the allowable method inputs. Note that the information provided by this command refers to optimizer parameters that are internal to SCOLIB, and which may differ from corresponding parameters used by the Dakota interface. The `misc_options` optional specification provides a means for inputting additional settings supported by the SCOLIB methods but which are not currently mapped through the Dakota input specification. Care must be taken in using this specification; they should only be employed by users familiar with the full range of parameter specifications available directly from SCOLIB and understand any differences that exist between those specifications and the ones available through Dakota.

**max_iterations**

- Keywords Area
- method
- coliny_solis_wets
- max_iterations

Number of iterations allowed for optimizers and adaptive UQ methods

**Topics**

This keyword is related to the topics:

- method_independent_controls

**Specification**

**Alias:** none

**Argument(s):** INTEGER  
**Default:** 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence} / efficient_global: 25*n)
6.2. **METHOD**

**Description**

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed $\text{max_iterations}$ iterations. See also $\text{max_function_evaluations}$.

**Default Behavior**

Default value is 100.

**convergence_tolerance**

- **Keywords Area**
- **method**
- **coliny_solis_wets**
- **convergence_tolerance**

Stopping criterion based on convergence of the objective function or statistics

**Topics**

This keyword is related to the topics:

- **method**
- **independent_controls**

**Specification**

Alias: none

Argument(s): REAL

Default: 1.e-4

**Description**

The $\text{convergence_tolerance}$ specification provides a real value for controlling the termination of iteration. For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by $\text{convergence_tolerance}$, then this convergence criterion is satisfied on the current iteration.

Therefore, permissible values are between 0 and 1, non-inclusive.

**Behavior Varies by Package/Library**

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- DOT: must be satisfied for two consecutive iterations
NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of convergence_tolerance approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., convergence_tolerance = 1.e-6 will result in approximately six digits of accuracy in the final objective function).

NL2SOL: See nl2sol

**max_function_evaluations**

- Keywords Area
- method
- coliny_solis_wets
- max_function_evaluations

Number of function evaluations allowed for optimizers

**Topics**

This keyword is related to the topics:

- method_independent_controls

**Specification**

Alias: none

Argument(s): INTEGER

Default: 1000

**Description**

The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed max_function_evaluations evaluations. See also max_iterations.

**Default Behavior**

Default value is 1000.

**scaling**

- Keywords Area
- method
- coliny_solis_wets
- scaling

Turn on scaling for variables, responses, and constraints
6.2. METHOD

Topics
This keyword is related to the topics:

- method_independent_controls

Specification
Alias: none
Argument(s): none
Default: no scaling

Description
Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by by providing the scaling keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the method, variables, and responses blocks. When the scaling keyword is omitted, all _scale_types and *scales specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.

- a *scales keyword, which gives characteristic values
- a *scale_type keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

Scale Types
There are four scale types:

1. none (default) - no scaling, value of *scales keyword is ignored
2. value - multiplicative scaling
3. auto - automatic scaling

First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:

- two-sided bounds scaled into the interval [0,1];
- one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
- no bounds or targets: no automatic scaling possible, therefore no scaling for this component

Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Futher, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into [0,1].
4. **log** - logarithmic scaling

First, any characteristic values from the optional *scales* specification are applied. Then logarithm base 10 scaling is applied.

Logarithmic scaling is not available for linear constraints.

When continuous design variables are log scaled, linear constraints are not allowed.

**Scales**

The *scales* keywords are used to specify the characteristic values. These must be non-zero real numbers. The numbers are used according to the corresponding *scale_type*, as described above.

Depending on the scale type, the characteristic values may be required or optional.

- **none**, **auto**, **log** - optional
- **value** - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than \(1.0\times10^{10}\). User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.

**Examples**

The two examples below are equivalent:

```plaintext
responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value"
  primary_scales = 1 1 100

responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value" "value" "value"
  primary_scales = 1 1 100
```

**model_pointer**

- **Keywords Area**
- **method**
- **coliny_solis_wets**
- **model_pointer**

Identifier for model block to be used by a method

**Topics**

This keyword is related to the topics:

- **block_pointer**
6.2. METHOD

Specification

Alias: none

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)

Description

The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.

Usage Tips

When doing advanced analyses that involve using multiple methods and multiple models, defining a model_pointer for each method is imperative.

See block_pointer for details about pointers.

Examples

environment
  tabular_graphics_data
  method_pointer = 'UQ'

method
  id_method = 'UQ'
  model_pointer = 'SURR'
  sampling,
    samples = 10
    seed = 98765 rng rnum2
    response_levels = 0.1 0.2 0.6
      0.1 0.2 0.6
    0.1 0.2 0.6
  sample_type lhs
  distribution cumulative

model
  id_model = 'SURR'
  surrogate global,
  dace_method_pointer = 'DACE'
  polynomial quadratic

method
  id_method = 'DACE'
  model_pointer = 'DACE_M'
  sampling sample_type lhs
    samples = 121 seed = 5034 rng rnum2

model
  id_model = 'DACE_M'
  single
  interface_pointer = 'I1'

variables
  uniform_certificate = 2
    lower_bounds = 0. 0.
    upper_bounds = 1. 1.
  descriptors = 'x1' 'x2'
interface

id_interface = 'I1'
system asynch evaluation_concurrency = 5
analysis_driver = 'text_book'

responses
response_functions = 3
no_gradients
no_hessians

6.2.38 coliny_cobyla

- Keywords Area
- method
- coliny_cobyla

Constrained Optimization BY Linear Approximations (COBYLA)

Topics
This keyword is related to the topics:

- package_scolib
- package_coliny
- local_optimization_methods
- constrained

Specification
Alias: none
Argument(s): none

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<th>Required/-</th>
<th>Description of</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional/Optional</td>
<td>Group</td>
<td>initial_delta</td>
<td>Description</td>
</tr>
<tr>
<td>Optional</td>
<td>threshold_delta</td>
<td>Reasonable initial changes to optimization variables</td>
<td>Required or expected accuracy in optimization variables.</td>
</tr>
<tr>
<td>Optional</td>
<td>solution_target</td>
<td>Stopping criteria based on objective function value</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>seed</td>
<td>Seed of the random number generator</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>show_misc_options</td>
<td>Show algorithm parameters not exposed in Dakota input</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>misc_options</td>
<td>Set method options not available through Dakota spec</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>max_iterations</td>
<td>Number of iterations allowed for optimizers and adaptive UQ methods</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>convergence_-tolerance</td>
<td>Stopping criterion based on convergence of the objective function or statistics</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>max_function_evaluations</td>
<td>Number of function evaluations allowed for optimizers</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>scaling</td>
<td>Turn on scaling for variables, responses, and constraints</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>model_pointer</td>
<td>Identifier for model block to be used by a method</td>
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</table>

**Description**

The Constrained Optimization BY Linear Approximations (COBYLA) algorithm is an extension to the Nelder-Mead simplex algorithm for handling general linear/nonlinear constraints and is invoked using the `coliny-cobyla` group specification. The COBYLA algorithm employs linear approximations to the objective and constraint functions, the approximations being formed by linear interpolation at N+1 points in the space of the variables. We regard these interpolation points as vertices of a simplex. The step length parameter controls the size of the simplex and it is reduced automatically from `initial_delta` to `threshold_delta`. One advantage that COBYLA has over many of its competitors is that it treats each constraint individually when calculating a
change to the variables, instead of lumping the constraints together into a single penalty function.

See the page package_scolib for important information regarding all SCOLIB methods
coliny_cobyla is inherently serial.

Stopping Criteria
COBYLA currently only supports termination based on

- `max_function_evaluations`
- `solution_target`

Other method-independent stopping criteria (`max_iterations` and `convergence_tolerance`) will be ignored if set.

Known Bugs
The implementation of the coliny_cobyla optimization method is such that the best function value is not always returned to Dakota for reporting. The user is advised to look through the Dakota screen output or the tabular output file (if generated) to confirm what the best function value and corresponding parameter values are.

The coliny_cobyla optimization method does not always respect bound constraints when scaling is turned on.

Neither bug will be fixed, as maintaining third-party source code (such as COBYLA) is outside of the Dakota project scope.

See Also
These keywords may also be of interest:

- coliny_beta
- coliny_direct
- coliny_pattern_search
- coliny_ea
- coliny_solis_wets

initial_delta

- Keywords Area
- method
- coliny_cobyla
- initial_delta

Reasonable initial changes to optimization variables

Specification

Alias: none

Argument(s): REAL

Default: 1.0 (COBYLA), 0.1*range (PS, SW)
6.2. METHOD

**Description**

*initial_delta* for COBYLA should be set to be a value that is reasonable for initial changes to the optimization variables. It represents a distance from the initial simplex within which linear approximation subproblems can be trusted to be sufficiently representative of the true problem. It is analogous to the initial trust-region size used in trust-region methods.

**Default Behavior**

The default value is 1.0.

**threshold_delta**

- Keywords Area
- method
- coliny_cobyla
- threshold_delta

Required or expected accuracy in optimization variables.

**Specification**

**Alias:** none

**Argument(s):** REAL

**Default:** 1.0e-4 (COBYLA), 1.0e-5 (PS), 1.0e-6 (SW)

**Description**

Unlike its use as a stopping criteria in other methods, *threshold_delta* is used to communicate the accuracy of the optimization variables to COBYLA. It represents the minimum distance from the simplex within which linear approximation subproblems can be trusted to be sufficiently representative of the true problem. It is analogous to the minimum trust-region size used in trust-region methods. Note that, per COBYLA documentation, the level of accuracy is not guaranteed.

**Default Behavior**

The default value is 0.0001.

**Additional Discussion**

While *threshold_delta* is not a stopping criteria for COBYLA, we note that it may have a side effect regarding convergence. In particular, if lower accuracy is required of the optimization variables, it may stop sooner than if higher accuracy is required.

**solution_target**

- Keywords Area
- method
- coliny_cobyla
- solution_target

Stopping criteria based on objective function value
CHAPTER 6. KEYWORDS AREA

Specification

Alias: solution_accuracy
  Argument(s): REAL
  Default: -DBL_MAX

Description

solution_target is a termination criterion. The algorithm will terminate when the function value falls below solution_target.

seed

- Keywords Area
- method
- coliny_cobyla
- seed

Seed of the random number generator

Specification

Alias: none
  Argument(s): INTEGER
  Default: system-generated (non-repeatable)

Description

The random seed control provides a mechanism for making a stochastic method repeatable. That is, the use of the same random seed in identical studies will generate identical results.

   Default Behavior
   If not specified, the seed is randomly generated.

   Expected Output
   If seed is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

   Usage Tips
   If a stochastic study was run without seed specified, and the user later wishes to repeat the study using the same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen. That value can then be added to the Dakota input file.

Examples

method
  sampling
    sample_type lhs
    samples = 10
    seed = 15347
show_misc_options

- Keywords Area
- method
- coliny_cobyla
- show_misc_options

Show algorithm parameters not exposed in Dakota input

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no dump of specification options

**Description**

All SCOLIB methods support the `show_misc_options` optional specification which results in a dump of all the allowable method inputs. Note that the information provided by this command refers to optimizer parameters that are internal to SCOLIB, and which may differ from corresponding parameters used by the Dakota interface. The `misc_options` optional specification provides a means for inputting additional settings supported by the SCOLIB methods but which are not currently mapped through the Dakota input specification. Care must be taken in using this specification; they should only be employed by users familiar with the full range of parameter specifications available directly from SCOLIB and understand any differences that exist between those specifications and the ones available through Dakota.

misc_options

- Keywords Area
- method
- coliny_cobyla
- misc_options

Set method options not available through Dakota spec

**Specification**

**Alias:** none

**Argument(s):** STRINGLIST

**Default:** no misc options
CHAPTER 6. KEYWORDS AREA

Description
All SCOLIB methods support the `show_misc_options` optional specification which results in a dump of all the allowable method inputs. Note that the information provided by this command refers to optimizer parameters that are internal to SCOLIB, and which may differ from corresponding parameters used by the Dakota interface. The `misc_options` optional specification provides a means for inputing additional settings supported by the SCOLIB methods but which are not currently mapped through the Dakota input specification. Care must be taken in using this specification; they should only be employed by users familiar with the full range of parameter specifications available directly from SCOLIB and understand any differences that exist between those specifications and the ones available through Dakota.

`max_iterations`
- **Keywords Area**
- **method**
- **coliny_cobyla**
- **max_iterations**

Number of iterations allowed for optimizers and adaptive UQ methods

Topics
This keyword is related to the topics:
- **method_independent_controls**

Specification
**Alias:** none
**Argument(s):** INTEGER
**Default:** 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence} / efficient_global: 25*n)

Description
The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed `max_iterations` iterations. See also `max_function_evaluations`.

**Default Behavior**
Default value is 100.

`convergence_tolerance`
- **Keywords Area**
- **method**
- **coliny_cobyla**
- **convergence_tolerance**

Stopping criterion based on convergence of the objective function or statistics
6.2. METHOD

Topics
This keyword is related to the topics:

- method
- independent
- controls

Specification
Alias: none
  Argument(s): REAL
  Default: 1.0e-4

Description
The convergence_tolerance specification provides a real value for controlling the termination of iteration. For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by convergence_tolerance, then this convergence criterion is satisfied on the current iteration.

Therefore, permissible values are between 0 and 1, non-inclusive.

Behavior Varies by Package/Library
This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:
- DOT: must be satisfied for two consecutive iterations
- NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of convergence_tolerance approximatively specifies the number of significant digits of accuracy desired in the final objective function (e.g., convergence_tolerance = 1.0e-6 will result in approximately six digits of accuracy in the final objective function).
- NL2SOL: See nl2sol

max_function_evaluations
- Keywords Area
- method
- coliny_cobyla
- max_function_evaluations

Number of function evaluations allowed for optimizers
Topics
This keyword is related to the topics:

- method_independent_controls

Specification
Alias: none
Argument(s): INTEGER
Default: 1000

Description
The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed \texttt{max\_function\_evaluations} evaluations. See also \texttt{max\_iterations}.

Default Behavior
Default value is 1000.

caln
- Keywords Area
- method
- coliny_cobyla
- scaling

Turn on scaling for variables, responses, and constraints

Topics
This keyword is related to the topics:

- method_independent_controls

Specification
Alias: none
Argument(s): none
Default: no scaling

Description
Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by by providing the \texttt{scaling} keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.
Scaling also requires the specification of additional keywords which are found in the method, variables, and responses blocks. When the scaling keyword is omitted, all _scale_types and *_scales specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.

- a *scales keyword, which gives characteristic values
- a *scale_type keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

**Scale Types**

There are four scale types:

1. **none** (default) - no scaling, value of *scales keyword is ignored
2. **value** - multiplicative scaling
3. **auto** - automatic scaling
   
   First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:
   - two-sided bounds scaled into the interval [0,1];
   - one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
   - no bounds or targets: no automatic scaling possible, therefore no scaling for this component

   Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into [0,1].

4. **log** - logarithmic scaling
   
   First, any characteristic values from the optional *scales specification are applied. Then logarithm base 10 scaling is applied.

   Logarithmic scaling is not available for linear constraints.

   When continuous design variables are log scaled, linear constraints are not allowed.

**Scales**

The *scales keywords are used to specify the characteristic values. These must be non-zero real numbers. The numbers are used according to the corresponding *scale_type, as described above.

Depending on the scale type, the characteristic values may be required or optional.

- **none, auto, log** - optional
- **value** - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than 1.0e10*DBL_MIN. User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.
Examples
The two examples below are equivalent:

```plaintext
responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value"
  primary_scales = 1 1 100

responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value" "value" "value"
  primary_scales = 1 1 100
```

**model_pointer**

- **Keywords Area**
- **method**
- **coliny_cobyla**
- **model_pointer**

Identifier for model block to be used by a method

**Topics**
This keyword is related to the topics:

- **block_pointer**

**Specification**

**Alias:** none

**Argument(s):** STRING

**Default:** method use of last model parsed (or use of default model if none parsed)

**Description**

The **model_pointer** is used to specify which **model** block will be used to perform the function evaluations needed by the Dakota method.

**Default Behavior**

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a **model** block in the Dakota input file that has a corresponding **id_model** with the same name.

**Usage Tips**

When doing advanced analyses that involve using multiple methods and multiple models, defining a **model-pointer** for each method is imperative.

See **block_pointer** for details about pointers.
6.2. METHOD

Examples

environment
tabular_graphics_data
method_pointer = 'UQ'

method
id_method = 'UQ'
model_pointer = 'Surr'
sampling,
samples = 10
seed = 98765 rng rnum2
response_levels = 0.1 0.2 0.6
0.1 0.2 0.6
0.1 0.2 0.6
sample_type lhs
distribution cumulative

model
id_model = 'Surr'
surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
id_method = 'DACE'
model_pointer = 'DACE_M'
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = 'DACE_M'
single
interface_pointer = 'I1'

variables
uniform_uncertain = 2
lower_bounds = 0. 0.
upper_bounds = 1. 1.
descriptors = 'x1' 'x2'

interface
id_interface = 'I1'
system asynch evaluation_concurrency = 5
analysis_driver = 'text_book'

responses
response_functions = 3
no_gradients
no_hessians

6.2.39 coliny_direct

- Keywords Area
- method
- coliny_direct

DIviding RECTangles method
CHAPTER 6. KEYWORDS AREA

Topics
This keyword is related to the topics:

- package_scolib
- package_coliny
- global_optimization_methods

Specification
Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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</thead>
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<tr>
<td>Optional</td>
<td></td>
<td>division</td>
<td>Determine how rectangles are subdivided</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>global_balance_ - parameter</td>
<td>Tolerance for whether a subregion is worth dividing</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>local_balance_ - parameter</td>
<td>Tolerance for whether a subregion is worth dividing</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>max_boxsize_limit</td>
<td>Stopping Criterion based on longest edge of hyperrectangle</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>min_boxsize_limit</td>
<td>Stopping Criterion based on shortest edge of hyperrectangle</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>constraint_penalty</td>
<td>Multiplier for the penalty function</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>solution_target</td>
<td>Stopping criteria based on objective function value</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>seed</td>
<td>Seed of the random number generator</td>
</tr>
</tbody>
</table>
6.2. METHOD

The DIviding RECTangles (DIRECT) optimization algorithm is a derivative free global optimization method that balances local search in promising regions of the design space with global search in unexplored regions. As shown in Figure 5.1, DIRECT adaptively subdivides the space of feasible design points so as to guarantee that iterates are generated in the neighborhood of a global minimum in finitely many iterations.

In practice, DIRECT has proven an effective heuristic for engineering design applications, for which it is able to quickly identify candidate solutions that can be further refined with fast local optimizers.

See the page package_scolib for important information regarding all SCOLIB methods

The DIRECT algorithm supports concurrency up to twice the number of variables being optimized. DIRECT uses the solution_target, constraint_penalty and show_misic_options specifications that are described in package_scolib. Note, however, that DIRECT uses a fixed penalty value for constraint violations (i.e. it is not dynamically adapted as is done in coliny_pattern_search).

### Search Parameters

<table>
<thead>
<tr>
<th>Optional</th>
<th>show_misic_options</th>
<th>Show algorithm parameters not exposed in Dakota input</th>
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<tbody>
<tr>
<td>Optional</td>
<td>misc_options</td>
<td>Set method options not available through Dakota spec</td>
</tr>
<tr>
<td>Optional</td>
<td>max_iterations</td>
<td>Number of iterations allowed for optimizers and adaptive UQ methods</td>
</tr>
<tr>
<td>Optional</td>
<td>convergence_tolerance</td>
<td>Stopping criterion based on convergence of the objective function or statistics</td>
</tr>
<tr>
<td>Optional</td>
<td>max_function_evaluations</td>
<td>Number of function evaluations allowed for optimizers</td>
</tr>
<tr>
<td>Optional</td>
<td>scaling</td>
<td>Turn on scaling for variables, responses, and constraints</td>
</tr>
<tr>
<td>Optional</td>
<td>model_pointer</td>
<td>Identifier for model block to be used by a method</td>
</tr>
</tbody>
</table>
The `global_balance_parameter` controls how much global search is performed by only allowing a subregion to be subdivided if the size of the subregion divided by the size of the largest subregion is at least \textit{global_balance_parameter}. Intuitively, this forces large subregions to be subdivided before the smallest subregions are refined. The `local_balance_parameter` provides a tolerance for estimating whether the smallest subregion can provide a sufficient decrease to be worth subdividing; the default value is a small value that is suitable for most applications.

**Stopping Criteria**

DIRECT can be terminated with:

- `max_function_evaluations`
- `max_iterations`
- `convergence_tolerance`
- `solution_target`
- `max_boxsize_limit`
- `min_boxsize_limit` - most effective in practice

**See Also**

These keywords may also be of interest:

- `coliny_beta`
- `coliny_pattern_search`
- `coliny_cobyla`
- `coliny_ea`
- `coliny_solis_wets`
- `ncsu_direct`

**division**

- `Keywords Area`
- `method`
- `coliny_direct`
- `division`

Determine how rectangles are subdivided

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** `major_dimension`
### Description

The division specification determines how DIRECT subdivides each subregion of the search space. If division is set to `major_dimension`, then the dimension representing the longest edge of the subregion is subdivided (this is the default). If division is set to `all_dimensions`, then all dimensions are simultaneously subdivided.

**major_dimension**

- Keywords Area
- method
- coliny_direct
- division
- `major_dimension`

  (default) Longest edge of subregion is subdivided

### Specification

**Alias:** none

**Argument(s):** none

### Description

Longest edge of subregion is subdivided

**all_dimensions**

- Keywords Area
- method
- coliny_direct
- division
- `all_dimensions`

All dimensions are simultaneously subdivided
Specification
Alias: none
Argument(s): none

Description
All dimensions are simultaneously subdivided

global_balance_parameter
- Keywords Area
- method
- coliny_direct
- global_balance_parameter

Tolerance for whether a subregion is worth dividing

Specification
Alias: none
Argument(s): REAL
Default: 0.0

Description
The global_balance_parameter controls how much global search is performed by only allowing a subregion to be subdivided if the size of the subregion divided by the size of the largest subregion is at least global_balance_parameter. Intuitively, this forces large subregions to be subdivided before the smallest subregions are refined.

local_balance_parameter
- Keywords Area
- method
- coliny_direct
- local_balance_parameter

Tolerance for whether a subregion is worth dividing

Specification
Alias: none
Argument(s): REAL
Default: 1.e-8
6.2. METHOD

Description

See parent page. The `local_balance` parameter provides a tolerance for estimating whether the smallest subregion can provide a sufficient decrease to be worth subdividing; the default value is a small value that is suitable for most applications.

`max_boxsize_limit`

- Keywords Area
- method
- coliny_direct
- `max_boxsize_limit`

Stopping Criterion based on longest edge of hyperrectangle

Specification

Alias: none
Argument(s): REAL
Default: 0.0

Description

Each subregion considered by DIRECT has a size, which corresponds to the longest diagonal of the subregion. `max_boxsize_limit` specification terminates DIRECT if the size of the largest subregion falls below this threshold.

`min_boxsize_limit`

- Keywords Area
- method
- coliny_direct
- `min_boxsize_limit`

Stopping Criterion based on shortest edge of hyperrectangle

Specification

Alias: none
Argument(s): REAL
Default: 1.0e-4
Description

`min_boxsize_limit` is a setting that terminates the optimization when the measure of a hyperrectangle $S$ with $f(c(S)) = f_{\text{min}}$ is less than `min_boxsize_limit`.

Each subregion considered by DIRECT has a size, which corresponds to the longest diagonal of the subregion. `min_boxsize_limit` specification terminates DIRECT if the size of the smallest subregion falls below this threshold.

In practice, this specification is likely to be more effective at limiting DIRECT’s search.

`constraint_penalty`

- Keywords Area
- method
- `coliny_direct`
- `constraint_penalty`

Multiplier for the penalty function

Specification

Alias: none

Argument(s): REAL

Default: 1000.0

Description

Most SCOLIB optimizers treat constraints with a simple penalty scheme that adds `constraint_penalty` times the sum of squares of the constraint violations to the objective function. The default value of `constraint_penalty` is 1000.0, except for methods that dynamically adapt their constraint penalty, for which the default value is 1.0.

`solution_target`

- Keywords Area
- method
- `coliny_direct`
- `solution_target`

Stopping criteria based on objective function value

Specification

Alias: `solution_accuracy`

Argument(s): REAL

Default: -DBL_MAX
6.2. METHOD

Description

`solution_target` is a termination criterion. The algorithm will terminate when the function value falls below `solution_target`.

`seed`

- **Keywords Area**
- **method**
- **coliny_direct**
- **seed**

Seed of the random number generator

Specification

**Alias:** none

**Argument(s):** INTEGER

**Default:** system-generated (non-repeatable)

Description

The random `seed` control provides a mechanism for making a stochastic method repeatable. That is, the use of the same random seed in identical studies will generate identical results.

**Default Behavior**

If not specified, the seed is randomly generated.

**Expected Output**

If `seed` is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

**Usage Tips**

If a stochastic study was run without `seed` specified, and the user later wishes to repeat the study using the same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen. That value can then be added to the Dakota input file.

Examples

```dakota
method
    sampling
        sample_type lhs
        samples = 10
        seed = 15347
```

**show_misc_options**

- **Keywords Area**
- **method**
- **coliny_direct**
- **show_misc_options**

Show algorithm parameters not exposed in Dakota input
Specified

Alias: none

Description

All SCOLIB methods support the `show_misc_options` optional specification which results in a dump of all the allowable method inputs. Note that the information provided by this command refers to optimizer parameters that are internal to SCOLIB, and which may differ from corresponding parameters used by the Dakota interface. The `misc_options` optional specification provides a means for inputting additional settings supported by the SCOLIB methods but which are not currently mapped through the Dakota input specification. Care must be taken in using this specification; they should only be employed by users familiar with the full range of parameter specifications available directly from SCOLIB and understand any differences that exist between those specifications and the ones available through Dakota.

**misc_options**

- Keywords Area
- method
- coliny_direct
- misc_options

Set method options not available through Dakota spec

Specified

Alias: none

Description

All SCOLIB methods support the `show_misc_options` optional specification which results in a dump of all the allowable method inputs. Note that the information provided by this command refers to optimizer parameters that are internal to SCOLIB, and which may differ from corresponding parameters used by the Dakota interface. The `misc_options` optional specification provides a means for inputting additional settings supported by the SCOLIB methods but which are not currently mapped through the Dakota input specification. Care must be taken in using this specification; they should only be employed by users familiar with the full range of parameter specifications available directly from SCOLIB and understand any differences that exist between those specifications and the ones available through Dakota.

**max_iterations**

- Keywords Area
- method
- coliny_direct
6.2. METHOD

- max_iterations

Number of iterations allowed for optimizers and adaptive UQ methods

**Topics**

This keyword is related to the topics:

- method_independent_controls

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence}/efficient-global: 25*n)

**Description**

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed max_iterations iterations. See also max_function_evaluations.

**Default Behavior**

Default value is 100.

**convergence_tolerance**

- Keywords Area

- method

- coliny_direct

- convergence_tolerance

Stopping criterion based on convergence of the objective function or statistics

**Topics**

This keyword is related to the topics:

- method_independent_controls

**Specification**

**Alias:** none

**Argument(s):** REAL

**Default:** 1.e-4
CHAPTER 6. KEYWORDS AREA

Description

The convergence_tolerance specification provides a real value for controlling the termination of iteration. For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by convergence_tolerance, then this convergence criterion is satisfied on the current iteration.

Therefore, permissible values are between 0 and 1, non-inclusive.

Behavior Varies by Package/Library

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- DOT: must be satisfied for two consecutive iterations
- NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of convergence_tolerance approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., convergence_tolerance = 1.e-6 will result in approximately six digits of accuracy in the final objective function).
- NL2SOL: See nl2sol

max_function_evaluations

- Keywords Area
- method
- coliny_direct
- max_function_evaluations

Number of function evaluations allowed for optimizers

Topics

This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none

Argument(s): INTEGER

Default: 1000
6.2. METHOD

Description

The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed max_function_evaluations evaluations. See also max_iterations.

Default Behavior

Default value is 1000.

scaling

- Keywords Area
- method
- coliny_direct
- scaling

Turn on scaling for variables, responses, and constraints

Topics

This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none

Argument(s): none

Default: no scaling

Description

Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by by providing the scaling keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the method, variables, and responses blocks. When the scaling keyword is omitted, all _scale_types and *scales specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.

- a *scales keyword, which gives characteristic values
- a *scale_type keyword, which determines how to use the characteristic values
The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

**Scale Types**

There are four scale types:

1. **none** (default) - no scaling, value of *scales* keyword is ignored
2. **value** - multiplicative scaling
3. **auto** - automatic scaling
   
   First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:
   
   - two-sided bounds scaled into the interval [0,1];
   - one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
   - no bounds or targets: no automatic scaling possible, therefore no scaling for this component

   Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into [0,1].

4. **log** - logarithmic scaling
   
   First, any characteristic values from the optional *scales* specification are applied. Then logarithm base 10 scaling is applied.

   Logarithmic scaling is not available for linear constraints. When continuous design variables are log scaled, linear constraints are not allowed.

**Scales**

The *scales* keywords are used to specify the characteristic values. These must be non-zero real numbers. Depending on the scale type, the characteristic values may be required or optional.

- **none, auto, log** - optional
- **value** - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than 1.0e10*DBL_MIN. User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.

**Examples**

The two examples below are equivalent:

```
responses
 objective_functions 3
 sense "maximize"
 primary_scale_types = "value"
 primary_scales = 1 1 100
```

```
responses
 objective_functions 3
 sense "maximize"
 primary_scale_types = "value" "value" "value"
 primary_scales = 1 1 100
```
model_pointer

• Keywords Area
• method
• coliny_direct
• model_pointer

Identifier for model block to be used by a method

Topics
This keyword is related to the topics:
• block_pointer

Specification
Alias: none
Argument(s): STRING
Default: method use of last model parsed (or use of default model if none parsed)

Description
The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior
If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.

Usage Tips
When doing advanced analyses that involve using multiple methods and multiple models, defining a model_pointer for each method is imperative.
See block_pointer for details about pointers.

Examples
environment
  tabular_graphics_data
  method_pointer = ’UQ’

method
  id_method = ’UQ’
  model_pointer = ’SURR’
  sampling,
    samples = 10
    seed = 98765 rng rnum2
    response_levels = 0.1 0.2 0.6
      0.1 0.2 0.6
        0.1 0.2 0.6
      sample_type lhs
distribution cumulative

model
  id_model = ’SURR’
surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
id_method = 'DACE'
model_pointer = 'DACE_M'
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = 'DACE_M'
single
interface_pointer = 'I1'

variables
uniform_uncertain = 2
lower_bounds = 0. 0.
upper_bounds = 1. 1.
descriptors = 'x1' 'x2'

interface
id_interface = 'I1'
system asynch evaluation_concurrency = 5
analysis_driver = 'text_book'

responses
response_functions = 3
no_gradients
no_hessians

6.2.40 coliny_ea

• Keywords Area

• method

• coliny_ea

Evolutionary Algorithm

Topics

This keyword is related to the topics:

• package_scolib

• package_coliny

• global_optimization_methods

Specification

Alias: none
Argument(s): none
### Required/-Optional

<table>
<thead>
<tr>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>population_size</td>
<td>Set the population size</td>
</tr>
<tr>
<td>Optional</td>
<td>initialization_type</td>
<td>Specify how to initialize the population</td>
</tr>
<tr>
<td>Optional</td>
<td>fitness_type</td>
<td>Select fitness type</td>
</tr>
<tr>
<td>Optional</td>
<td>replacement_type</td>
<td>Select a replacement type for SCOLIB evolutionary algorithm (coliny_ea)</td>
</tr>
<tr>
<td>Optional</td>
<td>crossover_rate</td>
<td>Specify the probability of a crossover event</td>
</tr>
<tr>
<td>Optional</td>
<td>crossover_type</td>
<td>Select a crossover type</td>
</tr>
<tr>
<td>Optional</td>
<td>mutation_rate</td>
<td>Set probability of a mutation type</td>
</tr>
<tr>
<td>Optional</td>
<td>mutation_type</td>
<td>Select a mutation type</td>
</tr>
<tr>
<td>Optional</td>
<td>constraint_penalty</td>
<td>Multiplier for the penalty function</td>
</tr>
<tr>
<td>Optional</td>
<td>solution_target</td>
<td>Stopping criteria based on objective function value</td>
</tr>
<tr>
<td>Optional</td>
<td>seed</td>
<td>Seed of the random number generator</td>
</tr>
<tr>
<td>Optional</td>
<td>show_misc_options</td>
<td>Show algorithm parameters not exposed in Dakota input</td>
</tr>
<tr>
<td>Optional</td>
<td>misc_options</td>
<td>Set method options not available through Dakota spec</td>
</tr>
</tbody>
</table>
CHAPTER 6. KEYWORDS AREA

<table>
<thead>
<tr>
<th>Optional</th>
<th>max_iterations</th>
<th>Number of iterations allowed for optimizers and adaptive UQ methods</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>convergence_-tolerance</td>
<td>Stopping criterion based on convergence of the objective function or statistics</td>
</tr>
<tr>
<td>Optional</td>
<td>max_function_-evaluations</td>
<td>Number of function evaluations allowed for optimizers</td>
</tr>
<tr>
<td>Optional</td>
<td>scaling</td>
<td>Turn on scaling for variables, responses, and constraints</td>
</tr>
<tr>
<td>Optional</td>
<td>model_pointer</td>
<td>Identifier for model block to be used by a method</td>
</tr>
</tbody>
</table>

Description

Evolutionary Algorithm

See the page package_scolib for important information regarding all SCOLIB methods

coliny_pattern_search supports concurrency up to the size of the population

The random seed control provides a mechanism for making a stochastic optimization repeatable. That is, the use of the same random seed in identical studies will generate identical results. The population_size control specifies how many individuals will comprise the EA’s population.

The initialization_type defines the type of initialization for the population of the EA. There are three types: simple_random, unique_random, and flat_file. simple_random creates initial solutions with random variable values according to a uniform random number distribution. It gives no consideration to any previously generated designs. The number of designs is specified by the population_size. unique_random is the same as simple_random, except that when a new solution is generated, it is checked against the rest of the solutions. If it duplicates any of them, it is rejected. flat_file allows the initial population to be read from a flat file. If flat_file is specified, a file name must be given.

The fitness_type controls how strongly differences in "fitness" (i.e., the objective function) are weighted in the process of selecting "parents" for crossover:

- the linear_rank setting uses a linear scaling of probability of selection based on the rank order of each individual’s objective function within the population

- the merit_function setting uses a proportional scaling of probability of selection based on the relative value of each individual’s objective function within the population
6.2. METHOD

The replacement_type controls how current populations and newly generated individuals are combined to create a new population. Each of the replacement_type selections accepts an integer value, which is referred to below as the replacement_size.

- The random setting creates a new population using (a) replacement_size randomly selected individuals from the current population, and (b) population_size - replacement_size individuals randomly selected from among the newly generated individuals (the number of which is optionally specified using new_solutions_generated) that are created for each generation (using the selection, crossover, and mutation procedures).

- The chc setting creates a new population using (a) the replacement_size best individuals from the combination of the current population and the newly generated individuals, and (b) population_size - replacement_size individuals randomly selected from among the remaining individuals in this combined pool. The chc setting is the preferred selection for many engineering problems.

- The elitist (default) setting creates a new population using (a) the replacement_size best individuals from the current population, (b) and population_size - replacement_size individuals randomly selected from the newly generated individuals. It is possible in this case to lose a good solution from the newly generated individuals if it is not randomly selected for replacement; however, the default new_solutions_generated value is set such that the entire set of newly generated individuals will be selected for replacement.

Note that new_solutions_generated is not recognized by Dakota as a valid keyword unless replacement_type has been specified.

Theory

The basic steps of an evolutionary algorithm are depicted in Figure 5.2.

![Figure 6.2: Depiction of evolutionary algorithm](image)

They can be enumerated as follows:
1. Select an initial population randomly and perform function evaluations on these individuals
2. Perform selection for parents based on relative fitness
3. Apply crossover and mutation to generate new solutions generated new individuals from the selected parents
   • Apply crossover with a fixed probability from two selected parents
   • If crossover is applied, apply mutation to the newly generated individual with a fixed probability
   • If crossover is not applied, apply mutation with a fixed probability to a single selected parent
4. Perform function evaluations on the new individuals
5. Perform replacement to determine the new population
6. Return to step 2 and continue the algorithm until convergence criteria are satisfied or iteration limits are exceeded

See Also
These keywords may also be of interest:

- coliny_beta
- coliny_direct
- coliny_pattern_search
- coliny_cobyla
- coliny_solis_wets

population_size

- Keywords Area
- method
- coliny_ea
- population_size

Set the population size

Specification

Alias: none

Argument(s): INTEGER
Default: 50

Description
The number of designs in the population is specified by the population_size.
6.2. METHOD

**initialization_type**

- **Keywords Area**
- **method**
- **coliny_ea**
- **initialization_type**

Specify how to initialize the population

**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** unique_random

<table>
<thead>
<tr>
<th>Required/Optional (Choose One)</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>simple_random</td>
<td>Create random initial solutions</td>
<td></td>
<td></td>
</tr>
<tr>
<td>unique_random</td>
<td>Create random initial solutions, but enforce uniqueness (default)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>flat_file</td>
<td>Read initial solutions from file</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Description**

The `initialization_type` defines how the initial population is created for the GA. There are three types:

1. **simple_random**
2. **unique_random** (default)
3. **flat_file**

Setting the size for the **flat_file** initializer has the effect of requiring a minimum number of designs to create. If this minimum number has not been created once the files are all read, the rest are created using the **unique_random** initializer and then the **simple_random** initializer if necessary.

**simple_random**

- **Keywords Area**
- **method**
- **coliny_ea**
- **initialization_type**
- **simple_random**

Create random initial solutions
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none
Argument(s): none

Description

simple_random creates initial solutions with random variable values according to a uniform random number distribution. It gives no consideration to any previously generated designs.

unique_random

- Keywords Area
- method
- coliny_ea
- initialization_type
- unique_random

Create random initial solutions, but enforce uniqueness (default)

Specification

Alias: none
Argument(s): none

Description

unique_random is the same as simple_random, except that when a new solution is generated, it is checked against the rest of the solutions. If it duplicates any of them, it is rejected.

flat_file

- Keywords Area
- method
- coliny_ea
- initialization_type
- flat_file

Read initial solutions from file

Specification

Alias: none
Argument(s): STRING
6.2. **METHOD**

**Description**

`flat_file` allows the initial population to be read from a flat file. If `flat_file` is specified, a file name must be given.

**fitness_type**

- **Keywords Area**
- **method**
- **coliny_ea**
- **fitness_type**

Select fitness type

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** linear_rank

<table>
<thead>
<tr>
<th>Required/-Optional Required</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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</thead>
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<td>Group 1</td>
<td>linear_rank</td>
<td>Set selection scaling</td>
</tr>
<tr>
<td></td>
<td></td>
<td>merit_function</td>
<td>Balance goals of reducing objective function and satisfying constraints</td>
</tr>
</tbody>
</table>

**Description**

The `fitness_type` controls how strongly differences in “fitness” (i.e., the objective function) are weighted in the process of selecting “parents” for crossover. It has two options, `linear_rank` and `merit_function`.

**linear_rank**

- **Keywords Area**
- **method**
- **coliny_ea**
- **fitness_type**
- **linear_rank**

Set selection scaling

**Specification**

**Alias:** none

**Argument(s):** none
CHAPTER 6. KEYWORDS AREA

Description
The linear_rank setting uses a linear scaling of probability of selection based on the rank order of each individual’s objective function within the population.

merit_function
- Keywords Area
- method
- coliny_ea
- fitness_type
- merit_function

Balance goals of reducing objective function and satisfying constraints.

Specification
Alias: none
Argument(s): none

Description
A merit_function is a function in constrained optimization that attempts to provide joint progress toward reducing the objective function and satisfying the constraints.

replacement_type
- Keywords Area
- method
- coliny_ea
- replacement_type

Select a replacement type for SCOLIB evolutionary algorithm (coliny_ea).

Specification
Alias: none
Argument(s): none
Default: elitist=1

<table>
<thead>
<tr>
<th>Required/Optional</th>
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<td><strong>random</strong></td>
<td><strong>random</strong></td>
</tr>
<tr>
<td>Create new population randomly</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
6.2. METHOD

<table>
<thead>
<tr>
<th>Replacement Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>chc</td>
<td>Create new population using replacement</td>
</tr>
<tr>
<td>elitist</td>
<td>Use the best designs to form a new population</td>
</tr>
<tr>
<td>new_solutions_generated</td>
<td>Replace population with individuals chosen from population</td>
</tr>
</tbody>
</table>

Optional

**Description**

The replacement_type controls how current populations and newly generated individuals are combined to create a new population. Each of the replacement_type selections accepts an associated integer value, which is specified by the replacement_size:

- The random setting creates a new population using (a) replacement_size randomly selected individuals from the current population, and (b) population_size - replacement_size individuals randomly selected from among the newly generated individuals (the number of which is optionally specified using new_solutions_generated) that are created for each generation (using the selection, crossover, and mutation procedures).

- The chc setting creates a new population using (a) the replacement_size best individuals from the combination of the current population and the newly generated individuals, and (b) population_size - replacement_size individuals randomly selected from among the remaining individuals in this combined pool. The chc setting is the preferred selection for many engineering problems.

- The elitist (default) setting creates a new population using (a) the replacement_size best individuals from the current population, (b) and population_size - replacement_size individuals randomly selected from the newly generated individuals. It is possible in this case to lose a good solution from the newly generated individuals if it is not randomly selected for replacement; however, the default new_solutions_generated value is set such that the entire set of newly generated individuals will be selected for replacement.

Note that new_solutions_generated is not recognized by Dakota as a valid keyword unless replacement_type has been specified.

**random**

- **Keywords Area**
- **method**
- **coliny_ea**
- **replacement_type**
- **random**

Create new population randomly

**Specification**

**Alias:** none

**Argument(s):** INTEGER
**Description**

The `replacement_type` controls how current populations and newly generated individuals are combined to create a new population. Each of the `replacement_type` selections accepts an integer value, which is referred to as the `replacement_size`:

The random setting creates a new population using:

- `replacement_size` randomly selected individuals from the current population, and
- `population_size - replacement_size` individuals randomly selected from among the newly generated individuals (the number of which is optionally specified using `new_solutions_generated`) that are created for each generation (using the selection, crossover, and mutation procedures).

**chc**

- Keywords Area
- method
- coliny_ea
- replacement_type
- chc

Create new population using replacement

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Description**

The `replacement_type` controls how current populations and newly generated individuals are combined to create a new population. Each of the `replacement_type` selections accepts an integer value, which is referred to as the `replacement_size`:

The chc setting creates a new population using (a) the `replacement_size` best individuals from the combination of the current population and the newly generated individuals, and (b) `population_size - replacement_size` individuals randomly selected from among the remaining individuals in this combined pool. The chc setting is the preferred selection for many engineering problems.

**elitist**

- Keywords Area
- method
- coliny_ea
- replacement_type
- elitist

Use the best designs to form a new population
6.2. **METHOD**

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Description**

The elitist (default) setting creates a new population using (a) the replacement_size best individuals from the current population, (b) and population_size - replacement_size individuals randomly selected from the newly generated individuals. It is possible in this case to lose a good solution from the newly generated individuals if it is not randomly selected for replacement; however, the default new_solutions_generated value is set such that the entire set of newly generated individuals will be selected for replacement.

new_solutions_generated

- Keywords Area
- method
- coliny_ea
- replacement_type
- new_solutions_generated

Replace population with individuals chosen from population

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** population_size - replacement_size

**Description**

- The random setting creates a new population using (a) replacement_size randomly selected individuals from the current population, and (b) population_size - replacement_size individuals randomly selected from among the newly generated individuals (the number of which is optionally specified using new_solutions_generated) that are created for each generation (using the selection, crossover, and mutation procedures).

crossover_rate

- Keywords Area
- method
- coliny_ea
- crossover_rate

Specify the probability of a crossover event
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): REAL

Default: 0.8

Description

The crossover_type controls what approach is employed for combining parent genetic information to create offspring, and the crossover_rate specifies the probability of a crossover operation being performed to generate a new offspring. The SCOLIB EA method supports three forms of crossover, two_point, blend, and uniform, which generate a new individual through combinations of two parent individuals. Two-point crossover divides each parent into three regions, where offspring are created from the combination of the middle region from one parent and the end regions from the other parent. Since the SCOLIB EA does not utilize bit representations of variable values, the crossover points only occur on coordinate boundaries, never within the bits of a particular coordinate. Uniform crossover creates offspring through random combination of coordinates from the two parents. Blend crossover generates a new individual randomly along the multidimensional vector connecting the two parents.

crossover_type

- Keywords Area
- method
- coliny_ea
- crossover_type

Select a crossover type

<table>
<thead>
<tr>
<th>Required-/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword</th>
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<tr>
<td>Required (Choose One)</td>
<td>Group 1</td>
<td>two_point</td>
<td>Description</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Combine middle of one parent with end of another</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Random blend of parents</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Randomly combine coordinates from parents</td>
</tr>
</tbody>
</table>

Description

The crossover_type controls what approach is employed for combining parent genetic information to create offspring. The SCOLIB EA method supports three forms of crossover, two_point, blend, and uniform, which generate a new individual through combinations of two parent individuals.
6.2. METHOD

two_point

- Keywords Area
- method
- coliny_ea
- crossover_type
- two_point

Combine middle of one parent with end of another

**Specification**

**Alias:** None

**Argument(s):** None

**Description**

Two-point crossover divides each parent into three regions, where offspring are created from the combination of the middle region from one parent and the end regions from the other parent. Since the SCOLIB EA does not utilize bit representations of variable values, the crossover points only occur on coordinate boundaries, never within the bits of a particular coordinate.

blend

- Keywords Area
- method
- coliny_ea
- crossover_type
- blend

Random blend of parents

**Specification**

**Alias:** None

**Argument(s):** None

**Description**

blend crossover generates a new individual randomly along the multidimensional vector connecting the two parents.
uniform
- Keywords Area
- method
- coliny_ea
- crossover_type
- uniform
  Randomly combine coordinates from parents

**Specification**

*Alias:* none

*Argument(s):* none

**Description**

Uniform crossover creates offspring through random combination of coordinates from the two parents.

**mutation_rate**

- Keywords Area
- method
- coliny_ea
- mutation_rate
  Set probability of a mutation

**Specification**

*Alias:* none

*Argument(s):* REAL

*Default:* 1.0

**Description**

The `mutation_rate` controls the probability of mutation being performed on an individual, both for new individuals generated by crossover (if crossover occurs) and for individuals from the existing population. It is the fraction of trial points that are mutated in a given iteration and therefore must be specified to be between 0 and 1.

**mutation_type**

- Keywords Area
- method
- coliny_ea
- mutation_type
  Select a mutation type
6.2. **METHOD**

### Specification

**Alias:** none  
**Argument(s):** none  
**Default:** offset_normal

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
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<tr>
<td><strong>Required</strong> <em>(Choose One)</em></td>
<td>Group 1</td>
<td>replace_uniform</td>
<td>Replace coordinate with randomly generated value</td>
</tr>
<tr>
<td>offset_normal</td>
<td></td>
<td></td>
<td>Set mutation offset to use a normal distribution</td>
</tr>
<tr>
<td>offset_cauchy</td>
<td></td>
<td></td>
<td>Use a Cauchy distribution for the mutation offset</td>
</tr>
<tr>
<td>offset_uniform</td>
<td></td>
<td></td>
<td>Set mutation offset to use a uniform distribution</td>
</tr>
<tr>
<td><strong>Optional</strong></td>
<td></td>
<td>non_adaptive</td>
<td>Disable self-adaptive mutation</td>
</tr>
</tbody>
</table>

### Description

The `mutation_type` controls what approach is employed in randomly modifying continuous design variables within the EA population. Each of the mutation methods generates coordinate-wise changes to individuals, usually by adding a random variable to a given coordinate value (an `offset_*` mutation), but also by replacing a given coordinate value with a random variable (a `replace_*` mutation).

Discrete design variables are always mutated using the `offset_uniform` method.

**replace_uniform**

- **Keywords Area**
- **method**
- **coliny_ea**
- **mutation_type**
- **replace_uniform**

Replace coordinate with randomly generated value

### Specification

**Alias:** none  
**Argument(s):** none
CHAPTER 6. KEYWORDS AREA

Description
The \texttt{replace.uniform} mutation type generates a replacement value for a coordinate using a uniformly distributed value over the total range for that coordinate.

\texttt{offset.normal}

- Keywords Area
- method
- coliny.ea
- mutation.type
- offset.normal

Set mutation offset to use a normal distribution

Specification
Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of</th>
<th>Dakota Keyword</th>
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<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>\texttt{mutation.scale}</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>\texttt{mutation.range}</td>
<td></td>
</tr>
</tbody>
</table>

Description
The \texttt{offset.normal} type is an “offset” mutation that adds a 0-mean random variable with a normal uniform distribution to the existing coordinate value. The offset is limited in magnitude by \texttt{mutation.scale}.

\texttt{mutation.scale}

- Keywords Area
- method
- coliny.ea
- mutation.type
- offset.normal
- \texttt{mutation.scale}

Scales mutation across range of parameter
6.2. METHOD

Specification

Alias: none
  Argument(s): REAL
  Default: 0.1

Description

The mutation_scale specifies a scale factor which scales continuous mutation offsets; this is a fraction of the total range of each dimension, so mutation_scale is a relative value between 0 and 1.

mutation_range
  • Keywords Area
  • method
  • coliny_ea
  • mutation_type
  • offset_normal
  • mutation_range

Set uniform offset control for discrete parameters

Specification

Alias: none
  Argument(s): INTEGER
  Default: 1

Description

The mutation_range is used to control offset_uniform mutation used for discrete parameters. The replacement discrete value is the original value plus or minus an integer value up to mutation_range.

offset_cauchy
  • Keywords Area
  • method
  • coliny_ea
  • mutation_type
  • offset_cauchy

Use a Cauchy distribution for the mutation offset

Specification

Alias: none
  Argument(s): none
CHAPTER 6. KEYWORDS AREA

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<thead>
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<th>Required/Optional</th>
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<tr>
<td>Optional</td>
<td></td>
<td>mutation_scale</td>
<td>Scales mutation across range of parameter</td>
</tr>
<tr>
<td></td>
<td></td>
<td>mutation_range</td>
<td>Set uniform offset control for discrete parameters</td>
</tr>
</tbody>
</table>

**Description**

The `offset_cauchy` type is an "offset" mutation that adds a 0-mean random variable with a cauchy distribution to the existing coordinate value. The offset is limited in magnitude by `mutation_scale`.

```
mutation_scale
  • Keywords Area
  • method
  • coliny_ea
  • mutation_type
  • offset_cauchy
  • mutation_scale
```

Scales mutation across range of parameter

**Specification**

**Alias:** none

**Argument(s):** REAL

**Default:** 0.1

**Description**

The `mutation_scale` specifies a scale factor which scales continuous mutation offsets; this is a fraction of the total range of each dimension, so `mutation_scale` is a relative value between 0 and 1.

```
mutation_range
  • Keywords Area
  • method
  • coliny_ea
  • mutation_type
  • offset_cauchy
  • mutation_range
```

Set uniform offset control for discrete parameters
6.2. METHOD

Specification

Alias: none
  Argument(s): INTEGER
  Default: 1

Description

The `mutation_range` is used to control `offset_uniform` mutation used for discrete parameters. The replacement discrete value is the original value plus or minus an integer value up to `mutation_range`.

(offset_uniform)

- Keywords Area
- method
- coliny_ea
- mutation_type
- offset_uniform

Set mutation offset to use a uniform distribution

Specification

Alias: none
  Argument(s): none

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword</th>
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<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>mutation_scale</td>
<td>mutation_range</td>
</tr>
</tbody>
</table>

Description

The `offset_uniform` type is an "offset" mutation that adds a 0-mean random variable with a uniform distribution to the existing coordinate value. The offset is limited in magnitude by `mutation_scale`.

For discrete design variables, `offset_uniform` is always used, and `mutation_range` controls the magnitude of the mutation.

`mutation_scale`

- Keywords Area
- method
- coliny_ea
- mutation_type
• offset_uniform
• mutation_scale

Scales mutation across range of parameter

Specification

Alias: none

Argument(s): REAL
Default: 0.1

Description

The mutation_scale specifies a scale factor which scales continuous mutation offsets; this is a fraction of the total range of each dimension, so mutation_scale is a relative value between 0 and 1.

mutation_range
• Keywords Area
• method
• coliny_ea
• mutation_type
• offset_uniform
• mutation_range

Set uniform offset control for discrete parameters

Specification

Alias: none

Argument(s): INTEGER
Default: 1

Description

The mutation_range is used to control offset_uniform mutation used for discrete parameters. The replacement discrete value is the original value plus or minus an integer value up to mutation_range.

non_adaptive
• Keywords Area
• method
• coliny_ea
• mutation_type
• non_adaptive

Disable self-adaptive mutation
6.2. **METHOD**

**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** Adaptive mutation

**Description**

The SCOLIB EA method uses self-adaptive mutation, which modifies the mutation scale dynamically. This mechanism is borrowed from EAs like evolution strategies. The `nonadaptive` flag can be used to deactivate the self-adaptation, which may facilitate a more global search.

Note that `nonadaptive` is not recognized by Dakota as a valid keyword unless `mutation_type` has been specified.

**constraint_penalty**

- **Keywords Area**
- method
- coliny_ea
- `constraint_penalty`

Multiplier for the penalty function

**Specification**

**Alias:** none  
**Argument(s):** REAL

**Description**

Most SCOLIB optimizers treat constraints with a simple penalty scheme that adds `constraint_penalty` times the sum of squares of the constraint violations to the objective function. The default value of `constraint_penalty` is 1000.0, except for methods that dynamically adapt their constraint penalty, for which the default value is 1.0.

**solution_target**

- **Keywords Area**
- method
- coliny_ea
- `solution_target`

Stopping criteria based on objective function value
CHAPTER 6. KEYWORDS AREA

Specification

Alias: solution_accuracy
  Argument(s): REAL
  Default: -DBL_MAX

Description

solution_target is a termination criterion. The algorithm will terminate when the function value falls below solution_target.

Seed of the random number generator

Specification

Alias: none
  Argument(s): INTEGER
  Default: system-generated (non-repeatable)

Description

The random seed control provides a mechanism for making a stochastic method repeatable. That is, the use of the same random seed in identical studies will generate identical results.

Default Behavior
  If not specified, the seed is randomly generated.

Expected Output
  If seed is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

Usage Tips
  If a stochastic study was run without seed specified, and the user later wishes to repeat the study using the same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen. That value can then be added to the Dakota input file.

Examples

method
  sampling
    sample_type lhs
    samples = 10
    seed = 15347
6.2. *METHOD*

**show_misc_options**

- **Keywords Area**
- **method**
- **coliny_ea**
- **show_misc_options**

Show algorithm parameters not exposed in Dakota input

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no dump of specification options

**Description**

All SCOLIB methods support the `show_misc_options` optional specification which results in a dump of all the allowable method inputs. Note that the information provided by this command refers to optimizer parameters that are internal to SCOLIB, and which may differ from corresponding parameters used by the Dakota interface. The `misc_options` optional specification provides a means for inputing additional settings supported by the SCOLIB methods but which are not currently mapped through the Dakota input specification. Care must be taken in using this specification; they should only be employed by users familiar with the full range of parameter specifications available directly from SCOLIB and understand any differences that exist between those specifications and the ones available through Dakota.

**misc_options**

- **Keywords Area**
- **method**
- **coliny_ea**
- **misc_options**

Set method options not available through Dakota spec

**Specification**

**Alias:** none

**Argument(s):** STRINGLIST

**Default:** no misc options
Description

All SCOLIB methods support the `show_misc_options` optional specification which results in a dump of all the allowable method inputs. Note that the information provided by this command refers to optimizer parameters that are internal to SCOLIB, and which may differ from corresponding parameters used by the Dakota interface. The `misc_options` optional specification provides a means for inputting additional settings supported by the SCOLIB methods but which are not currently mapped through the Dakota input specification. Care must be taken in using this specification; they should only be employed by users familiar with the full range of parameter specifications available directly from SCOLIB and understand any differences that exist between those specifications and the ones available through Dakota.

`max_iterations`

- Keywords Area
- method
- coliny_ea
- `max_iterations`

Number of iterations allowed for optimizers and adaptive UQ methods

Topics

This keyword is related to the topics:

- `method_independent_controls`

Specification

Alias: none

Argument(s): INTEGER

Default: 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence} / efficient-global: 25*n)

Description

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed `max_iterations` iterations. See also `max_function_evaluations`.

Default Behavior

Default value is 100.

`convergence_tolerance`

- Keywords Area
- method
- coliny_ea
- `convergence_tolerance`

Stopping criterion based on convergence of the objective function or statistics
6.2. METHOD

Topics
This keyword is related to the topics:

- method
- independent
- controls

Specification
Alias: none
Argument(s): REAL
Default: 1.e-4

Description
The convergence_tolerance specification provides a real value for controlling the termination of iteration. For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by convergence_tolerance, then this convergence criterion is satisfied on the current iteration. Therefore, permissible values are between 0 and 1, non-inclusive.

Behavior Varies by Package/Library
This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.
Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.
Notes on each library:

- DOT: must be satisfied for two consecutive iterations
- NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of convergence_tolerance approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., convergence_tolerance = 1.e-6 will result in approximately six digits of accuracy in the final objective function).
- NL2SOL: See nl2sol

max_function_evaluations

- Keywords Area
- method
- coliny_ea
- max_function_evaluations

Number of function evaluations allowed for optimizers
CHAPTER 6. KEYWORDS AREA

Topics
This keyword is related to the topics:

- `method_independent_controls`

Specification
Alias: none
Argument(s): INTEGER
Default: 1000

Description
The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed `max_function_evaluations` evaluations. See also `max_iterations`.

Default Behavior
Default value is 1000.

type

- `Keywords Area`
- `method`
- `coliny_ea`
- `scaling`

Turn on scaling for variables, responses, and constraints

Topics
This keyword is related to the topics:

- `method_independent_controls`

Specification
Alias: none
Argument(s): none
Default: no scaling

Description
Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by by providing the `scaling` keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.
6.2. METHOD

Scaling also requires the specification of additional keywords which are found in the method, variables, and responses blocks. When the scaling keyword is omitted, all _scale_types and *_scales specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.

- a *scales keyword, which gives characteristic values
- a *scale_type keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

**Scale Types**

There are four scale types:

1. none (default) - no scaling, value of *scales keyword is ignored
2. value - multiplicative scaling
3. auto - automatic scaling
   First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:
   - two-sided bounds scaled into the interval [0,1];
   - one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
   - no bounds or targets: no automatic scaling possible, therefore no scaling for this component

   Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into [0,1].
4. log - logarithmic scaling
   First, any characteristic values from the optional *scales specification are applied. Then logarithm base 10 scaling is applied.
   Logarithmic scaling is not available for linear constraints.
   When continuous design variables are log scaled, linear constraints are not allowed.

**Scales**

The *scales keywords are used to specify the characteristic values. These must be non-zero real numbers. The numbers are used according to the corresponding *scale_type, as described above.

Depending on the scale type, the characteristic values may be required or optional.

- none, auto, log - optional
- value - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than 1.0e10*DBL_MIN. User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.
Examples
The two examples below are equivalent:

```plaintext
responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value"
  primary_scales = 1 1 100

responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value" "value" "value"
  primary_scales = 1 1 100
```

**model_pointer**

- *Keywords Area*
- *method*
- *coliny_ea*
- *model_pointer*

Identifier for model block to be used by a method

Topics
This keyword is related to the topics:

- *block_pointer*

Specification
Alias: none

- **Argument(s):** STRING
- **Default:** method use of last model parsed (or use of default model if none parsed)

Description
The *model_pointer* is used to specify which *model* block will be used to perform the function evaluations needed by the Dakota method.

**Default Behavior**
If not specified, a Dakota method will use the last model block parsed. If specified, there must be a *model* block in the Dakota input file that has a corresponding *id_model* with the same name.

**Usage Tips**
When doing advanced analyses that involve using multiple methods and multiple models, defining a *model_pointer* for each method is imperative.

See *block_pointer* for details about pointers.
6.2. METHOD

Examples

environment
tabular_graphics_data
method_pointer = 'UQ'

method
id_method = 'UQ'
model_pointer = 'SURR'
sampling,
samples = 10
seed = 98765 rng rnum2
response_levels = 0.1 0.2 0.6
0.1 0.2 0.6
0.1 0.2 0.6
sample_type lhs
distribution cumulative

model
id_model = 'SURR'
surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
id_method = 'DACE'
model_pointer = 'DACE_M'
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = 'DACE_M'
single
interface_pointer = 'I1'

variables
uniform_uncertain = 2
lower_bounds = 0. 0.
upper_bounds = 1. 1.
descriptors = 'x1' 'x2'

interface
id_interface = 'I1'
system asynch evaluation_concurrency = 5
analysis_driver = 'text_book'

responses
response_functions = 3
no_gradients
no_hessians

6.2.41 coliny_beta

- Keywords Area
- method
- coliny_beta

(Experimental) Coliny beta solver
### Topics

This keyword is related to the topics:

- `package_scolib`
- `package_coliny`

### Specification

**Alias:** none  
**Argument(s):** none

<table>
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<tr>
<th>Required/-</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>beta_solver_name</td>
<td></td>
<td>Use an in-development SCOLIB solver</td>
</tr>
<tr>
<td>Optional</td>
<td>solution_target</td>
<td></td>
<td>Stopping criteria based on objective function value</td>
</tr>
<tr>
<td>Optional</td>
<td>seed</td>
<td></td>
<td>Seed of the random number generator</td>
</tr>
<tr>
<td>Optional</td>
<td>show_misc_options</td>
<td></td>
<td>Show algorithm parameters not exposed in Dakota input</td>
</tr>
<tr>
<td>Optional</td>
<td>misc_options</td>
<td></td>
<td>Set method options not available through Dakota spec</td>
</tr>
<tr>
<td>Optional</td>
<td>max_iterations</td>
<td></td>
<td>Number of iterations allowed for optimizers and adaptive UQ methods</td>
</tr>
<tr>
<td>Optional</td>
<td>convergence_-tolerance</td>
<td></td>
<td>Stopping criterion based on convergence of the objective function or statistics</td>
</tr>
</tbody>
</table>
6.2. METHOD

<table>
<thead>
<tr>
<th>Optional</th>
<th>max_function_evaluations</th>
<th>Optional scaling</th>
<th>Optional model_pointer</th>
</tr>
</thead>
</table>

**Description**

This method keyword allows testing of experimental (beta) Coliny (Scolib) optimization solvers during software development. It is intended primarily for developer use. Additional information on Coliny solvers is available at package_scolib.

**See Also**

These keywords may also be of interest:

- `coliny_direct`
- `coliny_pattern_search`
- `coliny_cobyla`
- `coliny_ea`
- `coliny_solis_wets`

**beta_solver_name**

- Keywords Area
- method
- `coliny_beta`
- `beta_solver_name`

Use an in-development SCOLIB solver

**Specification**

Alias: none

Argument(s): STRING
**Description**

This is a means of accessing new methods in SCOLIB before they are exposed through the Dakota interface. Seek help from a Dakota or SCOLIB developer or a Dakota developer.

**solution_target**

- **Keywords Area**
- **method**
- **coliny_beta**
- **solution_target**

Stopping criteria based on objective function value

**Specification**

Alias: solution_accuracy

- **Argument(s)**: REAL
- **Default**: -DBL_MAX

**Description**

*solution_target* is a termination criterion. The algorithm will terminate when the function value falls below *solution_target*.

**seed**

- **Keywords Area**
- **method**
- **coliny_beta**
- **seed**

Seed of the random number generator

**Specification**

Alias: none

- **Argument(s)**: INTEGER
- **Default**: system-generated (non-repeatable)
6.2. METHOD

Description

The random seed control provides a mechanism for making a stochastic method repeatable. That is, the use of the same random seed in identical studies will generate identical results.

**Default Behavior**

If not specified, the seed is randomly generated.

**Expected Output**

If seed is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

**Usage Tips**

If a stochastic study was run without seed specified, and the user later wishes to repeat the study using the same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen. That value can then be added to the Dakota input file.

Examples

```dakota
method
  sampling
    sample_type lhs
    samples = 10
    seed = 15347
```

**show_misc_options**

- Keywords Area
- method
- coliny_beta
- show_misc_options

Show algorithm parameters not exposed in Dakota input

Specification

**Alias:** none

**Argument(s):** none

**Default:** no dump of specification options

Description

All SCOLIB methods support the `show_misc_options` optional specification which results in a dump of all the allowable method inputs. Note that the information provided by this command refers to optimizer parameters that are internal to SCOLIB, and which may differ from corresponding parameters used by the Dakota interface. The `misc_options` optional specification provides a means for inputting additional settings supported by the SCOLIB methods but which are not currently mapped through the Dakota input specification. Care must be taken in using this specification; they should only be employed by users familiar with the full range of parameter specifications available directly from SCOLIB and understand any differences that exist between those specifications and the ones available through Dakota.
CHAPTER 6. KEYWORDS AREA

misc_options

- Keywords Area
- method
- coliny_beta
- misc_options

Set method options not available through Dakota spec

Specification

Alias: none
Argument(s): STRINGLIST
Default: no misc options

Description

All SCOLIB methods support the show_misc_options optional specification which results in a dump of all the allowable method inputs. Note that the information provided by this command refers to optimizer parameters that are internal to SCOLIB, and which may differ from corresponding parameters used by the Dakota interface. The misc_options optional specification provides a means for inputing additional settings supported by the SCOLIB methods but which are not currently mapped through the Dakota input specification. Care must be taken in using this specification; they should only be employed by users familiar with the full range of parameter specifications available directly from SCOLIB and understand any differences that exist between those specifications and the ones available through Dakota.

max_iterations

- Keywords Area
- method
- coliny_beta
- max_iterations

Number of iterations allowed for optimizers and adaptive UQ methods

Topics

This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none
Argument(s): INTEGER
Default: 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence} / efficient_global: 25*n)
6.2. METHOD

Description

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed $\text{max}_{-}\text{iterations}$. See also $\text{max}\_\text{function}\_\text{evaluations}$.

**Default Behavior**

Default value is 100.

**convergence_tolerance**

- **Keywords Area**
- **method**
- **coliny_beta**
- **convergence_tolerance**

Stopping criterion based on convergence of the objective function or statistics

**Topics**

This keyword is related to the topics:

- **method\_independent\_controls**

**Specification**

*Alias:* none

*Argument(s):* REAL

*Default:* 1.e-4

**Description**

The `convergence_tolerance` specification provides a real value for controlling the termination of iteration.

For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by convergence_tolerance, then this convergence criterion is satisfied on the current iteration.

Therefore, permissible values are between 0 and 1, non-inclusive.

**Behavior Varies by Package/Library**

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- **DOT:** must be satisfied for two consecutive iterations
• NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of convergence_tolerance approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., convergence_tolerance = 1.e-6 will result in approximately six digits of accuracy in the final objective function).

• NL2SOL: See nl2sol

max_function_evaluations

- Keywords Area
- method
- coliny_beta
- max_function_evaluations

Number of function evaluations allowed for optimizers

Topics

This keyword is related to the topics:

- method.independent.controls

Specification

Alias: none
Argument(s): INTEGER
Default: 1000

Description

The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed max_function_evaluations evaluations. See also max_iterations.

Default Behavior
Default value is 1000.

calculation

- Keywords Area
- method
- coliny_beta
- scaling

Turn on scaling for variables, responses, and constraints
6.2. **METHOD**

**Topics**
This keyword is related to the topics:

- `method.independent.controls`

**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** no scaling

**Description**

Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by by providing the `scaling` keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the `method`, `variables`, and `responses` blocks. When the `scaling` keyword is omitted, all `scale_type` and `*_scales` specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.

- a `*_scales` keyword, which gives characteristic values
- a `*_scale_type` keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

**Scale Types**

There are four scale types:

1. **none** (default) - no scaling, value of `*_scales` keyword is ignored
2. **value** - multiplicative scaling
3. **auto** - automatic scaling

First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:

- two-sided bounds scaled into the interval [0,1];
- one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
- no bounds or targets: no automatic scaling possible, therefore no scaling for this component

Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into [0,1].
4. **log** - logarithmic scaling

First, any characteristic values from the optional `*_scales` specification are applied. Then logarithm base 10 scaling is applied.

Logarithmic scaling is not available for linear constraints.

When continuous design variables are log scaled, linear constraints are not allowed.

**Scales**

The `*_scales` keywords are used to specify the characteristic values. These must be non-zero real numbers. The numbers are used according to the corresponding `*_scale_type`, as described above.

Depending on the scale type, the characteristic values may be required or optional.

- `none`, `auto`, `log` - optional
- `value` - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than `1.0e10*DBL_MIN`. User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.

**Examples**

The two examples below are equivalent:

```plaintext
responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value"
  primary_scales = 1 1 100

responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value" "value" "value"
  primary_scales = 1 1 100
```

**model_pointer**

- Keywords Area
- method
- coliny_beta
- model_pointer

Identifier for model block to be used by a method

**Topics**

This keyword is related to the topics:

- block_pointer
6.2. METHOD

Specification

Alias: none

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)

Description

The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.

Usage Tips

When doing advanced analyses that involve using multiple methods and multiple models, defining a model_pointer for each method is imperative.

See block_pointer for details about pointers.

Examples

environment
    tabular_graphics_data
    method_pointer = 'UQ'

method
    id_method = 'UQ'
    model_pointer = 'SURR'
    sampling,
        samples = 10
        seed = 98765 rng rnum2
        response_levels = 0.1 0.2 0.6
        0.1 0.2 0.6
        0.1 0.2 0.6
    sample_type lhs
    distribution cumulative

model
    id_model = 'SURR'
    surrogate global,
    dace_method_pointer = 'DACE'
    polynomial quadratic

method
    id_method = 'DACE'
    model_pointer = 'DACE_M'
    sampling sample_type lhs
        samples = 121 seed = 5034 rng rnum2

model
    id_model = 'DACE_M'
    single
    interface_pointer = 'I1'

variables
    uniform_uncertain = 2
    lower_bounds = 0. 0.
    upper_bounds = 1. 1.
    descriptors = 'x1' 'x2'
interface
    id_interface = 'I1'
    system asynch evaluation_concurrency = 5
    analysis_driver = 'text_book'

responses
    response_functions = 3
    no_gradients
    no_hessians

6.2.42 nl2sol

- Keywords Area
- method
- nl2sol

Trust-region method for nonlinear least squares

Topics
This keyword is related to the topics:

- nonlinear_least_squares

Specification
Alias: none
Argument(s): none

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<td>Optional</td>
<td>singular_conv_tol</td>
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<td>Singular convergence tolerance</td>
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### Optional

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<td>Turn on scaling for variables, responses, and constraints</td>
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<td>model_pointer</td>
<td>Identifier for model block to be used by a method</td>
</tr>
</tbody>
</table>

### Description

NL2SOL is available as `nl2sol` and addresses unconstrained and bound-constrained least squares problems. It uses a trust-region method (and thus can be viewed as a generalization of the Levenberg-Marquardt algorithm) and adaptively chooses between two Hessian approximations, the Gauss-Newton approximation alone and the Gauss-Newton approximation plus a quasi-Newton approximation to the rest of the Hessian. Even on small-residual problems, the latter Hessian approximation can be useful when the starting guess is far from the solution. On problems that are not over-parameterized (i.e., that do not involve more optimization variables than the data support), NL2SOL usually exhibits fast convergence.

Several internal NL2SOL convergence tolerances are adjusted in response to `function_precision`, which
gives the relative precision to which responses are computed. These tolerances may also be specified explicitly using:

- `convergence_tolerance` (NL2SOL’s `rfctol`)
- `x_conv_tol` (NL2SOL’s `xctol`)
- `absolute_conv_tol` (NL2SOL’s `afctol`)
- `singular_conv_tol` (NL2SOL’s `sctol`)
- `false_conv_tol` (NL2SOL’s `xftol`)
- `initial_trust_radius` (NL2SOL’s `lmax0`)

The internal NL2SOL defaults can be obtained for many of these controls by specifying the value `-1`. The internal defaults are often functions of machine epsilon (as limited by `function_precision`).

**Examples**

An example of `nl2sol` is given below, and is discussed in the User’s Manual.

Note that in this usage of `calibration_terms`, the driver script `rosenbrock`, is returning “residuals”, which the `nl2sol` method is attempting to minimize. Another use case is to provide a data file, which Dakota will attempt to match the model responses to. See `calibration_data_file`. Finally, as of Dakota 6.2, the field data capability may be used with `nl2sol`. That is, the user can specify field simulation data and field experiment data, and Dakota will interpolate and provide the proper residuals for the calibration.

```plaintext
# Dakota Input File: rosen_opt_nls.in
environment
tabular_data
  tabular_data_file = 'rosen_opt_nls.dat'
method
  max_iterations = 100
  convergence_tolerance = 1e-4
  nl2sol
model
  single
variables
  continuous_design = 2
  initial_point -1.2 1.0
  lower_bounds -2.0 -2.0
  upper_bounds 2.0 2.0
descriptors 'x1' "x2"
interface
  analysis_driver = 'rosenbrock'
direct
responses
  calibration_terms = 2
  analytic_gradients
  no_hessians
```
The NL2SOL has a variety of internal controls as described in AT&T Bell Labs CS TR 153 (http://cm.bell-labs.com/cm/cs/cstr/153.ps.gz). A number of existing Dakota controls (method independent controls and responses controls) are mapped into these NL2SOL internal controls. In particular, Dakota's convergence-tolerance, max.iterations, max.function_evaluations, and fd.gradient_step.size are mapped directly into NL2SOL's rfctol, mxiter, mxfcal, and dltfdj controls, respectively. In addition, Dakota's fd.hessian_step.size is mapped into both delta0 and dltfdc, and Dakota's output verbosity is mapped into NL2SOL's auxprt and outlev (for normal/verbose/debug output, NL2SOL prints initial guess, final solution, solution statistics, nondefault values, and changes to the active bound constraint set on every iteration; for quiet output, NL2SOL prints only the initial guess and final solution; and for silent output, NL2SOL output is suppressed).

**See Also**

These keywords may also be of interest:

- **nlssol_sqp**
- **optpp_g_newton**
- **field_calibration_terms**

**function_precision**

- **Keywords Area**
- **method**
- **nl2sol**
- **function_precision**

Specify the maximum precision of the analysis code responses

**Specification**

**Alias:** none

**Argument(s):** REAL

**Default:** 1.0e-10

**Description**

The function_precision control provides the algorithm with an estimate of the accuracy to which the problem functions can be computed. This is used to prevent the algorithm from trying to distinguish between function values that differ by less than the inherent error in the calculation.
absolute_conv_tol

- Keywords Area
- method
- nl2sol
- absolute_conv_tol

Absolute convergence tolerance

**Specification**

Alias: none
- **Argument(s):** REAL
- **Default:** -1. (use NL2SOL internal default)

**Description**

`absolute_conv_tol` (NL2SOL's `afctol`) is the absolute function convergence tolerance (stop when half the sum of squares is less than `absolute_conv_tol`, which is mainly of interest on zero-residual test problems). The internal default is a function of machine epsilon (as limited by `function_precision`). The default is selected with a value of -1.

x_conv_tol

- Keywords Area
- method
- nl2sol
- x_conv_tol

X-convergence tolerance

**Specification**

Alias: none
- **Argument(s):** REAL
- **Default:** -1. (use NL2SOL internal default)

**Description**

`x_conv_tol` maps to the internal NL2SOL control `xctol`. It is the X-convergence tolerance (scaled relative accuracy of the solution variables).

The internal default is a function of machine epsilon (as limited by `function_precision`). The default is selected with a value of -1.
6.2. **METHOD**

**singular_conv_tol**

- **Keywords Area**
- **method**
- **nl2sol**
- **singular_conv_tol**

Singular convergence tolerance

**Specification**

**Alias:** none

**Argument(s):** REAL

**Default:** -1. (use NL2SOL internal default)

**Description**

`singular_conv_tol` (NL2SOL’s `sctol`) is the singular convergence tolerance, which works in conjunction with `singular_radius` to test for underdetermined least-squares problems (stop when the relative reduction yet possible in the sum of squares appears less than `singular_conv_tol` for steps of scaled length at most `singular_radius`).

The internal default is a function of machine epsilon (as limited by `function_precision`). The default is selected with a value of -1.

**singular_radius**

- **Keywords Area**
- **method**
- **nl2sol**
- **singular_radius**

Singular radius

**Specification**

**Alias:** none

**Argument(s):** REAL

**Default:** -1. (use NL2SOL internal default of 1)

**Description**

`singular_radius` works in conjunction with `singular_conv_tol` to test for underdetermined least-squares problems (stop when the relative reduction yet possible in the sum of squares appears less than `singular_conv_tol` for steps of scaled length at most `singular_radius`).

The internal default results in the internal use of steps of length 1. The default is selected with a value of -1.
false_conv_tol

- Keywords Area
- method
- nl2sol
- false_conv_tol

False convergence tolerance

**Specification**

**Alias:** none

**Argument(s):** REAL  
**Default:** -1. (use NL2SOL internal default)

**Description**

false_conv_tol (NL2SOL's xftol) is the false-convergence tolerance (stop with a suspicion of discontinuity when a more favorable stopping test is not satisfied and a step of scaled length at most false_conv_tol is not accepted).

The internal default is a function of machine epsilon (as limited by function_precision). The default is selected with a value of -1.

initial_trust_radius

- Keywords Area
- method
- nl2sol
- initial_trust_radius

Initial trust region radius

**Specification**

**Alias:** none

**Argument(s):** REAL  
**Default:** -1. (use NL2SOL internal default of 1)

**Description**

initial_trust_radius specification (NL2SOL's lmax0) specifies the initial trust region radius for the algorithm.

The internal default results in the internal use of steps of length 1. The default is selected with a value of -1.
6.2. METHOD

covariance

- Keywords Area
- method
- nl2sol
- covariance

Determine how the final covariance matrix is computed

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** 0 (no covariance)

**Description**

covariance (NL2SOL's `covreq`) specifies whether and how NL2SOL computes a final covariance matrix. The desired covariance approximation:

- 0 = default = none
- 1 or -1 ==> \( \sigma^2 H^{-1} J^T J H^{-1} \)
- 2 or -2 ==> \( \sigma^2 H^{-1} \)
- 3 or -3 ==> \( \sigma^2 (J^T J)^{-1} \)
- Negative values ==> estimate the final Hessian H by finite differences of function values only (using `fd_hessian_step_size`)
- Positive values ==> differences of gradients (using `fd_hessian_step_size`)

regression_diagnostics

- Keywords Area
- method
- nl2sol
- regression_diagnostics

Turn on regression diagnostics

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no regression diagnostics
CHAPTER 6. KEYWORDS AREA

Description

When regression_diagnostics (NL2SOL’s rdreq) is specified and a positive-definite final Hessian approximation H is computed, NL2SOL computes and prints a regression diagnostic vector RD such that if omitting the i-th observation would cause alpha times the change in the solution that omitting the j-th observation would cause, then $RD[i] = |\alpha| RD[j]$. The finite-difference step-size tolerance affecting H is fd_step_size (NL2SOL’s delta0 and dltfdc).

convergence_tolerance

- Keywords Area
- method
- nl2sol
- convergence_tolerance

Stopping criterion based on convergence of the objective function or statistics

Topics

This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none

Argument(s): REAL

Default: 1.e-4

Description

The convergence_tolerance specification provides a real value for controlling the termination of iteration. For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by convergence_tolerance, then this convergence criterion is satisfied on the current iteration.

Therefore, permissible values are between 0 and 1, non-inclusive.

Behavior Varies by Package/Library

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- DOT: must be satisfied for two consecutive iterations
6.2. METHOD

- NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of `convergence_tolerance` approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., `convergence_tolerance = 1.e-6` will result in approximately six digits of accuracy in the final objective function).

- NL2SOL: See nl2sol

**max_iterations**

- Keywords Area
- method
- nl2sol
- max_iterations

Number of iterations allowed for optimizers and adaptive UQ methods

**Topics**

This keyword is related to the topics:

- `method_independent_controls`

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** 100 (exceptions: fsu_cv , local_reliability: 25; global_{reliability , interval_est , evidence} / efficient-global: 25∗n)

**Description**

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed `max_iterations` iterations. See also `max_function_evaluations`.

**Default Behavior**

Default value is 100.

**speculative**

- Keywords Area
- method
- nl2sol
- speculative

Compute speculative gradients
CHAPTER 6. KEYWORDS AREA

Topics
This keyword is related to the topics:

- method
  - independent

Specification
Alias: none
Argument(s): none
Default: no speculation

Description
When performing gradient-based optimization in parallel, speculative gradients can be selected to address the load imbalance that can occur between gradient evaluation and line search phases. In a typical gradient-based optimization, the line search phase consists primarily of evaluating the objective function and any constraints at a trial point, and then testing the trial point for a sufficient decrease in the objective function value and/or constraint violation. If a sufficient decrease is not observed, then one or more additional trial points may be attempted sequentially. However, if the trial point is accepted then the line search phase is complete and the gradient evaluation phase begins. By speculating that the gradient information associated with a given line search trial point will be used later, additional coarse grained parallelism can be introduced by computing the gradient information (either by finite difference or analytically) in parallel, at the same time as the line search phase trial-point function values. This balances the total amount of computation to be performed at each design point and allows for efficient utilization of multiple processors. While the total amount of work performed will generally increase (since some speculative gradients will not be used when a trial point is rejected in the line search phase), the run time will usually decrease (since gradient evaluations needed at the start of each new optimization cycle were already performed in parallel during the line search phase). Refer to [14] for additional details. The speculative specification is implemented for the gradient-based optimizers in the DOT, CONMIN, and OPT++ libraries, and it can be used with dakota numerical or analytic gradient selections in the responses specification (refer to responses gradient section for information on these specifications). It should not be selected with vendor numerical gradients since vendor internal finite difference algorithms have not been modified for this purpose. In full-Newton approaches, the Hessian is also computed speculatively. NPSOL and NLSSOL do not support speculative gradients, as their gradient-based line search in user-supplied gradient mode (dakota numerical or analytic gradients) is a superior approach for load-balanced parallel execution.

The speculative specification enables speculative computation of gradient and/or Hessian information, where applicable, for parallel optimization studies. By speculating that the derivative information at the current point will be used later, the complete data set (all available gradient/Hessian information) can be computed on every function evaluation. While some of these computations will be wasted, the positive effects are a consistent parallel load balance and usually shorter wall clock time. The speculative specification is applicable only when parallelism in the gradient calculations can be exploited by Dakota (it will be ignored for vendor numerical gradients).

max_function_evaluations

- Keywords Area
- method
- nl2sol
- max_function_evaluations
6.2. METHOD

Number of function evaluations allowed for optimizers

Topics
This keyword is related to the topics:

- method\_independent\_controls

Specification

Alias: none
Argument(s): INTEGER
Default: 1000

Description
The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed \texttt{max\_function\_evaluations} evaluations. See also \texttt{max\_iterations}.

Default Behavior
Default value is 1000.

scaling

- Keywords Area
- method
- nl2sol
- scaling

Turn on scaling for variables, responses, and constraints

Topics
This keyword is related to the topics:

- method\_independent\_controls

Specification

Alias: none
Argument(s): none
Default: no scaling
**Description**

Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by providing the `scaling` keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the method, variables, and responses blocks. When the `scaling` keyword is omitted, all `_scale_types` and `*_scales` specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.

- a `*_scales` keyword, which gives characteristic values
- a `*_scale_type` keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

**Scale Types**

There are four scale types:

1. **none** (default) - no scaling, value of `*_scales` keyword is ignored
2. **value** - multiplicative scaling
3. **auto** - automatic scaling
4. **log** - logarithmic scaling

First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:

- two-sided bounds scaled into the interval [0,1];
- one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
- no bounds or targets: no automatic scaling possible, therefore no scaling for this component

Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into [0,1].

4. **log** - logarithmic scaling

First, any characteristic values from the optional `*_scales` specification are applied. Then logarithm base 10 scaling is applied.

Logarithmic scaling is not available for linear constraints.

When continuous design variables are log scaled, linear constraints are not allowed.

**Scales**

The `*_scales` keywords are used to specify the characteristic values. These must be non-zero real numbers. The numbers are used according to the corresponding `*_scale_type`, as described above.

Depending on the scale type, the characteristic values may be required or optional.
6.2. **METHOD**

- none, auto, log - optional
- value - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than $1.0 \times 10^{-10} \times \text{DBL_MIN}$. User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.

**Examples**
The two examples below are equivalent:

```plaintext
responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value"
  primary_scales = 1 1 100

responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value" "value" "value"
  primary_scales = 1 1 100
```

**model_pointer**

- **Keywords Area**
- method
- nl2sol
- model_pointer

Identifier for model block to be used by a method

**Topics**

This keyword is related to the topics:

- **block_pointer**

**Specification**

**Alias:** none

**Argument(s):** STRING

**Default:** method use of last model parsed (or use of default model if none parsed)

**Description**

The `model_pointer` is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

**Default Behavior**

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding `id_model` with the same name.
Usage Tips
When doing advanced analyses that involve using multiple methods and multiple models, defining a model-pointer for each method is imperative. See block_pointer for details about pointers.

Examples

```plaintext
environment
tabular_graphics_data
method_pointer = 'UQ'

method
id_method = 'UQ'
model_pointer = 'SURR'
sampling,
samples = 10
seed = 98765 rng rnum2
response_levels = 0.1 0.2 0.6
0.1 0.2 0.6
0.1 0.2 0.6
sample_type lhs
distribution cumulative

model
id_model = 'SURR'
surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
id_method = 'DACE'
model_pointer = 'DACE_M'
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = 'DACE_M'
single
interface_pointer = 'I1'

variables
uniform_uncertain = 2
lower_bounds = 0. 0.
upper_bounds = 1. 1.
descriptors = 'x1' 'x2'

interface
id_interface = 'I1'
system asynch evaluation_concurrency = 5
analysis_driver = 'text_book'

responses
response_functions = 3
no_gradients
no_hessians
```

6.2.43 nonlinear_cg

- Keywords Area
6.2. METHOD

- method
- nonlinear_cg

(Experimental) nonlinear conjugate gradient optimization

Topics

This keyword is related to the topics:

- local_optimization_methods

Specification

Alias: none
Argument(s): none

<p>| Required/- | Description of | Dakota Keyword | Dakota Keyword |</p>
<table>
<thead>
<tr>
<th>Optional</th>
<th>Group</th>
<th></th>
<th>Description</th>
</tr>
</thead>
<tbody>
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<td></td>
<td>misc_options</td>
<td>Options for nonlinear CG optimizer</td>
</tr>
<tr>
<td>Optional</td>
<td>convergence_-tolerance</td>
<td></td>
<td>Stopping criterion based on convergence of the objective function or statistics</td>
</tr>
<tr>
<td>Optional</td>
<td>max_iterations</td>
<td></td>
<td>Number of iterations allowed for optimizers and adaptive UQ methods</td>
</tr>
<tr>
<td>Optional</td>
<td>scaling</td>
<td></td>
<td>Turn on scaling for variables, responses, and constraints</td>
</tr>
<tr>
<td>Optional</td>
<td>model_pointer</td>
<td></td>
<td>Identifier for model block to be used by a method</td>
</tr>
</tbody>
</table>

Description

This method is an incomplete experimental implementation of nonlinear conjugate gradient optimization, a local, gradient-based solver.
**misc_options**

- **Keywords Area**
- **method**
- **nonlinear_cg**
- **misc_options**

Options for nonlinear CG optimizer

**Specification**

**Alias:** none  
**Argument(s):** STRINGLIST  
**Default:** no misc options

**Description**

List of miscellaneous string options to pass to the experimental nonlinear CG solver (see NonlinearCGOptimizer.-cpp in the Dakota source code for available controls). Includes controls for step sizes, linesearch control, convergence, etc.

**convergence_tolerance**

- **Keywords Area**
- **method**
- **nonlinear_cg**
- **convergence_tolerance**

Stopping criterion based on convergence of the objective function or statistics

**Topics**

This keyword is related to the topics:

- **method_independent_controls**

**Specification**

**Alias:** none  
**Argument(s):** REAL  
**Default:** 1.e-4
6.2. METHOD

Description

The `convergence_tolerance` specification provides a real value for controlling the termination of iteration. For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by convergence_tolerance, then this convergence criterion is satisfied on the current iteration.

Therefore, permissible values are between 0 and 1, non-inclusive.

Behavior Varies by Package/Library

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- DOT: must be satisfied for two consecutive iterations
- NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of convergence_tolerance approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., convergence_tolerance = 1.e-6 will result in approximately six digits of accuracy in the final objective function).
- NL2SOL: See nl2sol

max_iterations

- Keywords Area
- method
- nonlinear_cg
- max_iterations

Number of iterations allowed for optimizers and adaptive UQ methods

Topics

This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none

Argument(s): INTEGER

Default: 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence}/efficient_global: 25*n)
CHAPTER 6. KEYWORDS AREA

Description

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed \( \text{max}_{\text{iterations}} \) iterations. See also \( \text{max.function_evaluations} \).

Default Behavior

Default value is 100.

scaling

- Keywords Area
- method
- nonlinear_cg
- scaling

Turn on scaling for variables, responses, and constraints

Topics

This keyword is related to the topics:

- method.independent_controls

Specification

Alias: none
Argument(s): none
Default: no scaling

Description

Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by by providing the scaling keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the method, variables, and responses blocks. When the scaling keyword is omitted, all \_scale_types and \_*scales specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.

- a \_*scales keyword, which gives characteristic values
- a \_*scale_type keyword, which determines how to use the characteristic values
6.2. METHOD

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to
the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the
examples below.

Scale Types
There are four scale types:

1. none (default) - no scaling, value of *scales keyword is ignored
2. value - multiplicative scaling
3. auto - automatic scaling
   First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according
to the following scheme:
   • two-sided bounds scaled into the interval [0,1];
   • one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and
     changing the sense of inequalities where necessary;
   • no bounds or targets: no automatic scaling possible, therefore no scaling for this component

   Automatic scaling is not available for objective functions nor calibration terms since they lack bound con-
   straints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not
   affinely scaled into [0,1].

4. log - logarithmic scaling
   First, any characteristic values from the optional *scales specification are applied. Then logarithm base
   10 scaling is applied.
   Logarithmic scaling is not available for linear constraints.
   When continuous design variables are log scaled, linear constraints are not allowed.

Scales
The *scales keywords are used to specify the characteristic values. These must be non-zero real numbers.
The numbers are used according to the corresponding *scale_type, as described above.
Depending on the scale type, the characteristic values may be required or optional.

• none, auto, log - optional

• value - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than 1.0e10*DBL_MIN.
User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated
scaling, the lower bound is enforced.

Examples
The two examples below are equivalent:

responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value"
  primary_scales = 1 1 100

responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value" "value" "value"
  primary_scales = 1 1 100
model_pointer

- Keywords Area
- method
- nonlinear_cg
- model_pointer

Identifier for model block to be used by a method

Topics

This keyword is related to the topics:

- block_pointer

Specification

Alias: none

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)

Description

The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.

Usage Tips

When doing advanced analyses that involve using multiple methods and multiple models, defining a model_pointer for each method is imperative.

See block_pointer for details about pointers.

Examples

environment
tabular_graphics_data
method_pointer = 'UQ'

method
id_method = 'UQ'
model_pointer = 'SURR'
sampling,
samples = 10
seed = 98765 rng rnum2
response_levels = 0.1 0.2 0.6
0.1 0.2 0.6
0.1 0.2 0.6
sample_type lhs
distribution cumulative

cmodel
id_model = 'SURR'
surrogate global,
edace_method_pointer = 'DACE'
polynomial quadratic

method
id_method = 'DACE'
model_pointer = 'DACE_M'
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = 'DACE_M'
single
interface_pointer = 'I1'

variables
uniform_uncertain = 2
lower_bounds = 0. 0.
upper_bounds = 1. 1.
descriptors = 'x1' 'x2'

interface
id_interface = 'I1'
system asynch evaluation_concurrency = 5
analysis_driver = 'text_book'

responses
response_functions = 3
no_gradients
no_hessians

6.2.44 ncsu_direct

- Keywords Area
- method
- ncsu_direct

DIviding RECTangles method

Topics
This keyword is related to the topics:
- global_optimization_methods

Specification
Alias: none
Argument(s): none
### Description
North Carolina State University (NCSU) has an implementation of the DIRECT algorithm (DIviding RECTangles algorithm that is outlined in the SCOLIB method section above). This version is documented in [28] We have found that the NCSU DIRECT implementation works better and is more robust for some problems than coliny-direct. Currently, we maintain both versions of DIRECT in Dakota; in the future, we may deprecate one.

The NCSU DIRECT method is selected with ncsu_direct. We have tried to maintain consistency between the keywords in SCOLIB and NCSU implementation of DIRECT, but the algorithms have different parameters, so the keywords sometimes have slightly different meaning.

#### Stopping Criteria
The algorithm stops based on:

<table>
<thead>
<tr>
<th>Optional</th>
<th>Keywords</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>solution_target</td>
<td>Specifies a globally optimal value toward which the optimizer should track</td>
</tr>
<tr>
<td>Optional</td>
<td>min_boxsize_limit</td>
<td>Stopping Criterion based on shortest edge of hyperrectangle</td>
</tr>
<tr>
<td>Optional</td>
<td>volume_boxsize_limit</td>
<td>Stopping criterion based on volume of search space</td>
</tr>
<tr>
<td>Optional</td>
<td>convergence_tolerance</td>
<td>Stopping criterion based on convergence of the objective function or statistics</td>
</tr>
<tr>
<td>Optional</td>
<td>max_iterations</td>
<td>Number of iterations allowed for optimizers and adaptive UQ methods</td>
</tr>
<tr>
<td>Optional</td>
<td>max_function_evaluations</td>
<td>Number of function evaluations allowed for optimizers</td>
</tr>
<tr>
<td>Optional</td>
<td>scaling</td>
<td>Turn on scaling for variables, responses, and constraints</td>
</tr>
<tr>
<td>Optional</td>
<td>model_pointer</td>
<td>Identifier for model block to be used by a method</td>
</tr>
</tbody>
</table>
6.2. METHOD

1. max_iterations - number of iterations
2. max_function_evaluations - number of function evaluations
3. solution_target and convergence_tolerance
4. min_boxsize_limit
5. volume_boxsize_limit

This method will always strictly respect the number of iterations, but may slightly exceed the number of
function evaluations, as it will always explore all sub-rectangles at the current level.

See Also
These keywords may also be of interest:

- coliny_direct

solution_target

- Keywords Area
- method
- ncsu_direct
- solution_target

Specifies a globally optimal value toward which the optimizer should track.

Specification

Alias: solution_accuracy
Argument(s): REAL
Default: 0

Description
The solution target specifies a goal toward which the optimizer should track.

This is used for test problems, when the true global minimum is known (call it solution_target - := f_global). Then, the optimization terminates when 100(f_min-f_global)/max(1,abs(f_global)) < convergence_tolerance. The default for f_global is -1.0e100 and the default for convergence tolerance is described at convergence._tolerance.

min_boxsize_limit

- Keywords Area
- method
- ncsu_direct
- min_boxsize_limit

Stopping Criterion based on shortest edge of hyperrectangle
Specification

Alias: none

Argument(s): REAL
Default: 1.0e-4

Description

min_boxsize_limit is a setting that terminates the optimization when the measure of a hyperrectangle S with \( f(c(S)) = f_{\text{min}} \) is less than \( \text{min\_boxsize\_limit} \).

Each subregion considered by DIRECT has a size, which corresponds to the longest diagonal of the subregion. \( \text{min\_boxsize\_limit} \) specification terminates DIRECT if the size of the smallest subregion falls below this threshold.

In practice, this specification is likely to be more effective at limiting DIRECT’s search.

volume_boxsize_limit

- Keywords Area
- method
- ncsu_direct
- volume_boxsize_limit

Stopping criterion based on volume of search space

Specification

Alias: none

Argument(s): REAL
Default: 1.0e-6

Description

volume_boxsize_limit is a setting that terminates the optimization when the volume of a hyperrectangle S with \( f(c(S)) = f_{\text{min}} \) is less than \( \text{volume\_boxsize\_limit} \) percent of the original hyperrectangle. Basically, volume_boxsize_limit stops the optimization when the volume of the particular rectangle which has \( f_{\text{min}} \) is less than a certain percentage of the whole volume.

convergence_tolerance

- Keywords Area
- method
- ncsu_direct
- convergence_tolerance

Stopping criterion based on convergence of the objective function or statistics
Topics
This keyword is related to the topics:

- method_independent_controls

Specification
Alias: none

Argument(s): REAL
Default: 1.e-4

Description
The convergence_tolerance specification provides a real value for controlling the termination of iteration. For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by convergence_tolerance, then this convergence criterion is satisfied on the current iteration. Therefore, permissible values are between 0 and 1, non-inclusive.

Behavior Varies by Package/Library
This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- DOT: must be satisfied for two consecutive iterations
- NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of convergence_tolerance approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., convergence_tolerance = 1.e-6 will result in approximately six digits of accuracy in the final objective function).
- NL2SOL: See nl2sol

max_iterations
- Keywords Area
- method
- ncsu_direct
- max_iterations

Number of iterations allowed for optimizers and adaptive UQ methods
Topics
This keyword is related to the topics:

- method_independent Controls

Specification
Alias: none
Argument(s): INTEGER
Default: 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence}/efficient_global: 25*n)

Description
The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed max_iterations iterations. See also max_function_evaluations.

Default Behavior
Default value is 100.

max_function_evaluations
- Keywords Area
- method
- ncsu_direct
- max_function_evaluations

Number of function evaluations allowed for optimizers

Topics
This keyword is related to the topics:

- method_independent Controls

Specification
Alias: none
Argument(s): INTEGER
Default: 1000

Description
The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed max_function_evaluations evaluations. See also max_iterations.

Default Behavior
Default value is 1000.
6.2. **METHOD**

**scaling**
- **Keywords Area**
- method
- ncsu_direct
- scaling

Turn on scaling for variables, responses, and constraints

**Topics**
This keyword is related to the topics:
- method_independent_controls

**Specification**

**Alias:** none
- **Argument(s):** none
- **Default:** no scaling

**Description**
Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by by providing the `scaling` keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the method, variables, and responses blocks. When the `scaling` keyword is omitted, all `_scale_types` and `*scales` specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.

- a `*scales` keyword, which gives characteristic values
- a `*scale_type` keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

**Scale Types**
There are four scale types:

1. **none** *(default) - no scaling, value of `*scales` keyword is ignored*
2. **value** - multiplicative scaling
3. **auto** - automatic scaling

First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:

- two-sided bounds scaled into the interval [0,1];
- one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
- no bounds or targets: no automatic scaling possible, therefore no scaling for this component

Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into [0,1].

4. **log** - logarithmic scaling

First, any characteristic values from the optional *scales specification are applied. Then logarithm base 10 scaling is applied.

Logarithmic scaling is not available for linear constraints.

When continuous design variables are log scaled, linear constraints are not allowed.

**Scales**

The *scales keywords are used to specify the characteristic values. These must be non-zero real numbers. The numbers are used according to the corresponding *scale_type, as described above.

Depending on the scale type, the characteristic values may be required or optional.

- none, auto, log - optional
- value - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than 1.0e10*DBL_MIN. User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.

**Examples**

The two examples below are equivalent:

```plaintext
responses
objective_functions 3
sense "maximize"
primary_scale_types = "value"
primary_scales = 1 1 100

responses
objective_functions 3
sense "maximize"
primary_scale_types = "value" "value" "value"
primary_scales = 1 1 100
```
model_pointer

- Keywords Area
- method
- ncsu_direct
- model_pointer

Identifier for model block to be used by a method

Topics

This keyword is related to the topics:
- block_pointer

Specification

Alias: none

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)

Description

The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.

Usage Tips

When doing advanced analyses that involve using multiple methods and multiple models, defining a model_pointer for each method is imperative.

See block_pointer for details about pointers.

Examples

```plaintext
environment
  tabular_graphics_data
  method_pointer = 'UQ'

method
  id_method = 'UQ'
  model_pointer = 'SURR'
  sampling,
    samples = 10
    seed = 98765 rng rnum2
    response_levels = 0.1 0.2 0.6
    0.1 0.2 0.6
    0.1 0.2 0.6
  sample_type lhs
  distribution cumulative

model
  id_model = 'SURR'
```
surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
id_method = 'DACE'
model_pointer = 'DACE_M'
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = 'DACE_M'
single
interface_pointer = 'I1'

variables
uniform_uncertain = 2
lower_bounds = 0. 0.
upper_bounds = 1. 1.
descriptors = 'x1' 'x2'

interface
id_interface = 'I1'
system asynch evaluation_concurrency = 5
analysis_driver = 'text_book'

responses
response_functions = 3
no_gradients
no_hessians

6.2.45 genie_opt_darts

- Keywords Area

- method

- genie_opt_darts

Voronoi-based high-dimensional global Lipschitzian optimization

Specification

Alias: none

Argument(s): none
6.2. Method

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>seed</td>
<td>Seed of the random number generator</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>max_function_evaluations</td>
<td>Number of function evaluations allowed for optimizers</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>scaling</td>
<td>Turn on scaling for variables, responses, and constraints</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>model_pointer</td>
<td>Identifier for model block to be used by a method</td>
</tr>
</tbody>
</table>

**Description**

OPT-Darts method is a fast alternative to DIRECT for global Lipschitzian optimization purposes. Instead of hyperrectangular, OPT-Darts decomposes a high-dimensional domain into Voronoi cells, and places samples via stochastic blue noise instead of deterministic cell division.

To refine a cell, OPT-Darts first adds a new sample within it via spoke-dart sampling, then set the conflict radius to the cells inscribed hypersphere radius, to avoid adding a sample point that is too close to a prior sample, then divide that cell (and update its neighboring cells) via the approximate Delaunay graph, and use the computed witnesses to decide the next refinement candidate. These two steps replace the corresponding deterministic center-sample and rectangular cell division in DIRECT, respectively.

OPT-Darts is the first exact stochastic Lipschitzian optimization technique that combines the benefits of guaranteed convergence in [Jones et al. 1993] and high dimensional efficiency in [Spall 2005]. Computing blue noise and Voronoi regions has been intractable in high dimensions, and are being done within OPT-Darts using Spoke-Darts.

**seed**

- **Keywords Area**
- **method**
- **genie_opt_darts**
- **seed**

Seed of the random number generator

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** system-generated (non-repeatable)
CHAPTER 6. KEYWORDS AREA

Description

The random seed control provides a mechanism for making a stochastic method repeatable. That is, the use of the same random seed in identical studies will generate identical results.

Default Behavior
If not specified, the seed is randomly generated.

Expected Output
If seed is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

Usage Tips
If a stochastic study was run without seed specified, and the user later wishes to repeat the study using the same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen. That value can then be added to the Dakota input file.

Examples

method
  sampling
    sample_type lhs
    samples = 10
    seed = 15347

max_function_evaluations

  * Keywords Area
  * method
  * genie_opt_darts
  * max_function_evaluations

Number of function evaluations allowed for optimizers

Topics

This keyword is related to the topics:

  * method_independent_controls

Specification

Alias: none
Argument(s): INTEGER
Default: 1000

Description

The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed max_function_evaluations evaluations. See also max_iterations.

Default Behavior
Default value is 1000.
6.2. METHOD

scaling

- Keywords Area
- method
- genie_opt_darts
- scaling

Turn on scaling for variables, responses, and constraints

Topics

This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none
- Argument(s): none
- Default: no scaling

Description

Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by by providing the scaling keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the method, variables, and responses blocks. When the scaling keyword is omitted, all _scale_types and *scales specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.

- a *scales keyword, which gives characteristic values
- a *scale_type keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

Scale Types

There are four scale types:

1. none (default) - no scaling, value of *scales keyword is ignored
2. value - multiplicative scaling
3. **auto** - automatic scaling

First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:

- two-sided bounds scaled into the interval \([0,1]\);
- one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
- no bounds or targets: no automatic scaling possible, therefore no scaling for this component

Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into \([0,1]\).

4. **log** - logarithmic scaling

First, any characteristic values from the optional `scales` specification are applied. Then logarithm base 10 scaling is applied.

Logarithmic scaling is not available for linear constraints.

When continuous design variables are log scaled, linear constraints are not allowed.

**Scales**

The `scales` keywords are used to specify the characteristic values. These must be non-zero real numbers. The numbers are used according to the corresponding `scale_type`, as described above.

Depending on the scale type, the characteristic values may be required or optional.

- **none**, **auto**, **log** - optional
- **value** - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than \(1.0 \times 10^{10}\). User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.

**Examples**

The two examples below are equivalent:

```plaintext
responses
objective_functions 3
sense "maximize"
primary_scale_types = "value"
primary_scales = 1 1 100

responses
objective_functions 3
sense "maximize"
primary_scale_types = "value" "value" "value"
primary_scales = 1 1 100
```
6.2. METHOD

model_pointer

- Keywords Area
- method
- genie_opt_darts
- model_pointer

Identifier for model block to be used by a method

Topics

This keyword is related to the topics:

- block_pointer

Specification

Alias: none

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)

Description

The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.

Usage Tips

When doing advanced analyses that involve using multiple methods and multiple models, defining a model_pointer for each method is imperative.

See block_pointer for details about pointers.

Examples

environment
  tabular_graphics_data
  method_pointer = 'UQ'

method
  id_method = 'UQ'
  model_pointer = 'SURR'
  sampling,
    samples = 10
    seed = 98765 rng rnum2
    response_levels = 0.1 0.2 0.6
    0.1 0.2 0.6
    0.1 0.2 0.6
  sample_type lhs
distribution cumulative

model
  id_model = 'SURR'
surrogate global,
dace_method_pointer = ‘DACE’
polynomial quadratic

method
id_method = ‘DACE’
model_pointer = ‘DACE_M’
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = ‘DACE_M’
single
interface_pointer = ‘I1’

variables
uniform_uncertain = 2
lower_bounds = 0. 0.  
upper_bounds = 1. 1.  
descriptors = ‘x1’ ‘x2’

interface
id_interface = ‘I1’
system asynch evaluation_concurrency = 5
analysis_driver = ‘text_book’

responses
response_functions = 3
no_gradients
no_hessians

6.2.46 genie_direct

• Keywords Area

• method

• genie_direct

Classical high-dimensional global Lipschitzian optimization

Specification

Alias: none

<table>
<thead>
<tr>
<th>Argument(s): none</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required/-Optional</td>
</tr>
<tr>
<td>-------------------</td>
</tr>
<tr>
<td>seed</td>
</tr>
</tbody>
</table>
### Description

DIRECT (DIviding RECTangles) partitions the domain into hyperrectangles and uses an iterative Lipschitzian optimization approach to search for a global optimal point.

DIRECT begins by scaling the domain into the unit hypercube by adopting a center-sampling strategy. The objective function is evaluated at the midpoint of the domain, where a lower bound is constructed. In one-dimension, the domain is tri-sected and two new center points are sampled. At each iteration (dividing and sampling), DIRECT identifies intervals that contain the best minimal value of the objective function found up to that point. This strategy of selecting and dividing gives DIRECT its performance and convergence properties compared to other deterministic methods.

The classical DIRECT method [Shubert 1972] has two limitations: poor scaling to high dimensions; and relying on a global K; whose exact value is often unknown. The enhanced DIRECT algorithm [Jones et al. 1993] generalizes [Shubert 1972] to higher dimensions and does not require knowledge of the Lipschitz constant.

### seed

- Keywords Area
- method
- genie_direct
- seed

Seed of the random number generator

### Specification

**Alias:** none  
**Argument(s):** INTEGER  
**Default:** system-generated (non-repeatable)

### Description

The random seed control provides a mechanism for making a stochastic method repeatable. That is, the use of the same random seed in identical studies will generate identical results.
**Default Behavior**
If not specified, the seed is randomly generated.

**Expected Output**
If `seed` is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

**Usage Tips**
If a stochastic study was run without `seed` specified, and the user later wishes to repeat the study using the same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen. That value can then be added to the Dakota input file.

**Examples**
```
method
  sampling
    sample_type lhs
    samples  = 10
    seed    = 15347
```

**max_function_evaluations**

- **Keywords Area**
- **method**
- **genie_direct**
- **max_function_evaluations**

Number of function evaluations allowed for optimizers

**Topics**
This keyword is related to the topics:

- **method_independent_controls**

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** 1000

**Description**
The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed `max_function_evaluations` evaluations. See also `max_iterations`.

**Default Behavior**
Default value is 1000.
6.2. METHOD

scaling
• Keywords Area
  • method
  • genie_direct
  • scaling

Turn on scaling for variables, responses, and constraints

Topics
This keyword is related to the topics:
• method_independent_controls

Specification
Alias: none
Argument(s): none
Default: no scaling

Description
Some of the optimization and calibration methods support scaling of continuous design variables, objective functions, calibration terms, and constraints. This is activated by by providing the `scaling` keyword. Discrete variable scaling is not supported.

When scaling is enabled, variables, functions, gradients, Hessians, etc., are transformed such that the method iterates in scaled variable space, whereas evaluations of the computational model as specified in the interface are performed on the original problem scale. Therefore using scaling does not require rewriting the interface to the simulation code.

Scaling also requires the specification of additional keywords which are found in the method, variables, and responses blocks. When the `scaling` keyword is omitted, all _scale_types and *scales specifications are ignored in the method, variables, and responses sections.

This page describes the usage of all scaling related keywords. The additional keywords come in pairs, one pair for each set of quantities to be scaled. These quantities can be constraint equations, variables, or responses.

• a *scales keyword, which gives characteristic values
• a *scale_type keyword, which determines how to use the characteristic values

The pair of keywords both take argument(s), and the length of the arguments can either be zero, one, or equal to the number of quantities to be scaled. If one argument is given, it will apply to all quantities in the set. See the examples below.

Scale Types
There are four scale types:

1. none (default) - no scaling, value of *scales keyword is ignored
2. value - multiplicative scaling
3. **auto** - automatic scaling

First the quantity is scaled by the characteristic value, then automatic scaling will be attempted according to the following scheme:

- two-sided bounds scaled into the interval \[0,1\];
- one-sided bound or targets are scaled by the characteristic value, moving the bound or target to 1 and changing the sense of inequalities where necessary;
- no bounds or targets: no automatic scaling possible, therefore no scaling for this component

Automatic scaling is not available for objective functions nor calibration terms since they lack bound constraints. Further, when automatically scaled, linear constraints are scaled by characteristic values only, not affinely scaled into \([0,1]\).

4. **log** - logarithmic scaling

First, any characteristic values from the optional \(*_scales\) specification are applied. Then logarithm base 10 scaling is applied.

Logarithmic scaling is not available for linear constraints.

When continuous design variables are log scaled, linear constraints are not allowed.

**Scales**

The \(*_scales\) keywords are used to specify the characteristic values. These must be non-zero real numbers. The numbers are used according to the corresponding \(_scale\_type\), as described above.

Depending on the scale type, the characteristic values may be required or optional.

- **none, auto, log** - optional
- **value** - required.

A warning is issued if scaling would result in division by a value smaller in magnitude than \(1.0e10*DBL\_MIN\). User-provided values violating this lower bound are accepted unaltered, whereas for automatically calculated scaling, the lower bound is enforced.

**Examples**

The two examples below are equivalent:

```
responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value"
  primary_scales = 1 1 100

responses
  objective_functions 3
  sense "maximize"
  primary_scale_types = "value" "value" "value"
  primary_scales = 1 1 100
```
6.2. METHOD

model_pointer

- Keywords Area
- method
- genie_direct
- model_pointer

Identifier for model block to be used by a method

Topics

This keyword is related to the topics:

- block_pointer

Specification

Alias: none

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)

Description

The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.

Usage Tips

When doing advanced analyses that involve using multiple methods and multiple models, defining a model_pointer for each method is imperative.

See block_pointer for details about pointers.

Examples

```plaintext
environment
    tabular_graphics_data
    method_pointer = 'UQ'

method
    id_method = 'UQ'
    model_pointer = 'Surr'
    sampling,
    samples = 10
    seed = 98765 rng rnum2
    response_levels = 0.1 0.2 0.6
    0.1 0.2 0.6
    0.1 0.2 0.6
    sample_type lhs
    distribution cumulative

model
    id_model = 'Surr'
```
surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
  id_method = 'DACE'
  model_pointer = 'DACE_M'
  sampling sample_type lhs
  samples = 121 seed = 5034 rng rnum2

model
  id_model = 'DACE_M'
single
  interface_pointer = 'I1'

variables
  uniform_uncertain = 2
  lower_bounds = 0.0
  upper_bounds = 1.1
  descriptors = 'x1' 'x2'

interface
  id_interface = 'I1'
  system asynch evaluation_concurrency = 5
  analysis_driver = 'text_book'

responses
  response_functions = 3
  no_gradients
  no_hessians

6.2.47 efficient_global

- Keywords Area
- method
- efficient_global

Global Surrogate Based Optimization, a.k.a. EGO

Topics

This keyword is related to the topics:

- global_optimization_methods
- surrogate_based_optimization_methods

Specification

Alias: none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>none</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
6.2. METHOD

| Optional | initial_samples | Initial number of samples for sampling-based methods |
| Optional | seed | Seed of the random number generator |
| Optional | max_iterations | Number of iterations allowed for optimizers and adaptive UQ methods |
| Optional | gaussian_process | Gaussian Process surrogate model |
| Optional | use_derivatives | Use derivative data to construct surrogate models |
| Optional | import_build_points_file | File containing points you wish to use to build a surrogate |
| Optional | export_approx_points_file | Output file for evaluations of a surrogate model |
| Optional | model_pointer | Identifier for model block to be used by a method |

**Description**

The Efficient Global Optimization (EGO) method was first developed by Jones, Schonlau, and Welch[54]. In EGO, a stochastic response surface approximation for the objective function is developed based on some sample points from the “true” simulation.

Note that several major differences exist between our implementation and that of[54]. First, rather than using a branch and bound method to find the point which maximizes the EIF, we use the DIRECT global optimization method.

Second, we support both global optimization and global nonlinear least squares as well as general nonlinear constraints through abstraction and subproblem recasting.

The efficient global method is in prototype form. Currently, we do not expose any specification controls for the underlying Gaussian process model used or for the optimization of the expected improvement function (which is currently performed by the NCSU DIRECT algorithm using its internal defaults).

By default, EGO uses the Surfpack GP (Kriging) model, but the Dakota implementation may be selected instead. If use_derivatives is specified the GP model will be built using available derivative data (Surfpack...
Theory

The particular response surface used is a Gaussian process (GP). The GP allows one to calculate the prediction at a new input location as well as the uncertainty associated with that prediction. The key idea in EGO is to maximize the Expected Improvement Function (EIF). The EIF is used to select the location at which a new training point should be added to the Gaussian process model by maximizing the amount of improvement in the objective function that can be expected by adding that point. A point could be expected to produce an improvement in the objective function if its predicted value is better than the current best solution, or if the uncertainty in its prediction is such that the probability of it producing a better solution is high. Because the uncertainty is higher in regions of the design space with few observations, this provides a balance between exploiting areas of the design space that predict good solutions, and exploring areas where more information is needed. EGO trades off this “exploitation vs. exploration.” The general procedure for these EGO-type methods is:

- Build an initial Gaussian process model of the objective function
- Find the point that maximizes the EIF. If the EIF value at this point is sufficiently small, stop.
- Evaluate the objective function at the point where the EIF is maximized. Update the Gaussian process model using this new point.
- Return to the previous step.

See Also

These keywords may also be of interest:

- surrogate_based_local
- surrogate_based_global

initial_samples

- Keywords Area
- method
- efficient_global
- initial_samples

Initial number of samples for sampling-based methods

Specification

Alias: none

Argument(s): INTEGER

Default: \((d+1)(d+2)/2\)
6.2. METHOD

Description

The initial_samples keyword is used to define the number of initial samples (i.e., randomly chosen sets of variable values) at which to execute a model. The initial samples may later be augmented in an iterative process.

Default Behavior

By default, Dakota will use the minimum number of samples required by the chosen method.

Usage Tips

To obtain linear sensitivities or to construct a linear response surface, at least \( \text{dim}+1 \) samples should be used, where "dim" is the number of variables. For sensitivities to quadratic terms or quadratic response surfaces, at least \( (\text{dim}+1)(\text{dim}+2)/2 \) samples are needed. For uncertainty quantification, we recommend at least \( 10 \times \text{dim} \) samples. For variance_based_decomp, we recommend hundreds to thousands of samples. Note that for variance_based_decomp, the number of simulations performed will be \( N \times (\text{dim}+2) \).

Examples

```plaintext
method sampling
  sample_type random
  initial_samples = 20
  refinement_samples = 5

seed
  * Keywords Area
  * method
  * efficient_global
  * seed

Seed of the random number generator

Specification

Alias: none

Argument(s): INTEGER

Default: system-generated (non-repeatable)

Description

The random seed control provides a mechanism for making a stochastic method repeatable. That is, the use of the same random seed in identical studies will generate identical results.

Default Behavior

If not specified, the seed is randomly generated.

Expected Output

If seed is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

Usage Tips

If a stochastic study was run without seed specified, and the user later wishes to repeat the study using the same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen. That value can then be added to the Dakota input file.
Examples

method
  sampling
    sample_type lhs
    samples = 10
    seed = 15347

max_iterations
  - Keywords Area
  - method
  - efficient_global
  - max_iterations

Number of iterations allowed for optimizers and adaptive UQ methods

Topics

This keyword is related to the topics:
  - method_independent_controls

Specification

Alias: none
  Argument(s): INTEGER
  Default: 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence} / efficient_global: \(25 \times n\))

Description

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed \(\text{max\_iterations} \times n\) iterations. See also max_function_evaluations.

Default Behavior

Default value is 100.

gaussian_process
  - Keywords Area
  - method
  - efficient_global
  - gaussian_process

Gaussian Process surrogate model
6.2. METHOD

Specification

Alias: kriging
- Argument(s): none
- Default: Surfpack Gaussian process
CHAPTER 6. KEYWORDS AREA

<table>
<thead>
<tr>
<th>Required/Optional Required (Choose One)</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<tbody>
<tr>
<td></td>
<td></td>
<td>surfpack</td>
<td>Use the Surfpack version of Gaussian Process surrogates</td>
</tr>
</tbody>
</table>

**Description**

Use the Gaussian process (GP) surrogate from Surfpack, which is specified using the `surfpack` keyword.

An alternate version of GP surrogates was available in prior versions of Dakota. **For now, both versions are supported but the dakota version is deprecated and intended to be removed in a future release.**

**Known Issue:** When using discrete variables, there have been sometimes significant differences in surrogate behavior observed across computing platforms in some cases. The cause has not yet been fully diagnosed and is currently under investigation. In addition, guidance on appropriate construction and use of surrogates with discrete variables is under development. In the meantime, users should therefore be aware that there is a risk of inaccurate results when using surrogates with discrete variables.

**surfpack**
- Keywords Area
- method
- efficient_global
- gaussian_process
- surfpack

Use the Surfpack version of Gaussian Process surrogates

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

This keyword specifies the use of the Gaussian process that is incorporated in our surface fitting library called Surfpack.

Several user options are available:

1. **Optimization methods:**
   - Maximum Likelihood Estimation (MLE) is used to find the optimal values of the hyper-parameters governing the trend and correlation functions. By default the global optimization method DIRECT is used for MLE, but other options for the optimization method are available. See `optimization_method`.
   - The total number of evaluations of the likelihood function can be controlled using the `max_trials` keyword followed by a positive integer. Note that the likelihood function does not require running the "truth" model, and is relatively inexpensive to compute.
2. Trend Function:
   The GP models incorporate a parametric trend function whose purpose is to capture large-scale variations. See trend.

3. Correlation Lengths:
   Correlation lengths are usually optimized by Surfpack, however, the user can specify the lengths manually. See correlation_lengths.

4. Ill-conditioning
   One of the major problems in determining the governing values for a Gaussian process or Kriging model is the fact that the correlation matrix can easily become ill-conditioned when there are too many input points close together. Since the predictions from the Gaussian process model involve inverting the correlation matrix, ill-conditioning can lead to poor predictive capability and should be avoided.
   Note that a sufficiently bad sample design could require correlation lengths to be so short that any interpolatory GP model would become inept at extrapolation and interpolation.
   The surfpack model handles ill-conditioning internally by default, but behavior can be modified using

5. Gradient Enhanced Kriging (GEK).
   The use_derivatives keyword will cause the Surfpack GP to be constructed from a combination of function value and gradient information (if available).
   See notes in the Theory section.

Theory

Gradient Enhanced Kriging

Incorporating gradient information will only be beneficial if accurate and inexpensive derivative information is available, and the derivatives are not infinite or nearly so. Here “inexpensive” means that the cost of evaluating a function value plus gradient is comparable to the cost of evaluating only the function value, for example gradients computed by analytical, automatic differentiation, or continuous adjoint techniques. It is not cost effective to use derivatives computed by finite differences. In tests, GEK models built from finite difference derivatives were also significantly less accurate than those built from analytical derivatives. Note that GEK’s correlation matrix tends to have a significantly worse condition number than Kriging for the same sample design.

This issue was addressed by using a pivoted Cholesky factorization of Kriging’s correlation matrix (which is a small sub-matrix within GEK’s correlation matrix) to rank points by how much unique information they contain. This reordering is then applied to whole points (the function value at a point immediately followed by gradient information at the same point) in GEK’s correlation matrix. A standard non-pivoted Cholesky is then applied to the reordered GEK correlation matrix and a bisection search is used to find the last equation that meets the constraint on the (estimate of) condition number. The cost of performing pivoted Cholesky on Kriging’s correlation matrix is usually negligible compared to the cost of the non-pivoted Cholesky factorization of GEK’s correlation matrix. In tests, it also resulted in more accurate GEK models than when pivoted Cholesky or whole-point-block pivoted Cholesky was performed on GEK’s correlation matrix.

dakota

- Keywords Area
- method
- efficient_global
• **gaussian_process**

• **dakota**

Select the built in Gaussian Process surrogate

### Specification

**Alias:** none

**Argument(s):** none

### Description

A second version of GP surrogates was available in prior versions of Dakota. **For now, both versions are supported but the dakota version is deprecated and intended to be removed in a future release.**

Historically these models were drastically different, but in Dakota 5.1, they became quite similar. They now differ in that the Surfpack GP has a richer set of features/options and tends to be more accurate than the Dakota version. Due to how the Surfpack GP handles ill-conditioned correlation matrices (which significantly contributes to its greater accuracy), the Surfpack GP can be a factor of two or three slower than Dakota’s. As of Dakota 5.2, the Surfpack implementation is the default in all contexts except Bayesian calibration.

More details on the **gaussian_process** dakota model can be found in[58].

Dakota’s GP deals with ill-conditioning in two ways. First, when it encounters a non-invertible correlation matrix it iteratively increases the size of a "nugget," but in such cases the resulting approximation smooths rather than interpolates the data. Second, it has a **point_selection** option (default off) that uses a greedy algorithm to select a well-spaced subset of points prior to the construction of the GP. In this case, the GP will only interpolate the selected subset. Typically, one should not need point selection in trust-region methods because a small number of points are used to develop a surrogate within each trust region. Point selection is most beneficial when constructing with a large number of points, typically more than order one hundred, though this depends on the number of variables and spacing of the sample points.

This differs from the **point_selection** option of the Dakota GP which initially chooses a well-spaced subset of points and finds the correlation parameters that are most likely for that one subset.

### use_derivatives

- **Keywords Area**
- **method**
- **efficient_global**
- **use_derivatives**

Use derivative data to construct surrogate models

### Specification

**Alias:** none

**Argument(s):** none

**Default:** use function values only
6.2. **METHOD**

**Description**

The `use_derivatives` flag specifies that any available derivative information should be used in global approximation builds, for those global surrogate types that support it (currently, polynomial regression and the Surfpack Gaussian process).

However, its use with Surfpack Gaussian process is not recommended.

**import_build_points_file**

- **Keywords Area**
- **method**
- **efficient_global**
- **import_build_points_file**

File containing points you wish to use to build a surrogate

**Specification**

**Alias:** import_points_file  
**Argument(s):** STRING  
**Default:** no point import from a file

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
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<td>Optional/Choose One</td>
<td>Tabular Format (Group 1)</td>
<td>annotated</td>
</tr>
<tr>
<td></td>
<td></td>
<td>custom_annotated</td>
</tr>
<tr>
<td></td>
<td></td>
<td>freeform</td>
</tr>
<tr>
<td>Optional</td>
<td>active_only</td>
<td>Import only active variables from tabular data file</td>
</tr>
</tbody>
</table>

**Description**

The `import_build_points_file` allows the user to specify a file that contains a list of points and truth model responses used to construct a surrogate model. These can be used by all methods that (explicitly, e.g. surrogate-based optimization, or implicitly, e.g. efficient global optimization) operate on a surrogate. In particular, these points and responses are used in place of truth model evaluations to construct the initial surrogate. When used to construct surrogate models or emulators these are often called build points or training data.

**Default Behavior**

By default, methods do not import points from a file.

**Usage Tips**
Dakota parses input files without regard to whitespace, but the `import_build_points_file` must be in one of three formats:

- annotated (default)
- custom.annotated
- freeform

**Examples**

```plaintext
method
  polynomial_chaos
  expansion_order = 4
  import_build_points_file = 'dakota_uq_rosenbrock_pce_import.annot.pts.dat'
```

**Topics**

This keyword is related to the topics:

- file_formats

**Specification**

Alias: none

**Argument(s):** none

**Default:** annotated format

**Description**

An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

**Default Behavior**

By default, Dakota imports and exports tabular files in annotated format. The `annotated` keyword can be used to explicitly specify this.

**Usage Tips**

- To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify `custom.annotated header eval_id`
6.2. METHOD

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```python
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
annotated

Resulting tabular file:

```
%eval_id interface x1 x2 obj_fn nln_ineq_con_1 nln_ineq_con_2
1 NO_ID 0.9 1.1 0.0002 0.26 0.76
2 NO_ID 0.90009 1.1 0.0001996404857 0.2601620081 0.759955
3 NO_ID 0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...```

custom_annotated

- Keywords Area
- method
- efficient_global
- import_build_points_file
- custom_annotated

Selects custom-annotated tabular file format

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none

Argument(s): none

Default: annotated format

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<tbody>
<tr>
<td>Optional</td>
<td></td>
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</tr>
</tbody>
</table>
CHAPTER 6. KEYWORDS AREA

<table>
<thead>
<tr>
<th>Optional</th>
<th>header</th>
<th>Enable header row in custom-annotated tabular file</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>eval id</td>
<td>Enable evaluation ID column in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td>interface id</td>
<td>Enable interface ID column in custom-annotated tabular file</td>
</tr>
</tbody>
</table>

Description

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval id column, and interface id column appear in the tabular file, thus bridging freeform and (fully) annotated.

Default Behavior

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

Usage Tips

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval id (no interface_id), and data for variables and responses. Input file fragment:

```plaintext
environment
  tabular_data
    tabular_data_file = 'dakota_summary.dat'
    custom_annotated header eval_id

Resulting tabular file:

%eval_id   x1   x2   obj_fn   nln_ineq_con_1   nln_ineq_con_2
1   0.9   1.1   0.0002   0.26   0.76
2   0.90009   1.1   0.0001996404857   0.2601620081   0.759955
3   0.89991   1.1   0.0002003604863   0.2598380081   0.760045
...```
6.2. METHOD

header
- Keywords Area
- method
- efficient_global
- import_build_points_file
- custom_annotated
- header

Enable header row in custom-annotated tabular file

Specification
Alias: none
- Argument(s): none
- Default: no header

Description
See description of parent custom_annotated

eval_id
- Keywords Area
- method
- efficient_global
- import_build_points_file
- custom_annotated
- eval_id

Enable evaluation ID column in custom-annotated tabular file

Specification
Alias: none
- Argument(s): none
- Default: no eval_id column

Description
See description of parent custom_annotated
interface_id

- Keywords Area
- method
- efficient_global
- import_build_points_file
- custom_annotated
- interface_id

Enable interface ID column in custom-annotated tabular file

**Specification**

**Alias:** none

Argument(s): none
Default: no interface_id column

**Description**

See description of parent custom_annotated

**freeform**

- Keywords Area
- method
- efficient_global
- import_build_points_file
- freeform

Selects freeform file format

**Topics**

This keyword is related to the topics:

- file_formats

**Specification**

**Alias:** none

Argument(s): none
Default: annotated format
6.2. METHOD

Description
A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior
The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips
- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples
Export a freeform tabular file containing only data for variables and responses. Input file fragment:
```python
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
freeform
```

Resulting tabular file:
```
0.9 1.1 0.0002 0.26 0.76
0.90009 1.1 0.0001996404857 0.2601620081 0.759955
0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...
```

active_only
- Keywords Area
- method
- efficient_global
- import_build_points_file
- active_only
Import only active variables from tabular data file

Topics
This keyword is related to the topics:
**CHAPTER 6. KEYWORDS AREA**

**Specification**

**Alias:** none  
**Argument(s):** none

**Description**

By default, files for tabular data imports are expected to contain columns for all variables, active and inactive. The keyword `active_only` indicates that the file to import contains only the active variables.

This option should only be used in contexts where the inactive variables have no influence, for example, building a surrogate over active variables, with the state variables held at nominal. It should not be used in more complex nested contexts, where the values of inactive variables are relevant to the function evaluations used to build the surrogate.

---

**export_approx_points_file**

- **Keywords Area**
- **method**
- **efficient_global**
- **export_approx_points_file**

Output file for evaluations of a surrogate model

**Specification**

**Alias:** export_points_file  
**Argument(s):** STRING  
**Default:** no point export to a file

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional (Choose One)</td>
<td>Tabular Format (Group 1)</td>
<td>annotated</td>
<td>Selects annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>custom_annotated</td>
<td>Selects custom-annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>freeform</td>
<td>Selects freeform file format</td>
</tr>
</tbody>
</table>

**Description**

The `export_approx_points_file` keyword allows the user to specify a file in which the points (input variable values) at which the surrogate model is evaluated and corresponding response values computed by the surrogate model will be written. The response values are the surrogate’s predicted approximation to the truth model responses at those points.

**Usage Tips**

Dakota exports tabular data in one of three formats:
6.2. METHOD

- annotated (default)
- custom.annotated
- freeform

annotated

- Keywords Area
- method
- efficient_global
- export.approx_points_file
- annotated

Selects annotated tabular file format

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none
Argument(s): none
Default: annotated format

Description

An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior

By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips

- To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify custom.annotated header eval.id

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.
Examples
Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```python
environment
tabular_data
    tabular_data_file = 'dakota_summary.dat'
annotated
```

Resulting tabular file:

```
%eval_id interface x1 x2 obj_fn nln_ineq_con_1 nln_ineq_con_2
1 NO_ID 0.9 1.1 0.0002 0.26 0.76
2 NO_ID 0.90009 1.1 0.0001996404857 0.2601620081 0.759955
3 NO_ID 0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...```

custom_annotated

- Keywords Area
- method
- efficient_global
- export_approx_points_file
- custom_annotated

Selects custom-annotated tabular file format

Topics
This keyword is related to the topics:

- file_formats

Specification
Alias: none
Argument(s): none
Default: annotated format

<p>| Required/- | Description of | Dakota Keyword | Dakota Keyword |</p>
<table>
<thead>
<tr>
<th>Optional</th>
<th>Group</th>
<th>header</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Enable header row in custom-annotated tabular file</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
6.2. METHOD

### Description

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

#### Default Behavior

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

#### Usage Tips

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

#### Examples

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
custom_annotated header eval_id
```

Resulting tabular file:

<table>
<thead>
<tr>
<th>%eval_id</th>
<th>x1</th>
<th>x2</th>
<th>obj_fn</th>
<th>nln_ineq_con_1</th>
<th>nln_ineq_con_2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.9</td>
<td>1.1</td>
<td>0.0002</td>
<td>0.26</td>
<td>0.76</td>
</tr>
<tr>
<td>2</td>
<td>0.90009</td>
<td>1.1</td>
<td>0.0001996404857</td>
<td>0.2601620081</td>
<td>0.759955</td>
</tr>
<tr>
<td>3</td>
<td>0.89991</td>
<td>1.1</td>
<td>0.0002003604863</td>
<td>0.2598380081</td>
<td>0.760045</td>
</tr>
<tr>
<td>...</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Keywords Area

- method
- efficient_global
• export_approx_points_file
• custom_annotated
• header

Enable header row in custom-annotated tabular file

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no header

**Description**

See description of parent `custom_annotated`

eval_id

• Keywords Area
• method
• efficient_global
• export_approx_points_file
• custom_annotated

• eval_id

Enable evaluation ID column in custom-annotated tabular file

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no eval_id column

**Description**

See description of parent `custom_annotated`

interface_id

• Keywords Area
• method
• efficient_global
• export_approx_points_file
• custom_annotated

• interface_id

Enable interface ID column in custom-annotated tabular file
6.2. METHOD

Specification

Alias: none

Argument(s): none

Default: no interface_id column

Description

See description of parent custom.annotated

freeform

- Keywords Area
- method
- efficient_global
- export.approx_points_file
- freeform

Selects freeform file format

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none

Argument(s): none

Default: annotated format

Description

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior

The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips

- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
• In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).

• Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples
Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
  tabular_data_file = 'dakota_summary.dat'
  freeform
```

Resulting tabular file:

```
0.9  1.1  0.0002  0.26  0.76
0.90009  1.1  0.0001996404857  0.2601620081  0.759955
0.89991  1.1  0.0002003604863  0.2598380081  0.760045
...
```

model_pointer

• Keywords Area

• method

• efficient_global

• model_pointer

Identifier for model block to be used by a method

Topics
This keyword is related to the topics:

• block_pointer

Specification

Alias: none

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)

Description
The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior
If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.

Usage Tips
When doing advanced analyses that involve using multiple methods and multiple models, defining a model-pointer for each method is imperative.

See block_pointer for details about pointers.
6.2. METHOD

Examples

environment
  tabular_graphics_data
  method_pointer = 'UQ'

method
  id_method = 'UQ'
  model_pointer = 'SURR'
  sampling,
  samples = 10
  seed = 98765 rng rnum2
  response_levels = 0.1 0.2 0.6
  0.1 0.2 0.6
  0.1 0.2 0.6
  sample_type lhs
distribution cumulative

model
  id_model = 'SURR'
surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
  id_method = 'DACE'
  model_pointer = 'DACE_M'
sampling sample_type lhs
  samples = 121 seed = 5034 rng rnum2

model
  id_model = 'DACE_M'
single
  interface_pointer = 'I1'

variables
  uniform_uncertain = 2
  lower_bounds = 0. 0.
  upper_bounds = 1. 1.
  descriptors = 'x1' 'x2'

interface
  id_interface = 'I1'
system asynch evaluation_concurrency = 5
  analysis_driver = 'text_book'

responses
  response_functions = 3
  no_gradients
  no_hessians

6.2.48 polynomial_chaos

- Keywords Area
- method
- polynomial_chaos

Uncertainty quantification using polynomial chaos expansions
Specification

Alias: nond_polynomial_chaos

Argument(s): none
### 6.2. METHOD

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>samples_on_emulator</td>
<td></td>
<td>Number of samples at which to evaluate an emulator (surrogate)</td>
</tr>
<tr>
<td>Optional</td>
<td>seed</td>
<td></td>
<td>Seed of the random number generator</td>
</tr>
<tr>
<td>Optional</td>
<td>fixed_seed</td>
<td></td>
<td>Reuses the same seed value for multiple random sampling sets</td>
</tr>
<tr>
<td>Optional</td>
<td>max_refinement_iterations</td>
<td></td>
<td>Maximum number of expansion refinement iterations</td>
</tr>
<tr>
<td>Optional</td>
<td>convergence_tolerance</td>
<td></td>
<td>Stopping criterion based on convergence of the objective function or statistics</td>
</tr>
<tr>
<td>Optional</td>
<td>final_moments</td>
<td></td>
<td>Output moments of the specified type and include them within the set of final statistics.</td>
</tr>
<tr>
<td>Optional</td>
<td>p_refinement</td>
<td></td>
<td>Automatic polynomial order refinement</td>
</tr>
<tr>
<td>Optional(Choose One)</td>
<td>askey</td>
<td></td>
<td>Select the standardized random variables (and associated basis polynomials) from the Askey family that best match the user-specified random variables.</td>
</tr>
<tr>
<td>Optional(Choose One)</td>
<td>wiener</td>
<td></td>
<td>Use standard normal random variables (along with Hermite orthogonal basis polynomials) when transforming to a standardized probability space.</td>
</tr>
<tr>
<td><strong>Required (Choose One)</strong></td>
<td><strong>Coefficient estimation approach (Group 2)</strong></td>
<td><strong>quadrature_order_sequence</strong></td>
<td><strong>Order for tensor-products of Gaussian quadrature rules</strong></td>
</tr>
<tr>
<td>--------------------------</td>
<td>-----------------------------------------</td>
<td>-----------</td>
<td>--------------------------------------------------</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Level to use in sparse grid integration or interpolation</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Cubature using Stroud rules and their extensions</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>The (initial) order of a polynomial expansion</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Build a polynomial chaos expansion from simulation samples using orthogonal least interpolation.</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Build a Polynomial Chaos Expansion (PCE) by import coefficients and a multi-index from a file</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Activates global sensitivity analysis based on decomposition of response variance into main, interaction, and total effects</td>
</tr>
</tbody>
</table>

**Optional**

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td><strong>variance_based_decomp</strong></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### Optional (Choose One)

<table>
<thead>
<tr>
<th>Covariance type (Group 3)</th>
<th>diagonal_covariance</th>
<th>full_covariance</th>
</tr>
</thead>
<tbody>
<tr>
<td>Display only the diagonal terms of the covariance matrix</td>
<td>Display the full covariance matrix</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Optional</th>
</tr>
</thead>
<tbody>
<tr>
<td>normalized</td>
</tr>
<tr>
<td>The normalized specification requests output of PCE coefficients that correspond to normalized orthogonal basis polynomials</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Optional</th>
</tr>
</thead>
<tbody>
<tr>
<td>sample_type</td>
</tr>
<tr>
<td>Selection of sampling strategy</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Optional</th>
</tr>
</thead>
<tbody>
<tr>
<td>probability_refinement</td>
</tr>
<tr>
<td>Allow refinement of probability and generalized reliability results using importance sampling</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Optional</th>
</tr>
</thead>
<tbody>
<tr>
<td>import_approx_points_file</td>
</tr>
<tr>
<td>Filename for points at which to evaluate the PCE/SC surrogate</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Optional</th>
</tr>
</thead>
<tbody>
<tr>
<td>export_approx_points_file</td>
</tr>
<tr>
<td>Output file for evaluations of a surrogate model</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Optional</th>
</tr>
</thead>
<tbody>
<tr>
<td>export_expansion_file</td>
</tr>
<tr>
<td>Export the coefficients and multi-index of a Polynomial Chaos Expansion (PCE) to a file</td>
</tr>
</tbody>
</table>
| Optional | reliability_levels | Specify reliability levels at which the response values will be estimated.
| Optional | response_levels | Values at which to estimate desired statistics for each response.
| Optional | distribution | Selection of cumulative or complementary cumulative functions.
| Optional | probability_levels | Specify probability levels at which to estimate the corresponding response value.
| Optional | gen_reliability_levels | Specify generalized reliability levels at which to estimate the corresponding response value.
| Optional | rng | Selection of a random number generator.
| Optional | model_pointer | Identifier for model block to be used by a method.

**Description**

The polynomial chaos expansion (PCE) is a general framework for the approximate representation of random response functions in terms of finite-dimensional series expansions in standardized random variables

\[ R = \sum_{i=0}^{P} \alpha_i \Psi_i(\xi) \]

where \(\alpha_i\) is a deterministic coefficient, \(\Psi_i\) is a multidimensional orthogonal polynomial and \(\xi\) is a vector of standardized random variables. An important distinguishing feature of the methodology is that the functional relationship between random inputs and outputs is captured, not merely the output statistics as in the case of many nondeterministic methodologies.

**Basis polynomial family (Group 1)**

Group 1 keywords are used to select the type of basis, \(\Psi_i\), of the expansion. Three approaches may be employed:
6.2. **METHOD**

- **Wiener**: employs standard normal random variables in a transformed probability space, corresponding to Hermite orthogonal basis polynomials (see [wiener](#)).

- **Askey**: employs standard normal, standard uniform, standard exponential, standard beta, and standard gamma random variables in a transformed probability space, corresponding to Hermite, Legendre, Laguerre, Jacobi, and generalized Laguerre orthogonal basis polynomials, respectively (see [askey](#)).

- **Extended** (default if no option is selected): The Extended option avoids the use of any nonlinear variable transformations by augmenting the Askey approach with numerically-generated orthogonal polynomials for non-Askey probability density functions. Extended polynomial selections replace each of the sub-optimal Askey basis selections for bounded normal, lognormal, bounded lognormal, loguniform, triangular, gumbel, frechet, weibull, and bin-based histogram.

For supporting correlated random variables, certain fallbacks must be implemented.

- The Extended option is the default and supports only Gaussian correlations.

- If needed to support prescribed correlations (not under user control), the Extended and Askey options will fall back to the Wiener option *on a per variable basis*. If the prescribed correlations are also unsupported by Wiener expansions, then Dakota will exit with an error.

Refer to variable support for additional information on supported variable types, with and without correlation.

**Coefficient estimation approach (Group 2)**

To obtain the coefficients $\alpha_i$ of the expansion, seven options are provided:

1. multidimensional integration by a tensor-product of Gaussian quadrature rules (specified with `quadrature-order`, and, optionally, `dimension_preference`).

2. multidimensional integration by the Smolyak sparse grid method (specified with `sparse_grid_level` and, optionally, `dimension_preference`).

3. multidimensional integration by Stroud cubature rules and extensions as specified with `cubature-integrand`.

4. multidimensional integration by Latin hypercube sampling (specified with `expansion_order` and `expansion-samples`).

5. linear regression (specified with `expansion_order` and either `collocation_points` or `collocation-ratio`), using either over-determined (least squares) or under-determined (compressed sensing) approaches.

6. orthogonal least interpolation (specified with `orthogonal_least_interpolation` and `collocation-points`).

7. coefficient import from a file (specified with `import_expansion_file`). The expansion can be comprised of a general set of expansion terms, as indicated by the multi-index annotation within the file.

It is important to note that, while `quadrature_order`, `sparse_grid_level`, and `expansion_order` are array inputs, only one scalar from these arrays is active at a time for a particular expansion estimation. These scalars can be augmented with `dimension_preference` to support anisotropy across the random dimension set. The array inputs are present to support advanced use cases such as multifidelity UQ, where multiple grid resolutions can be employed.

**Active Variables**

The default behavior is to form expansions over aleatory uncertain continuous variables. To form expansions over a broader set of variables, one needs to specify `active` followed by `state`, `epistemic`, `design`, or `all` in the variables specification block.
For continuous design, continuous state, and continuous epistemic uncertain variables included in the expansion, Legendre chaos bases are used to model the bounded intervals for these variables. However, these variables are not assumed to have any particular probability distribution, only that they are independent variables. Moreover, when probability integrals are evaluated, only the aleatory random variable domain is integrated, leaving behind a polynomial relationship between the statistics and the remaining design/state/epistemic variables.

**Covariance type (Group 3)**

These two keywords are used to specify how this method computes, stores, and outputs the covariance of the responses. In particular, the diagonal covariance option is provided for reducing post-processing overhead and output volume in high dimensional applications.

**Optional Keywords regarding method outputs**

Each of these sampling specifications refer to sampling on the PCE approximation for the purposes of generating approximate statistics.

- sample_type
- samples
- seed
- fixed_seed
- rng
- probability_refinement
- distribution
- reliability_levels
- response_levels
- probability_levels
- gen_reliability_levels

which should be distinguished from simulation sampling for generating the PCE coefficients as described in options 4, 5, and 6 above (although these options will share the sample_type, seed, and rng settings, if provided).

When using the probability_refinement control, the number of refinement samples is not under the user’s control (these evaluations are approximation-based, so management of this expense is less critical). This option allows for refinement of probability and generalized reliability results using importance sampling.

**Multifidelity PCE**

The advanced use case of multifidelity UQ using PCE automatically becomes active if the model selected for iteration by the method specification is a multifidelity surrogate model (see hierarchical). In this case, an expansion will first be formed for the low fidelity surrogate model, using the first value within the quadrature_order_sequence, sparse_grid_level_sequence, or expansion_order_sequence (if multiple values are present; the first is reused if not present) along with any specified refinement strategy. Second, expansions are formed for one or more model discrepancies (the difference between response results if additive correction or the ratio of results if multiplicative correction), using all subsequent values in the quadrature_order_sequence, sparse_grid_level_sequence, or expansion_order_sequence along with any specified refinement strategy. The number of discrepancy expansions is determined by the length of the ordered_model_sequence within the hierarchical model specification (see hierarchical). Then each of these expansions are combined (added or multiplied) into an expansion that approximates the high fidelity model, from which the final set of statistics are generated. For polynomial chaos expansions, this high fidelity
expansion can differ significantly in form from the low fidelity and discrepancy expansions, particularly in the multiplicative case where it is expanded to include all of the basis products.

**Multilevel PCE**

Experimental: For the case of regression-based PCE (either least squares or compressed sensing), an optimal sample allocation procedure can be applied for the resolution of each level within a multilevel sampling procedure as in multilevel_sampling. The core difference is that a Monte Carlo estimator of the statistics is replaced with a PCE-based estimator of the statistics, requiring approximation of the variance of these estimators.

Initial prototypes for multilevel PCE can be explored using dakota/test/dakota_uq_diffusion-mlpce.in, and will be stabilized in future releases.

**Usage Tips**

If \( n \) is small (e.g., two or three), then tensor-product Gaussian quadrature is quite effective and can be the preferred choice. For moderate to large \( n \) (e.g., five or more), tensor-product quadrature quickly becomes too expensive and the sparse grid and regression approaches are preferred. Random sampling for coefficient estimation is generally not recommended due to its slow convergence rate. For incremental studies, approaches 4 and 5 support reuse of previous samples through the incremental_lhs and reuse_points specifications, respectively.

In the quadrature and sparse grid cases, growth rates for nested and non-nested rules can be synchronized for consistency. For a non-nested Gauss rule used within a sparse grid, linear one-dimensional growth rules of \( m = 2l + 1 \) are used to enforce odd quadrature orders, where \( l \) is the grid level and \( m \) is the number of points in the rule. The precision of this Gauss rule is then \( i = 2m - 1 = 4l + 1 \). For nested rules, order growth with level is typically exponential; however, the default behavior is to restrict the number of points to be the lowest order rule that is available that meets the one-dimensional precision requirement implied by either a level \( l \) for a sparse grid ( \( i = 4l + 1 \) ) or an order \( m \) for a tensor grid ( \( i = 2m - 1 \) ). This behavior is known as “restricted growth” or “delayed sequences.” To override this default behavior in the case of sparse grids, the unrestricted keyword can be used; it cannot be overridden for tensor grids using nested rules since it also provides a mapping to the available nested rule quadrature orders. An exception to the default usage of restricted growth is the dimension_adaptive_p_refinement generalized sparse grid case described previously, since the ability to evolve the index sets of a sparse grid in an unstructured manner eliminates the motivation for restricting the exponential growth of nested rules.

**Additional Resources**


**Examples**

```plaintext
method,
    polynomial_chaos
    sparse_grid_level = 2
    samples = 10000 seed = 12347 rng rnum2
    response_levels = .1 1. 50. 100. 500. 1000.
    variance_based_decomp
```

**See Also**

These keywords may also be of interest:

- adaptive_sampling
- gpais
- local_reliability
- global_reliability
- sampling
- importance_sampling
- stoch_collocation

samples_on_emulator
- Keywords Area
- method
- polynomial_chaos
- samples_on_emulator

Number of samples at which to evaluate an emulator (surrogate)

Specification
Alias: samples
Argument(s): INTEGER

Description
How many approximate function evaluations to perform on the emulator model, e.g., to compute statistics

Default Behavior
The default number of samples is method-dependent.

Examples
Perform 10000 samples on the PCE approximation of the true model:

```
method
  polynomial_chaos
    quadrature_order  = 2
  samples_on_emulator  = 10000
```

seed
- Keywords Area
- method
- polynomial_chaos
- seed

Seed of the random number generator
6.2. METHOD

Specification

Alias: none
  Argument(s): INTEGER
  Default: system-generated (non-repeatable)

Description

The random seed control provides a mechanism for making a stochastic method repeatable. That is, the use of the same random seed in identical studies will generate identical results.

  Default Behavior
  If not specified, the seed is randomly generated.

  Expected Output
  If seed is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

  Usage Tips
  If a stochastic study was run without seed specified, and the user later wishes to repeat the study using the same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen. That value can then be added to the Dakota input file.

Examples

```
method sampling
  sample_type lhs
  samples = 10
  seed = 15347
```

fixed_seed

- Keywords Area
- method
- polynomial_chaos
- fixed_seed

Reuses the same seed value for multiple random sampling sets

Specification

Alias: none
  Argument(s): none
  Default: not fixed; pattern varies run-to-run

Description

The fixed_seed flag is relevant if multiple sampling sets will be generated over the coarse of a Dakota analysis. This occurs when using advance methods (e.g., surrogate-based optimization, optimization under uncertainty). The same seed value is reused for each of these multiple sampling sets, which can be important for reducing variability in the sampling results.

  Default Behavior
The default behavior is to not use a fixed seed, as the repetition of the same sampling pattern can result in a modeling weakness that an optimizer could potentially exploit (resulting in actual reliabilities that are lower than the estimated reliabilities). For repeatable studies, the seed must also be specified.

**Examples**

```
method
  sampling
    sample_type lhs
    samples = 10
    fixed_seed
```

**max_refinement_iterations**

- Keywords Area
- method
- polynomial_chaos
- max_refinement_iterations

Maximum number of expansion refinement iterations

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** 100

**Description**

Limits the number of times the expansion can be refined under various refinement strategies.

**Examples**

```
method,
  polynomial_chaos
    dimension_adaptive generalized p_refinement
      max_refinement_iterations = 20
      convergence_tol = 1.e-4
      sparse_grid_level = 1
```

**convergence_tolerance**

- Keywords Area
- method
- polynomial_chaos
- convergence_tolerance

Stopping criterion based on convergence of the objective function or statistics
Topics

This keyword is related to the topics:

- method independent controls

Specification

Alias: none

- Argument(s): REAL
- Default: 1.e-4

Description

The convergence_tolerance specification provides a real value for controlling the termination of iteration. For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by convergence_tolerance, then this convergence criterion is satisfied on the current iteration. Therefore, permissible values are between 0 and 1, non-inclusive.

Behavior Varies by Package/Library

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- DOT: must be satisfied for two consecutive iterations
- NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of convergence_tolerance approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., convergence_tolerance = 1.e-6 will result in approximately six digits of accuracy in the final objective function).
- NL2SOL: See nl2sol

final_moments

- Keywords Area
- method
- polynomial_chaos
- final_moments

Output moments of the specified type and include them within the set of final statistics.
Specification

Alias: none

Argument(s): none

Default: standard
### 6.2. METHOD

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group Objective Formulation (Group 1)</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required (Choose One)</td>
<td>none</td>
<td>standard</td>
<td>Omit moments from the set of final statistics.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>central</td>
<td>Output central moments and include them within the set of final statistics.</td>
</tr>
</tbody>
</table>

#### Description

When performing a nested study that may employ moment statistics on the inner loop, it can be desirable to control the type of these moments. The `final_moments` specification supports options of `none`, `standard` (default), or `central`, corresponding to omission of moments, standardized moments (mean, standard deviation, skewness, and excess kurtosis), or central moments (mean, variance, 3rd central, and 4th central).

The presence or omission of moment results in the final statistics influences the outer level mappings in the case of a nested study. For example, `final_moments none` can allow for a more compact specification of primary and/or secondary response mappings.

#### Examples

The following method specification overrides the default to print `central` moments and include them in the set of final statistics.

```dakota
method, sampling
  samples = 50 seed = 1234
  response_levels = 3.6e+11 1.2e+05 3.5e+05
  final_moments central
```

Overriding the default to `none` as follows:

```dakota
method, sampling
  samples = 50 seed = 1234
  response_levels = 3.6e+11 1.2e+05 3.5e+05
  final_moments none
```

allows associated nested model mappings to be simplified from:

```dakota
model
  nested
    sub_method_pointer = ’UQ’
    primary_response_mapping  = 0. 0. 1. 0. 0. 1. 0. 0. 0.
    secondary_response_mapping = 0. 0. 0. 0. 0. 0. 0. 0. 1.
```
to a more compact version focused only on the response level mappings (two leading zeros per response
function for moment mappings have been removed):

```python
model
    nested
        sub_method_pointer = 'UQ'
        primary_response_mapping  = 1. 1. 0.
        secondary_response_mapping = 0. 0. 1.
```

none

- Keywords Area
- method
- polynomial_chaos
- final_moments
- none

Omit moments from the set of final statistics.

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

The omission of moment results from the final statistics can allow for a more compact definition of primary and/or secondary response mappings within a nested model specification.

**Examples**

```python
method,
    sampling
        samples = 50 seed = 1234
        response_levels = 3.6e+11 1.2e+05 3.5e+05
        final_moments none
```

**standard**

- Keywords Area
- method
- polynomial_chaos
- final_moments
- standard

Output standardized moments and include them within the set of final statistics.
6.2. METHOD

Specification

Alias: none
  Argument(s): none

Description

Output standardized moments (mean, standard deviation, skewness, and excess kurtosis) and include the first two within the set of final statistics to be used at a higher level (e.g., optimization under uncertainty, mixed aleatory-epistemic UQ). This inclusion of moment results affects the primary and/or secondary response mappings in a nested model specification.

Examples

The following method specification overrides the default to print central moments and include them in the set of final statistics.

```
method, sampling
  samples = 50 seed = 1234
  response_levels = 3.6e+11 1.2e+05 3.5e+05
  final_moments standard
```

central

- Keywords Area
- method
- polynomial_ chaos
- final_moments
- central

Output central moments and include them within the set of final statistics.

Specification

Alias: none
  Argument(s): none

Description

Output central moments (mean, variance, 3rd central, and 4th central) and include the first two within the set of final statistics to be used at a higher level (e.g., optimization under uncertainty, mixed aleatory-epistemic UQ). This inclusion of moment results affects the primary and/or secondary response mappings in a nested model specification.
CHAPTER 6. KEYWORDS AREA

Examples
The following method specification overrides the default to print central moments and include them in the set of final statistics.

```
method, sampling
  samples = 50 seed = 1234
  response_levels = 3.6e+11 1.2e+05 3.5e+05
  final_moments central
```

**p_refinement**

- Keywords Area
- method
- polynomial_chaos
- p_refinement

Automatic polynomial order refinement

**Specification**

Alias: none

**Argument(s):** none

**Default:** no refinement

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required (Choose One)</td>
<td>p-refinement type (Group 1)</td>
<td>uniform</td>
<td>Refine an expansion uniformly in all dimensions.</td>
</tr>
<tr>
<td>dimension-adaptive</td>
<td>Perform anisotropic expansion refinement by preferentially adapting in dimensions that are detected to have higher ‘importance’.</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Description**

The `p_refinement` keyword specifies the usage of automated polynomial order refinement, which can be either `uniform` or `dimension_adaptive`.

The `dimension_adaptive` option is supported for the tensor-product quadrature and Smolyak sparse grid options and `uniform` is supported for tensor and sparse grids as well as regression approaches (`collocation_points` or `collocation_ratio`).
Each of these refinement cases makes use of the `max_iterations` and `convergence_tolerance` method independent controls. The former control limits the number of refinement iterations, and the latter control terminates refinement when the two-norm of the change in the response covariance matrix (or, in goal-oriented approaches, the two-norm of change in the statistical quantities of interest (QOI)) falls below the tolerance.

The `dimension_adaptive` case can be further specified to utilize `sobol`, `decay`, or `generalized` refinement controls. The former two cases employ anisotropic tensor/sparse grids in which the anisotropic dimension preference (leading to anisotropic integrations/expansions with differing refinement levels for different random dimensions) is determined using either total Sobol’ indices from variance-based decomposition (sobol case: high indices result in high dimension preference) or using spectral coefficient decay rates from a rate estimation technique similar to Richardson extrapolation (decay case: low decay rates result in high dimension preference). In these two cases as well as the `uniform` refinement case, the `quadrature_order` or `sparse_grid_level` are ramped by one on each refinement iteration until either of the two convergence controls is satisfied. For the `uniform` refinement case with regression approaches, the `expansion_order` is ramped by one on each iteration while the oversampling ratio (either defined by `collocation_ratio` or inferred from `collocation_points` based on the initial expansion) is held fixed. Finally, the `generalized dimension_adaptive` case is the default adaptive approach; it refers to the generalized sparse grid algorithm, a greedy approach in which candidate index sets are evaluated for their impact on the statistical QOI, the most influential sets are selected and used to generate additional candidates, and the index set frontier of a sparse grid is evolved in an unstructured and goal-oriented manner (refer to User’s Manual PCE descriptions for additional specifics).

For the case of p-refinement or the case of an explicit nested override, Gauss-Hermite rules are replaced with Genz-Keister nested rules and Gauss-Legendre rules are replaced with Gauss-Patterson nested rules, both of which exchange lower integrand precision for greater point reuse.

**uniform**

- Keywords Area
- method
- polynomial_choas
- p_refinement
- uniform

Refine an expansion uniformly in all dimensions.

**Specification**

Alias: none

Argument(s): none

**Description**

The `quadrature_order` or `sparse_grid_level` are ramped by one on each refinement iteration until either of the two convergence controls is satisfied. For the uniform refinement case with regression approaches, the `expansion_order` is ramped by one on each iteration while the oversampling ratio (either defined by `collocation_ratio` or inferred from `collocation_points` based on the initial expansion) is held fixed.
Perform anisotropic expansion refinement by preferentially adapting in dimensions that are detected to have higher ‘importance’.

**Specification**

**Alias:** none  
**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>required (choose one)</td>
<td>dimension adaptivity estimation approach (Group 1)</td>
<td>sobol</td>
<td>Estimate dimension preference for automated refinement of stochastic expansion using total Sobol’ sensitivity indices.</td>
</tr>
<tr>
<td></td>
<td>decay</td>
<td></td>
<td>Estimate spectral coefficient decay rates to guide dimension-adaptive refinement.</td>
</tr>
<tr>
<td></td>
<td>generalized</td>
<td></td>
<td>Use the generalized sparse grid dimension adaptive algorithm to refine a sparse grid approximation of stochastic expansion.</td>
</tr>
</tbody>
</table>

**Description**

Perform anisotropic expansion refinement by preferentially adapting in dimensions that are detected to hold higher ‘importance’ in resolving statistical quantities of interest.
Dimension importance must be estimated as part of the refinement process. Techniques include either sobol or generalized for stochastic collocation and either sobol, decay, or generalized for polynomial chaos. Each of these automated refinement approaches makes use of the max_iterations and convergence_tolerance iteration controls.

**sobol**
- **Keywords Area**
- **method**
- **polynomial_chaos**
- **p_refinement**
- **dimension_adaptive**
- **sobol**

Estimate dimension preference for automated refinement of stochastic expansion using total Sobol’ sensitivity indices.

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** generalized

**Description**

Determine dimension preference for refinement of a stochastic expansion from the total Sobol’ sensitivity indices obtained from global sensitivity analysis. High indices indicate high importance for resolving statistical quantities of interest and therefore result in high dimension preference.

**Examples**

```plaintext
method,
    polynomial_chaos
    sparse_grid_level = 3
    dimension_adaptive p_refinement sobol
    max_iterations = 20
    convergence_tol = 1.e-4
```

**decay**
- **Keywords Area**
- **method**
- **polynomial_chaos**
- **p_refinement**
- **dimension_adaptive**
- **decay**

Estimate spectral coefficient decay rates to guide dimension-adaptive refinement.
CHAPTER 6. KEYWORDS AREA

Specification
Alias: none
  Argument(s): none

Description
Estimate spectral coefficient decay rates from a rate estimation technique similar to Richardson extrapolation. These decay rates are used to guide dimension-adaptive refinement, where slower decay rates result in higher dimension preference.

Examples
method,
  polynomial_chaos
  sparse_grid_level = 3
  dimension_adaptive p_refinement decay
  max_iterations = 20
  convergence_tol = 1.e-4

  generalized
  • Keywords Area
  • method
  • polynomial_chaos
  • p_refinement
  • dimension_adaptive
  • generalized

  Use the generalized sparse grid dimension adaptive algorithm to refine a sparse grid approximation of stochastic expansion.

Specification
Alias: none
  Argument(s): none

Description
The generalized sparse grid algorithm is a greedy approach in which candidate index sets are evaluated for their impact on the statistical QOI, the most influential sets are selected and used to generate additional candidates, and the index set frontier of a sparse grid is evolved in an unstructured and goal-oriented manner (refer to User’s Manual PCE descriptions for additional specifics).

Examples
method,
  polynomial_chaos
  sparse_grid_level = 3
  dimension_adaptive p_refinement generalized
  max_iterations = 20
  convergence_tol = 1.e-4
6.2. METHOD

askey

- Keywords Area
- method
- polynomial_chaos
- askey

Select the standardized random variables (and associated basis polynomials) from the Askey family that best match the user-specified random variables.

Specification

Alias: none

Argument(s): none

Default: extended (Askey + numerically-generated)

Description

The Askey option employs standard normal, standard uniform, standard exponential, standard beta, and standard gamma random variables in a transformed probability space. These selections correspond to Hermite, Legendre, Laguerre, Jacobi, and generalized Laguerre orthogonal polynomials, respectively.

Specific mappings for the basis polynomials are based on a closest match criterion, and include Hermite for normal (optimal) as well as bounded normal, lognormal, bounded lognormal, gumbel, frechet, and weibull (sub-optimal); Legendre for uniform (optimal) as well as loguniform, triangular, and bin-based histogram (sub-optimal); Laguerre for exponential (optimal); Jacobi for beta (optimal); and generalized Laguerre for gamma (optimal).

See Also

These keywords may also be of interest:

- polynomial_chaos
- wiener

wiener

- Keywords Area
- method
- polynomial_chaos
- wiener

Use standard normal random variables (along with Hermite orthogonal basis polynomials) when transforming to a standardized probability space.
CHAPTER 6. KEYWORDS AREA

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** extended (Askey + numerically-generated)

**Description**

The Wiener option employs standard normal random variables in a transformed probability space, corresponding to a Hermite orthogonal polynomial basis. This is the same nonlinear variable transformation used by local and global reliability methods (and therefore has the same variable support).

**See Also**

These keywords may also be of interest:

- polynomial_chaos
- askey

**quadrature_order_sequence**

- Keywords Area
- method
- polynomial_chaos
- quadrature_order_sequence

Order for tensor-products of Gaussian quadrature rules

**Specification**

**Alias:** none

**Argument(s):** INTEGERLIST

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>dimension_preference</td>
<td>A set of weights specifying the relative importance of each uncertain variable (dimension)</td>
</tr>
</tbody>
</table>
6.2. METHOD

<table>
<thead>
<tr>
<th>Optional(Choose One)</th>
<th>Nesting of quadrature rules (Group 1)</th>
<th>nested</th>
<th>Enforce use of nested quadrature rules if available</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>non_nested</td>
<td></td>
<td>Enforce use of non-nested quadrature rules</td>
</tr>
</tbody>
</table>

**Description**

Multidimensional integration by a tensor-product of Gaussian quadrature rules (specified with `quadrature_order`, and, optionally, `dimension_preference`). The default rule selection is to employ non_nested Gauss rules including Gauss-Hermite (for normals or transformed normals), Gauss-Legendre (for uniforms or transformed uniforms), Gauss-Jacobi (for betas), Gauss-Laguerre (for exponentials), generalized Gauss-Laguerre (for gammas), and numerically-generated Gauss rules (for other distributions when using an Extended basis). For the case of `p.refinement` or the case of an explicit nested override, Gauss-Hermite rules are replaced with Genz-Keister nested rules and Gauss-Legendre rules are replaced with Gauss-Patterson nested rules, both of which exchange lower integrand precision for greater point reuse. By specifying a `dimension_preference`, where higher preference leads to higher order polynomial resolution, the tensor grid may be rendered anisotropic. The dimension specified to have highest preference will be set to the specified `quadrature_order` and all other dimensions will be reduced in proportion to their reduced preference; any non-integral portion is truncated.

To synchronize with tensor-product integration, a tensor-product expansion is used, where the order $p_i$ of the expansion in each dimension is selected to be half of the integrand precision available from the rule in use, rounded down. In the case of non-nested Gauss rules with integrand precision $2m_i - 1$, $p_i$ is one less than the quadrature order $m_i$ in each dimension (a one-dimensional expansion contains the same number of terms, $p + 1$, as the number of Gauss points). The total number of terms, $N$, in a tensor-product expansion involving $n$ uncertain input variables is

$$N = 1 + P = \prod_{i=1}^{n} (p_i + 1)$$

In some advanced use cases (e.g., multifidelity UQ), multiple grid resolutions can be employed; for this reason, the `quadrature_order` specification supports an array input.

**Usage Tips**

For most use cases, this keyword will specify a single integer order. In more advanced UQ studies with hierarchical models, the list of integers can apply to different models and/or model levels.

`dimension_preference`

- Keywords Area
- method
- polynomial_chaos
- `quadrature_order_sequence`
- `dimension_preference`

A set of weights specifying the relative importance of each uncertain variable (dimension)
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none
  Argument(s): REALLIST
  Default: isotropic grids

Description

A set of weights specifying the relative importance of each uncertain variable (dimension). Using this specification leads to anisotropic integrations with differing refinement levels for different random dimensions.

See Also

These keywords may also be of interest:
- sobol
- decay

The keywords may also be of interest:
- Keywords Area
- method
- polynomial_chaos
- quadrature_order_sequence
- nested
  Enforce use of nested quadrature rules if available

Specification

Alias: none
  Argument(s): none
  Default: quadrature: non_nested unless automated refinement; sparse grids: nested

Description

Enforce use of nested quadrature rules if available. For instance if the aleatory variables are Gaussian use the Nested Genz-Keister rule instead of the default non-nested Gauss-Hermite rule variables are non_nested

- Keywords Area
- method
- polynomial_chaos
- quadrature_order_sequence
- non_nested
  Enforce use of non-nested quadrature rules
6.2. METHOD

Specification
Alias: none
Argument(s): none

Description
Enforce use of non-nested quadrature rules if available. For instance if the aleatory variables are Gaussian use the non-nested Gauss-Hermite rule

sparse_grid_level_sequence
- Keywords Area
- method
- polynomial_chaos
- sparse_grid_level_sequence

Level to use in sparse grid integration or interpolation

Specification
Alias: none
Argument(s): INTEGERLIST

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>Choose One</td>
<td>Group 1</td>
<td>restricted</td>
</tr>
<tr>
<td>unrestricted</td>
<td>Override the default restriction of growth rates for nested and non-nested rules that are by default synchronized for consistency.</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### Description

Multi-dimensional integration by the Smolyak sparse grid method (specified with `sparse_grid_level` and, optionally, `dimension_preference`). The underlying one-dimensional integration rules are the same as for the tensor-product quadrature case; however, the default rule selection is nested for sparse grids (Genz-Keister for normals/transformed normals and Gauss-Patterson for uniforms/transformed uniforms). This default can be overridden with an explicit `non_nested` specification (resulting in Gauss-Hermite for normals/transformed normals and Gauss-Legendre for uniforms/transformed uniforms). As for tensor quadrature, the `dimension_preference` specification enables the use of anisotropic sparse grids (refer to the PCE description in the User’s Manual for the anisotropic index set constraint definition). Similar to anisotropic tensor grids, the dimension with greatest preference will have resolution at the full `sparse_grid_level` and all other dimension resolutions will be reduced in proportion to their reduced preference. For PCE with either isotropic or anisotropic sparse grids, a summation of tensor-product expansions is used, where each anisotropic tensor-product quadrature rule underlying the sparse grid construction results in its own anisotropic tensor-product expansion as described in case 1. These anisotropic tensor-product expansions are summed into a sparse PCE using the standard Smolyak summation (again, refer to the User’s Manual for additional details). As for `quadrature_order`, the `sparse_grid_level` specification admits an array input for enabling specification of multiple grid resolutions used by certain advanced solution methodologies.

### Usage Tips

This keyword can be used when using sparse grid integration to calculate PCE coefficients or when generating samples for sparse grid collocation.

For most use cases, this keyword will specify a single integer level. In more advanced UQ studies with hierarchical models, the list of integers can apply to different models and/or model levels.

### restricted

- **Keywords Area**
- **method**
- **polynomial_chaos**
- **sparse_grid_level_sequence**
- **restricted**

Restrict the growth rates for nested and non-nested rules can be synchronized for consistency.
6.2. METHOD

Specification

Alias: none
Argument(s): none
Default: restricted (except for generalized sparse grids)

Description

In the quadrature and sparse grid cases, growth rates for nested and non-nested rules can be synchronized for consistency. For a non-nested Gauss rule used within a sparse grid, linear one-dimensional growth rules of \( m = 2l + 1 \) are used to enforce odd quadrature orders, where \( l \) is the grid level and \( m \) is the number of points in the rule. The precision of this Gauss rule is then \( i = 2m - 1 = 4l + 1 \). For nested rules, order growth with level is typically exponential; however, the default behavior is to restrict the number of points to be the lowest order rule that is available that meets the one-dimensional precision requirement implied by either a level \( l \) for a sparse grid \( (i = 4l + 1) \) or an order \( m \) for a tensor grid \( (i = 2m - 1) \). This behavior is known as "restricted growth" or "delayed sequences." To override this default behavior in the case of sparse grids, the unrestricted keyword can be used; it cannot be overridden for tensor grids using nested rules since it also provides a mapping to the available nested rule quadrature orders. An exception to the default usage of restricted growth is the dimension_adaptive p refinement generalized sparse grid case described previously, since the ability to evolve the index sets of a sparse grid in an unstructured manner eliminates the motivation for restricting the exponential growth of nested rules.

unrestricted

- Keywords Area
- method
- polynomial_chaos
- sparse_grid_level_sequence
- unrestricted

Override the default restriction of growth rates for nested and non-nested rules that are by default synchronized for consistency.

Specification

Alias: none
Argument(s): none

Description

In the quadrature and sparse grid cases, growth rates for nested and non-nested rules can be synchronized for consistency. For a non-nested Gauss rule used within a sparse grid, linear one-dimensional growth rules of \( m = 2l + 1 \) are used to enforce odd quadrature orders, where \( l \) is the grid level and \( m \) is the number of points in the rule. The precision of this Gauss rule is then \( i = 2m - 1 = 4l + 1 \). For nested rules, order growth with level is typically exponential; however, the default behavior is to restrict the number of points to be the lowest order rule that is available that meets the one-dimensional precision requirement implied by either a level \( l \) for a sparse grid \( (i = 4l + 1) \) or an order \( m \) for a tensor grid \( (i = 2m - 1) \). This behavior is known as "restricted growth" or "delayed sequences." To override this default behavior in the case of sparse grids, the unrestricted keyword can be used; it cannot be overridden for tensor grids using nested rules since it also provides a mapping to the available
nested rule quadrature orders. An exception to the default usage of restricted growth is the dimension Adaptive p-
.refinement generalized sparse grid case described previously, since the ability to evolve the index sets of a sparse
grid in an unstructured manner eliminates the motivation for restricting the exponential growth of nested rules.

dimension_preference

- Keywords Area
- method
- polynomial_choas
- sparse_grid_level_sequence
- dimension_preference

A set of weights specifying the relative importance of each uncertain variable (dimension)

Specification

Alias: none
Argument(s): REALLIST
Default: isotropic grids

Description

A set of weights specifying the relative importance of each uncertain variable (dimension). Using this specification
leads to anisotropic integrations with differing refinement levels for different random dimensions.

See Also

These keywords may also be of interest:
- sobol
- decay

nested

- Keywords Area
- method
- polynomial_choas
- sparse_grid_level_sequence
- nested

Enforce use of nested quadrature rules if available

Specification

Alias: none
Argument(s): none
Default: quadrature: non_nested unless automated refinement; sparse grids: nested
6.2. METHOD

Description

Enforce use of nested quadrature rules if available. For instance if the aleatory variables are Gaussian use the Nested Genz-Keister rule instead of the default non-nested Gauss-Hermite rule variables are non_nested

- Keywords Area
- method
- polynomial_chaos
- sparse_grid_level_sequence
- non_nested

Enforce use of non-nested quadrature rules

Specification

Alias: none
Argument(s): none

Description

Enforce use of non-nested quadrature rules if available. For instance if the aleatory variables are Gaussian use the non-nested Gauss-Hermite rule

cubature_integrand

- Keywords Area
- method
- polynomial_chaos
- cubature_integrand

Cubature using Stroud rules and their extensions

Specification

Alias: none
Argument(s): INTEGER
CHAPTER 6. KEYWORDS AREA

Description

Multi-dimensional integration by Stroud cubature rules [77] and extensions [91], as specified with `cubature-integrand`. A total-order expansion is used, where the isotropic order \( p \) of the expansion is half of the integrand order, rounded down. The total number of terms \( N \) for an isotropic total-order expansion of order \( p \) over \( n \) variables is given by

\[
N = 1 + P = 1 + \sum_{s=1}^{p} \frac{1}{s!} \prod_{r=0}^{s-1} (n + r) = \frac{(n + p)!}{n!p!}
\]

Since the maximum integrand order is currently five for normal and uniform and two for all other types, at most second- and first-order expansions, respectively, will be used. As a result, cubature is primarily useful for global sensitivity analysis, where the Sobol’ indices will provide main effects and, at most, two-way interactions. In addition, the random variable set must be independent and identically distributed (\( iid \)), so the use of `askey` or `wiener` transformations may be required to create \( iid \) variable sets in the transformed space (as well as to allow usage of the higher order cubature rules for normal and uniform). Note that global sensitivity analysis often assumes uniform bounded regions, rather than precise probability distributions, so the \( iid \) restriction would not be problematic in that case.

expansion_order_sequence

- Keywords Area
- method
- polynomial_chaos
- expansion_order_sequence

The (initial) order of a polynomial expansion

Specification

Alias: none

<table>
<thead>
<tr>
<th>Argument(s): INTEGERLIST</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required/-Optional</td>
</tr>
<tr>
<td>Description of Group</td>
</tr>
<tr>
<td>Dakota Keyword</td>
</tr>
<tr>
<td>Dakota Keyword Description</td>
</tr>
<tr>
<td>dimension_preference</td>
</tr>
</tbody>
</table>
6.2. METHOD

### Required (Choose One)

<table>
<thead>
<tr>
<th>Optional</th>
<th>Required (Choose One)</th>
<th>Group 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>basis_type</td>
<td>collocation_points_sequence</td>
<td>Specify the type of truncation to be used with a Polynomial Chaos Expansion. Number of collocation points to estimate PCE coefficients</td>
</tr>
<tr>
<td>collocation_points_sequence</td>
<td>collocation_ratio</td>
<td>Set the number of points used to build a PCE via regression to be proportional to the number of terms in the expansion.</td>
</tr>
<tr>
<td>expansion_samples_sequence</td>
<td></td>
<td>Number of simulation samples to estimate the PCE coefficients</td>
</tr>
<tr>
<td>import_build-points_file</td>
<td></td>
<td>File containing points you wish to use to build a surrogate</td>
</tr>
</tbody>
</table>

### Description

When the expansion_order for a polynomial chaos expansion is specified, the coefficients may be computed by integration based on random samples or by regression using either random or sub-sampled tensor product quadrature points.

Multidimensional integration by Latin hypercube sampling (specified with `expansion_samples`). In this case, the expansion order $p$ cannot be inferred from the numerical integration specification and it is necessary to provide an `expansion_order` to specify $p$ for a total-order expansion.

Linear regression (specified with either `collocation_points` or `collocation_ratio`). A total-order expansion is used and must be specified using `expansion_order` as described in the previous option. To avoid requiring the user to calculate $N$ from $n$ and $p$), the `collocation_ratio` allows for specification of a constant factor applied to $N$ (e.g., `collocation_ratio = 2`, produces samples $= 2N$). In addition, the default linear relationship with $N$ can be overridden using a real-valued exponent specified using `ratio_order`. In this case, the number of samples becomes $cN^o$ where $c$ is the `collocation_ratio` and $o$ is the `ratio_order`. The `use_derivatives` flag informs the regression approach to include derivative matching equations (limited to gradients at present) in the least squares solutions, enabling the use of fewer collocation points for a given expansion order and dimension (number of points required becomes $\frac{cN^o}{n+1}$). When admissible, a constrained least squares approach is employed in which response values are first reproduced exactly and error in reproducing response derivatives is minimized. Two collocation grid options are supported: the default is Latin hypercube sampling (“point collocation”), and an alternate approach of “probabilistic collocation” is also available through inclusion of the `tensor_grid` keyword. In this alternate case, the collocation grid is defined using a subset of
tensor-product quadrature points: the order of the tensor-product grid is selected as one more than the expansion order in each dimension (to avoid sampling at roots of the basis polynomials) and then the tensor multi-index is uniformly sampled to generate a non-repeated subset of tensor quadrature points.

If `collocation_points` or `collocation_ratio` is specified, the PCE coefficients will be determined by regression. If no regression specification is provided, appropriate defaults are defined. Specifically SVD-based least-squares will be used for solving over-determined systems and under-determined systems will be solved using LASSO. For the situation when the number of function values is smaller than the number of terms in a PCE, but the total number of samples including gradient values is greater than the number of terms, the resulting over-determined system will be solved using equality constrained least squares. Technical information on the various methods listed below can be found in the Linear regression section of the Theory Manual. Some of the regression methods (OMP, LASSO, and LARS) are able to produce a set of possible PCE coefficient vectors (see the Linear regression section in the Theory Manual). If cross validation is inactive, then only one solution, consistent with the noise_tolerance, will be returned. If cross validation is active, Dakota will choose between possible coefficient vectors found internally by the regression method across the set of expansion orders (1,...,expansion_order) and the set of specified noise tolerances and return the one with the lowest cross validation error indicator.

**Usage Tips**

For most use cases, this keyword will specify a single integer order. In more advanced UQ studies with hierarchical models, the list of integers can apply to different models and/or model levels.

dimension_preference

- Keywords Area
- method
- polynomial_chaos
- expansion_order_sequence
- dimension_preference

A set of weights specifying the relative importance of each uncertain variable (dimension).

**Specification**

Alias: none  
**Argument(s):** REALLIST  
**Default:** isotropic grids

**Description**

A set of weights specifying the relative importance of each uncertain variable (dimension). Using this specification leads to anisotropic integrations with differing refinement levels for different random dimensions.

**See Also**

These keywords may also be of interest:

- `sobol`
- `decay`
6.2. METHOD

basis_type

- Keywords Area
- method
- polynomial_chaos
- expansion_order_sequence
- basis_type

Specify the type of truncation to be used with a Polynomial Chaos Expansion.

**Specification**

**Alias:** none
**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Required (Choose One)</strong></td>
<td>Group 1</td>
<td>tensor_product</td>
<td>Use a tensor-product index set to construct a polynomial chaos expansion.</td>
</tr>
<tr>
<td>total_order</td>
<td></td>
<td></td>
<td>Use a total-order index set to construct a polynomial chaos expansion.</td>
</tr>
<tr>
<td>adapted</td>
<td></td>
<td></td>
<td>Use adaptive basis selection to choose the basis terms in a polynomial chaos expansion.</td>
</tr>
</tbody>
</table>

**Description**

Specify the type of truncation to be used with a Polynomial Chaos Expansion.

**tensor_product**

- Keywords Area
- method
- polynomial_chaos
- expansion_order_sequence
- basis_type
- tensor_product

Use a tensor-product index set to construct a polynomial chaos expansion.
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none
  Argument(s): none

Description

Use a tensor-product index set to construct a polynomial chaos expansion. That is for a given order \( p \) keep all terms with \( d \)-dimensional multi index \( \mathbf{i} = (i_1, \ldots, i_d) \) that satisfies
\[
\max(i_1, \ldots, i_d) \leq p
\]

**total_order**
- Keywords Area
- method
- polynomial_chaos
- expansion_order_sequence
- basis_type
- total_order

Use a total-order index set to construct a polynomial chaos expansion.

Specification

Alias: none
  Argument(s): none

Description

Use the traditional total-order index set to construct a polynomial chaos expansion. That is for a given order \( p \) keep all terms with a \( d \)-dimensional multi index \( \mathbf{i} = (i_1, \ldots, i_d) \) that satisfies
\[
\sum_{k=1}^{d} i_k \leq p
\]

**adapted**
- Keywords Area
- method
- polynomial_chaos
- expansion_order_sequence
- basis_type
- adapted

Use adaptive basis selection to choose the basis terms in a polynomial chaos expansion.
6.2. **METHOD**

### Specification

**Alias:** none  
**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Optional</th>
<th>Description of</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>Group</td>
<td>advancements</td>
<td>soft_convergence_limit</td>
<td>The maximum number of steps used to expand a basis step. The maximum number of times no improvement in cross validation error is allowed before the algorithm is terminated.</td>
</tr>
</tbody>
</table>

### Description

Use adaptive basis selection to choose the basis terms in a polynomial chaos expansion. Basis selection uses compressed sensing to identify a initial set of non zero PCE coefficients. Then these non-zero terms are expanded a set number of times (we suggest 3) and compressed sensing is then applied to these three new index sets. Cross validation is used to choose the best candidate basis. The best basis is then restricted again to the non-zero terms and expanded until no improvement can be gained by adding additional terms.

- **Advancements**
  - **Keywords Area**
  - **method**
  - **polynomial_choa**
  - **expansion_order_sequence**
  - **basis_type**
  - **adapted**
  - **advancements**

  The maximum number of steps used to expand a basis step.

### Specification

**Alias:** none  
**Argument(s):** INTEGER
Description

Use adaptive basis selection to choose the basis terms in a polynomial chaos expansion. Basis selection uses compressed sensing to identify a initial set of non zero PCE coefficients. Then these non-zero terms are expanded a set number of times (we suggest 3) and compressed sensing is then applied to these three new index sets. Cross validation is used to choose the best candidate basis. The best basis is then restricted again to the non-zero terms and expanded until no improvement can be gained by adding additional terms.

**soft_convergence_limit**

- Keywords Area
- method
- polynomial_chaos
- expansion_order_sequence
- basis_type
- adapted
- soft_convergence_limit

The maximum number of times no improvement in cross validation error is allowed before the algorithm is terminated.

Specification

Alias: none

Argument(s): INTEGER

Description

Use adaptive basis selection to choose the basis terms in a polynomial chaos expansion. Basis selection uses compressed sensing to identify a initial set of non zero PCE coefficients. Then these non-zero terms are expanded a set number of times (we suggest 3) and compressed sensing is then applied to these three new index sets. Cross validation is used to choose the best candidate basis. The best basis is then restricted again to the non-zero terms and expanded until no improvement can be gained by adding additional terms.

**collocation_points_sequence**

- Keywords Area
- method
- polynomial_chaos
- expansion_order_sequence
- collocation_points_sequence

Number of collocation points to estimate PCE coefficients
6.2. METHOD

Specification

Alias: none

Argument(s): INTEGERLIST
<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional (Choose One)</td>
<td>Group 1</td>
<td>ratio_order</td>
<td>Specify a non-linear relationship between the expansion order of a polynomial chaos expansion and the number of samples that will be used to compute the PCE coefficients. Compute the coefficients of a polynomial expansion using least squares.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>least_squares</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>orthogonal_matching_pursuit</td>
<td>Compute the coefficients of a polynomial expansion using orthogonal matching pursuit (OMP).</td>
</tr>
<tr>
<td></td>
<td></td>
<td>basis_pursuit</td>
<td>Compute the coefficients of a polynomial expansion by solving the Basis Pursuit $\ell_1$-minimization problem using linear programming.</td>
</tr>
</tbody>
</table>
### 6.2. METHOD

<table>
<thead>
<tr>
<th>Technique</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>basis_pursuit_denoising</strong></td>
<td>Compute the coefficients of a polynomial expansion by solving the Basis Pursuit Denoising ( \ell_1 )-minimization problem using second order cone optimization.</td>
</tr>
<tr>
<td><strong>least_angle_regression</strong></td>
<td>Compute the coefficients of a polynomial expansion by using the greedy least angle regression (LAR) method.</td>
</tr>
<tr>
<td><strong>least_absolute_shrinkage</strong></td>
<td>Compute the coefficients of a polynomial expansion by using the LASSO problem.</td>
</tr>
<tr>
<td><strong>cross_validation</strong></td>
<td>Use cross validation to choose the 'best' polynomial order of a polynomial chaos expansion. Use derivative data to construct surrogate models.</td>
</tr>
<tr>
<td><strong>use_derivatives</strong></td>
<td>Use sub-sampled tensor-product quadrature points to build a polynomial chaos expansion.</td>
</tr>
<tr>
<td><strong>tensor_grid</strong></td>
<td></td>
</tr>
</tbody>
</table>
CHAPTER 6. KEYWORDS AREA

| Optional | reuse_points | This describes the behavior of reuse of points in constructing polynomial chaos expansion models. Number of iterations allowed for optimizers and adaptive UQ methods |
| Optional | max_iterations | Maximum iterations in determining polynomial coefficients |
| Optional | max_solver_iterations |

**Description**

Specify the number of collocation points used to estimate PCE coefficients using regression or orthogonal-least-interpolation.

**Usage Tips**

For most use cases, this keyword will specify a single integer number of points. In more advanced UQ studies with hierarchical models, the list of integers can apply to different models and/or model levels.

**ratio_order**

- Keywords Area
- method
- polynomial_chaos
- expansion_order_sequence
- collocation_points_sequence
- ratio_order

Specify a non-linear the relationship between the expansion order of a polynomial chaos expansion and the number of samples that will be used to compute the PCE coefficients.

**Specification**

Alias: none

Argument(s): REAL

Default: 1.
6.2. METHOD

Description

When using regression type methods (specified with either collocation_points or collocation_ratio), a total-order expansion can be specified using expansion_order. To avoid requiring the user to calculate N from n and p, the collocation_ratio allows for specification of a constant factor applied to N (e.g., collocation_ratio = 2. produces samples = 2N). In addition, the default linear relationship with N can be overridden using a real-valued exponent specified using ratio_order. In this case, the number of samples becomes $cN^o$ where $c$ is the collocation_ratio and $o$ is the ratio_order.

least_squares

- Keywords Area
- method
- polynomial_chaos
- expansion_order_sequence
- collocation_points_sequence
- least_squares

Compute the coefficients of a polynomial expansion using least squares

Specification

Alias: none
Argument(s): none
Default: svd

<table>
<thead>
<tr>
<th>Required/-Optional/Optional/Choose One</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Group 1</td>
<td>svd</td>
<td>Calculate the coefficients of a polynomial chaos expansion using the singular value decomposition.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>equality_-constrained</td>
<td>Calculate the coefficients of a polynomial chaos expansion using equality constrained least squares.</td>
</tr>
</tbody>
</table>

Description

Compute the coefficients of a polynomial expansion using least squares. Specifically SVD-based least-squares will be used for solving over-determined systems. For the situation when the number of function values is smaller than the number of terms in a PCE, but the total number of samples including gradient values is greater than the number of terms, the resulting over-determined system will be solved using equality constrained least squares.
CHAPTER 6. KEYWORDS AREA

svd
  • Keywords Area
  • method
  • polynomial_chaos
  • expansion_order_sequence
  • collocation_points_sequence
  • least_squares
  • svd

Calculate the coefficients of a polynomial chaos expansion using the singular value decomposition.

Specification
Alias: none
Argument(s): none

Description
Calculate the coefficients of a polynomial chaos expansion using the singular value decomposition. When the number of model runs exceeds the number of terms in the PCE, the solution returned will be the least-squares solution, otherwise the solution will be the minimum norm solution computed using the pseudo-inverse.

equality_constrained
  • Keywords Area
  • method
  • polynomial_chaos
  • expansion_order_sequence
  • collocation_points_sequence
  • least_squares
  • equality_constrained

Calculate the coefficients of a polynomial chaos expansion using equality constrained least squares.

Specification
Alias: none
Argument(s): none

Description
Calculate the coefficients of a polynomial chaos expansion using equality constrained least squares.
6.2. METHOD

orthogonal_matching_pursuit

• Keywords Area
• method
• polynomial_chaos
• expansion_order_sequence
• collocation_points_sequence
• orthogonal_matching_pursuit

Compute the coefficients of a polynomial expansion using orthogonal matching pursuit (OMP)

Specification

Alias: omp
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>noise_tolerance</td>
<td>noise_tolerance</td>
<td>The noise tolerance used when performing cross validation in the presence of noise or truncation errors.</td>
</tr>
</tbody>
</table>

Description

Compute the coefficients of a polynomial expansion using orthogonal matching pursuit (OMP). Orthogonal matching pursuit (OMP) is a greedy algorithm that is useful when solving underdetermined linear systems.

noise_tolerance

• Keywords Area
• method
• polynomial_chaos
• expansion_order_sequence
• collocation_points_sequence
• orthogonal_matching_pursuit
• noise_tolerance

The noise tolerance used when performing cross validation in the presence of noise or truncation errors.
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): REALLIST

Default: 1e-3 for BPDN, 0. otherwise (algorithms run until termination)

Description

The noise tolerance used when performing cross validation in the presence of noise or truncation errors.

basis_pursuit

- Keywords Area
- method
- polynomial_chaos
- expansion_order_sequence
- collocation_points_sequence
- basis_pursuit

Compute the coefficients of a polynomial expansion by solving the Basis Pursuit $\ell_1$-minimization problem using linear programming.

Specification

Alias: bp

Argument(s): none

Description

Compute the coefficients of a polynomial expansion by solving the Basis Pursuit $\ell_1$-minimization problem using linear programming.

basis_pursuit_denoising

- Keywords Area
- method
- polynomial_chaos
- expansion_order_sequence
- collocation_points_sequence
- basis_pursuit_denoising

Compute the coefficients of a polynomial expansion by solving the Basis Pursuit Denoising $\ell_1$-minimization problem using second order cone optimization.

Specification

Alias: bpdn

Argument(s): none
6.2. METHOD

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<tbody>
<tr>
<td>Optional</td>
<td>noise_tolerance</td>
<td>noise_tolerance</td>
<td>The noise tolerance used when performing cross validation in the presence of noise or truncation errors.</td>
</tr>
</tbody>
</table>

**Description**

Compute the coefficients of a polynomial expansion by solving the Basis Pursuit Denoising $\ell_1$-minimization problem using second order cone optimization.

noise_tolerance
- Keywords Area
  - method
  - polynomial_chaos
  - expansion_order_sequence
  - collocation_points_sequence
  - basis_pursuit_denoising
  - noise_tolerance

The noise tolerance used when performing cross validation in the presence of noise or truncation errors.

**Specification**

Alias: none

Argument(s): REALLIST

Default: 1e-3 for BPDN, 0. otherwise (algorithms run until termination)

**Description**

The noise tolerance used when performing cross validation in the presence of noise or truncation errors.

least_angle_regression
- Keywords Area
  - method
  - polynomial_chaos
  - expansion_order_sequence
  - collocation_points_sequence
  - least_angle_regression

Compute the coefficients of a polynomial expansion by using the greedy least angle regression (LAR) method.
CHAPTER 6. KEYWORDS AREA

Specification

Alias: lars
Argument(s): none

<table>
<thead>
<tr>
<th>Required/Optional Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>noise_tolerance</td>
<td></td>
<td>noise_tolerance</td>
<td>The noise tolerance used when performing cross validation in the presence of noise or truncation errors.</td>
</tr>
</tbody>
</table>

Description

Compute the coefficients of a polynomial expansion by using the greedy least angle regression (LAR) method.

noise_tolerance

- Keywords Area
- method
- polynomial_chaos
- expansion_order_sequence
- collocation_points_sequence
- least_angle_regression
- noise_tolerance

The noise tolerance used when performing cross validation in the presence of noise or truncation errors.

Specification

Alias: none
Argument(s): REALLIST
Default: 1e-3 for BPDN, 0. otherwise (algorithms run until termination)

Description

The noise tolerance used when performing cross validation in the presence of noise or truncation errors.

least_absolute_shrinkage

- Keywords Area
- method
- polynomial_chaos
6.2. METHOD

- expansion_order_sequence
- collocation_points_sequence
- least_absolute_shrinkage

Compute the coefficients of a polynomial expansion by using the LASSO problem.

Specification

Alias: lasso

Argument(s): none

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>noise_tolerance</td>
<td>The noise tolerance used when performing cross validation in the presence of noise or truncation errors.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>l2_penalty</td>
<td>The $l_2$ penalty used when performing compressed sensing with elastic net.</td>
</tr>
</tbody>
</table>

Description

Compute the coefficients of a polynomial expansion by using the LASSO problem.

noise_tolerance

- Keywords Area
- method
- polynomial_chaos
- expansion_order_sequence
- collocation_points_sequence
- least_absolute_shrinkage
- noise_tolerance

The noise tolerance used when performing cross validation in the presence of noise or truncation errors.

Specification

Alias: none

Argument(s): REALLIST
Default: 1e-3 for BPDN, 0. otherwise (algorithms run until termination)
Description
The noise tolerance used when performing cross validation in the presence of noise or truncation errors.

\texttt{l2\_penalty}
- Keywords Area
- method
- polynomial\_chaos
- expansion\_order\_sequence
- collocation\_points\_sequence
- least\_absolute\_shrinkage
- l2\_penalty

The \(l_2\) penalty used when performing compressed sensing with elastic net.

Specification
Alias: none
Argument(s): REAL
Default: 0. (reverts to standard LASSO formulation)

Description
The \(l_2\) penalty used when performing compressed sensing with elastic net.

\texttt{cross\_validation}
- Keywords Area
- method
- polynomial\_chaos
- expansion\_order\_sequence
- collocation\_points\_sequence
- cross\_validation

Use cross validation to choose the ‘best’ polynomial order of a polynomial chaos expansion.

Specification
Alias: none
Argument(s): none
### Description

Use cross validation to choose the 'best' polynomial degree of a polynomial chaos expansion. 10 fold cross validation is used to estimate the cross validation error of a total-order polynomial expansion for orders 1 through to order. The order chosen is the one that produces the lowest cross validation error. If there are not enough points to perform 10 fold cross validation then one-at-a-time cross validation will be performed.

**noise_only**

- **Keywords Area**
- **method**
- **polynomial_choas**
- **expansion_order_sequence**
- **collocation_points_sequence**
- **cross_validation**
- **noise_only**

Restrict the cross validation process to estimating only the best noise tolerance.

### Specification

**Alias:** none

**Argument(s):** none

**Default:** false

### Description

By default, cross validation estimates both the best noise tolerance and the best candidate basis order. For reasons of reducing computational cost by reducing the number of candidate solves, the user may wish to restrict this process to estimating only the best noise tolerance.

Generally speaking, computing the best noise tolerance through cross validation mitigates issues with overfitting the data. Computing the best candidate basis order can also mitigate overfitting, while also controlling levels of mutual coherence resulting from high-order Vandermonde-like matrix systems.
CHAPTER 6. KEYWORDS AREA

use_derivatives

- Keywords Area
- method
- polynomial_chaos
- expansion_order_sequence
- collocation_points_sequence
- use_derivatives

Use derivative data to construct surrogate models

**Specification**

Alias: none

Argument(s): none

Default: use function values only

**Description**

The `use_derivatives` flag specifies that any available derivative information should be used in global approximation builds, for those global surrogate types that support it (currently, polynomial regression and the Surfpack Gaussian process).

However, it’s use with Surfpack Gaussian process is not recommended.

tensor_grid

- Keywords Area
- method
- polynomial_chaos
- expansion_order_sequence
- collocation_points_sequence
- tensor_grid

Use sub-sampled tensor-product quadrature points to build a polynomial chaos expansion.

**Specification**

Alias: none

Argument(s): none

Default: regression with LHS sample set (point collocation)
6.2. **METHOD**

**Description**

The collocation grid is defined using a subset of tensor-product quadrature points: the order of the tensor-product grid is selected as one more than the expansion order in each dimension (to avoid sampling at roots of the basis polynomials) and then the tensor multi-index is uniformly sampled to generate a non-repeated subset of tensor quadrature points.

**reuse_points**

- **Keywords Area**
- **method**
- **polynomial_chaos**
- **expansion_order_sequence**
- **collocation_points_sequence**
- **reuse_points**

This describes the behavior of reuse of points in constructing polynomial chaos expansion models.

**Specification**

**Alias:** reuse_samples

**Argument(s):** none

**Default:** no sample reuse in coefficient estimation

**Description**

The **reuse_points** option controls the reuse behavior of points for various types of polynomial chaos expansions, including: collocation_points, collocation_ratio, expansion_samples, or orthogonal_least_interpolation. If any of these approaches are specified to create a set of points for the polynomial chaos expansion, one can specify **reuse_points** so that any points that have been previously generated (for example, from the import_points file) can be reused.

**max_iterations**

- **Keywords Area**
- **method**
- **polynomial_chaos**
- **expansion_order_sequence**
- **collocation_points_sequence**
- **max_iterations**

Number of iterations allowed for optimizers and adaptive UQ methods.
**Topics**

This keyword is related to the topics:

- `method_independent_controls`

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** 100 (exceptions: `fsu_cvt`, `local_reliability`: 25; `global_{reliability, interval_est, evidence}` / `efficient-global`: 25\(\ast n\))

**Description**

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed `max_iterations` iterations. See also `max_function_evaluations`.

**Default Behavior**

Default value is 100.

`max_solver_iterations`

- **Keywords Area**
- **method**
- **polynomial_chaos**
- **expansion_order_sequence**
- **collocation_points_sequence**
- **max_solver_iterations**

Maximum iterations in determining polynomial coefficients

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** 100

**Description**

When using an iterative polynomial coefficient estimation approach, e.g., cross-validation-based solvers, limits the maximum iterations in the coefficient solver.
collocation_ratio

- Keywords Area
- method
- polynomial_chaos
- expansion_order_sequence
- collocation_ratio

Set the number of points used to build a PCE via regression to be proportional to the number of terms in the expansion.

**Specification**

**Alias:** none  
**Argument(s):** REAL

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>ratio_order</td>
<td>Specify a non-linear the relationship between the expansion order of a polynomial chaos expansion and the number of samples that will be used to compute the PCE coefficients.</td>
</tr>
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</table>

<table>
<thead>
<tr>
<th>Optional(Choose One)</th>
<th>Group 1</th>
<th>least_squares</th>
</tr>
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<tbody>
<tr>
<td></td>
<td></td>
<td>least squares</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Optional</th>
<th>Group 1</th>
<th>orthogonal_matching_pursuit</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Compute the coefficients of a polynomial expansion using orthogonal matching pursuit (OMP)</td>
</tr>
<tr>
<td><strong>basis_pursuit</strong></td>
<td>Compute the coefficients of a polynomial expansion by solving the Basis Pursuit $\ell_1$-minimization problem using linear programming.</td>
<td></td>
</tr>
<tr>
<td><strong>basis_pursuit_denoising</strong></td>
<td>Compute the coefficients of a polynomial expansion by solving the Basis Pursuit Denoising $\ell_1$-minimization problem using second order cone optimization.</td>
<td></td>
</tr>
<tr>
<td><strong>least_angle_regression</strong></td>
<td>Compute the coefficients of a polynomial expansion by using the greedy least angle regression (LAR) method.</td>
<td></td>
</tr>
<tr>
<td><strong>least_absolute_shrinkage</strong></td>
<td>Compute the coefficients of a polynomial expansion by using the LASSO problem.</td>
<td></td>
</tr>
<tr>
<td><strong>Optional</strong></td>
<td>Use cross validation to choose the ‘best’ polynomial order of a polynomial chaos expansion.</td>
<td></td>
</tr>
</tbody>
</table>
### Optional

<table>
<thead>
<tr>
<th>use_derivatives</th>
<th>Optional use derivative data to construct surrogate models</th>
</tr>
</thead>
<tbody>
<tr>
<td>tensor_grid</td>
<td>Use sub-sampled tensor-product quadrature points to build a polynomial chaos expansion.</td>
</tr>
<tr>
<td>reuse_points</td>
<td>This describes the behavior of reuse of points in constructing polynomial chaos expansion models.</td>
</tr>
<tr>
<td>max_iterations</td>
<td>Number of iterations allowed for optimizers and adaptive UQ methods</td>
</tr>
<tr>
<td>max_solver_iterations</td>
<td>Maximum iterations in determining polynomial coefficients</td>
</tr>
</tbody>
</table>

### Description

Set the number of points used to build a PCE via regression to be proportional to the number of terms in the expansion. To avoid requiring the user to calculate N from n and p, the collocation_ratio allows for specification of a constant factor applied to N (e.g., collocation\_ratio = 2. produces samples = 2N). In addition, the default linear relationship with N can be overridden using a real-valued exponent specified using ratio\_order. In this case, the number of samples becomes \(cN^o\) where \(c\) is the collocation\_ratio and \(o\) is the ratio\_order. The use\_derivatives flag informs the regression approach to include derivative matching equations (limited to gradients at present) in the least squares solutions, enabling the use of fewer collocation points for a given expansion order and dimension (number of points required becomes \(\frac{cN^o}{n+1}\)).

#### ratio\_order

- Keywords Area
- method
- polynomial\_chaos
- expansion\_order\_sequence
- collocation\_ratio
• **ratio_order**

Specify a non-linear the relationship between the expansion order of a polynomial chaos expansion and the number of samples that will be used to compute the PCE coefficients.

**Specification**

Alias: none

**Argument(s):** REAL

**Default:** 1.

**Description**

When using regression type methods (specified with either collocation_points or collocation_ratio), a total-order expansion can be specified using expansion_order. To avoid requiring the user to calculate \( N \) from \( n \) and \( p \), the collocation_ratio allows for specification of a constant factor applied to \( N \) (e.g., collocation_ratio = 2 produces samples = 2N). In addition, the default linear relationship with \( N \) can be overridden using a real-valued exponent specified using ratio_order. In this case, the number of samples becomes \( cN^{o} \) where \( c \) is the collocation_ratio and \( o \) is the ratio_order.

**least_squares**

• Keywords Area

• method

• polynomial_chaos

• expansion_order_sequence

• collocation_ratio

• least_squares

Compute the coefficients of a polynomial expansion using least squares

**Specification**

Alias: none

**Argument(s):** none

**Default:** svd
### Description

Compute the coefficients of a polynomial expansion using least squares. Specifically SVD-based least-squares will be used for solving over-determined systems. For the situation when the number of function values is smaller than the number of terms in a PCE, but the total number of samples including gradient values is greater than the number of terms, the resulting over-determined system will be solved using equality constrained least squares.

svd

- Keywords Area
- method
- polynomial\_chaos
- expansion\_order\_sequence
- collocation\_ratio
- least\_squares
- svd

Calculate the coefficients of a polynomial chaos expansion using the singular value decomposition.

### Specification

**Alias:** none

**Argument(s):** none

### Description

Calculate the coefficients of a polynomial chaos expansion using the singular value decomposition. When the number of model runs exceeds the number of terms in the PCE, the solution returned will be the least-squares solution, otherwise the solution will be the minimum norm solution computed using the pseudo-inverse.
equality_constrained

- Keywords Area
- method
- polynomial_chaos
- expansion_order_sequence
- collocation_ratio
- least_squares
- equality_constrained

Calculate the coefficients of a polynomial chaos expansion using equality constrained least squares.

**Specification**

*Alias:* none
  *Argument(s):* none

**Description**

Calculate the coefficients of a polynomial chaos expansion using equality constrained least squares.

**orthogonal_matching_pursuit**

- Keywords Area
- method
- polynomial_chaos
- expansion_order_sequence
- collocation_ratio
- orthogonal_matching_pursuit

Compute the coefficients of a polynomial expansion using orthogonal matching pursuit (OMP)

**Specification**

*Alias:* omp
  *Argument(s):* none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>noise_tolerance</td>
<td></td>
<td>The noise tolerance used when performing cross validation in the presence of noise or truncation errors.</td>
</tr>
</tbody>
</table>


6.2. **METHOD**

**Description**

Compute the coefficients of a polynomial expansion using orthogonal matching pursuit (OMP). Orthogonal matching pursuit (OMP) is a greedy algorithm that is useful when solving underdetermined linear systems.

**noise_tolerance**

- **Keywords Area**
- **method**
- **polynomial_chaos**
- **expansion_order_sequence**
- **collocation_ratio**
- **orthogonal_matching_pursuit**
- **noise_tolerance**

The noise tolerance used when performing cross validation in the presence of noise or truncation errors.

**Specification**

**Alias:** none

**Argument(s):** REALLIST

**Default:** 1e-3 for BPDN, 0. otherwise (algorithms run until termination)

**Description**

The noise tolerance used when performing cross validation in the presence of noise or truncation errors.

**basis_pursuit**

- **Keywords Area**
- **method**
- **polynomial_chaos**
- **expansion_order_sequence**
- **collocation_ratio**
- **basis_pursuit**

Compute the coefficients of a polynomial expansion by solving the Basis Pursuit $\ell_1$-minimization problem using linear programming.

**Specification**

**Alias:** bp

**Argument(s):** none
CHAPTER 6. KEYWORDS AREA

Description
Compute the coefficients of a polynomial expansion by solving the Basis Pursuit $\ell_1$-minimization problem using linear programming.

basis_pursuit_denoising
- Keywords Area
- method
- polynomial_chaos
- expansion_order_sequence
- collocation_ratio
- basis_pursuit_denoising

Compute the coefficients of a polynomial expansion by solving the Basis Pursuit Denoising $\ell_1$-minimization problem using second order cone optimization.

Specification
Alias: bpdn
Argument(s): none

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>noise_tolerance</td>
<td>noise_tolerance</td>
<td>The noise tolerance used when performing cross validation in the presence of noise or truncation errors.</td>
</tr>
</tbody>
</table>

Description
Compute the coefficients of a polynomial expansion by solving the Basis Pursuit Denoising $\ell_1$-minimization problem using second order cone optimization.

noise_tolerance
- Keywords Area
- method
- polynomial_chaos
- expansion_order_sequence
- collocation_ratio
- basis_pursuit_denoising
- noise_tolerance

The noise tolerance used when performing cross validation in the presence of noise or truncation errors.
6.2. METHOD

Specification

Alias: none

Argument(s): REALIST

Default: 1e-3 for BPDN, 0. otherwise (algorithms run until termination)

Description

The noise tolerance used when performing cross validation in the presence of noise or truncation errors.

least_angle_regression

- Keywords Area
- method
- polynomial_chaos
- expansion_order_sequence
- collocation_ratio
- least_angle_regression

Compute the coefficients of a polynomial expansion by using the greedy least angle regression (LAR) method.

Specification

Alias: lars

Argument(s): none

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
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<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>noise_tolerance</td>
<td></td>
<td>noise_tolerance</td>
<td>The noise tolerance used when performing cross validation in the presence of noise or truncation errors.</td>
</tr>
</tbody>
</table>

Description

Compute the coefficients of a polynomial expansion by using the greedy least angle regression (LAR) method.

noise_tolerance

- Keywords Area
- method
- polynomial_chaos
- expansion_order_sequence
• collocation_ratio
• least_angle_regression
• noise_tolerance

The noise tolerance used when performing cross validation in the presence of noise or truncation errors.

**Specification**

**Alias:** none

**Argument(s):** REALLIST

**Default:** 1e-3 for BPDN, 0. otherwise (algorithms run until termination)

**Description**

The noise tolerance used when performing cross validation in the presence of noise or truncation errors.

**least_absolute_shrinkage**

• Keywords Area
• method
• polynomial_chaos
• expansion_order_sequence
• collocation_ratio
• least_absolute_shrinkage

Compute the coefficients of a polynomial expansion by using the LASSO problem.

**Specification**

**Alias:** lasso

**Argument(s):** none
6.2. METHOD

Optional | l2_penalty | The $l_2$ penalty used when performing compressed sensing with elastic net.

**Description**

Compute the coefficients of a polynomial expansion by using the LASSO problem.

```
noise_tolerance
```

- Keywords Area
- method
- polynomial_chaos
- expansion_order_sequence
- collocation_ratio
- least_absolute_shrinkage
- noise_tolerance

The noise tolerance used when performing cross validation in the presence of noise or truncation errors.

**Specification**

Alias: none

Argument(s): REALLIST

Default: 1e-3 for BPDN, 0. otherwise (algorithms run until termination)

**Description**

The noise tolerance used when performing cross validation in the presence of noise or truncation errors.

```
l2_penalty
```

- Keywords Area
- method
- polynomial_chaos
- expansion_order_sequence
- collocation_ratio
- least_absolute_shrinkage
- l2_penalty

The $l_2$ penalty used when performing compressed sensing with elastic net.
CHAPTER 6. KEYWORDS AREA

**Specification**

Alias: none

Argument(s): REAL

Default: 0. (reverts to standard LASSO formulation)

**Description**

The $l_2$ penalty used when performing compressed sensing with elastic net.

cross_validation

- Keywords Area
- method
- polynomial.chaos
- expansion_order_sequence
- collocation_ratio
- cross.validation

Use cross validation to choose the 'best' polynomial order of a polynomial chaos expansion.

**Specification**

Alias: none

Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>noise_only</td>
<td></td>
<td></td>
<td>Restrict the cross validation process to estimating only the best noise tolerance.</td>
</tr>
</tbody>
</table>

**Description**

Use cross validation to choose the 'best' polynomial degree of a polynomial chaos expansion. 10 fold cross validation is used to estimate the cross validation error of a total-order polynomial expansion for orders 1 through to order. The order chosen is the one that produces the lowest cross validation error. If there are not enough points to perform 10 fold cross validation then one-at-a-time cross validation will be performed.

noise_only

- Keywords Area
- method
- polynomial.chaos
6.2. METHOD

- expansion_order_sequence
- collocation_ratio
- cross_validation
- noise_only

Restrict the cross validation process to estimating only the best noise tolerance.

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** false

**Description**

By default, cross validation estimates both the best noise tolerance and the best candidate basis order. For reasons of reducing computational cost by reducing the number of candidate solves, the user may wish to restrict this process to estimating only the best noise tolerance.

Generally speaking, computing the best noise tolerance through cross validation mitigates issues with overfitting the data. Computing the best candidate basis order can also mitigate overfitting, while also controlling levels of mutual coherence resulting from high-order Vandermonde-like matrix systems.

**use_derivatives**

- Keywords Area
- method
- polynomial_chaos
- expansion_order_sequence
- collocation_ratio
- use_derivatives

Use derivative data to construct surrogate models

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** use function values only

**Description**

The **use_derivatives** flag specifies that any available derivative information should be used in global approximation builds, for those global surrogate types that support it (currently, polynomial regression and the Surfpack Gaussian process).

However, it’s use with Surfpack Gaussian process is not recommended.
Use sub-sampled tensor-product quadrature points to build a polynomial chaos expansion.

**Specification**

**Alias:** none

- **Argument(s):** none
- **Default:** regression with LHS sample set (point collocation)

**Description**

The collocation grid is defined using a subset of tensor-product quadrature points: the order of the tensor-product grid is selected as one more than the expansion order in each dimension (to avoid sampling at roots of the basis polynomials) and then the tensor multi-index is uniformly sampled to generate a non-repeated subset of tensor quadrature points.

This describes the behavior of reuse of points in constructing polynomial chaos expansion models.

**Specification**

**Alias:** reuse_samples

- **Argument(s):** none
- **Default:** no sample reuse in coefficient estimation
6.2. METHOD

Description

The `reuse_points` option controls the reuse behavior of points for various types of polynomial chaos expansions, including: `collocation_points`, `collocation_ratio`, `expansion_samples`, or `orthogonal_least_interpolation`. If any of these approaches are specified to create a set of points for the polynomial chaos expansion, one can specify `reuse_points` so that any points that have been previously generated (for example, from the `import_points` file) can be reused.

**max_iterations**

- **Keywords Area**
- **method**
- **polynomial_chaos**
- **expansion_order_sequence**
- **collocation_ratio**
- **max_iterations**

Number of iterations allowed for optimizers and adaptive UQ methods

Topics

This keyword is related to the topics:

- **method_independent_controls**

Specification

**Alias:** none  
**Argument(s):** INTEGER  
**Default:** 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence} / efficient_global: 25*n)

Description

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed `max_iterations` iterations. See also `max_function_evaluations`.

**Default Behavior**

Default value is 100.

**max_solver_iterations**

- **Keywords Area**
- **method**
- **polynomial_chaos**
- **expansion_order_sequence**
• collocation_ratio
• max_solver_iterations

Maximum iterations in determining polynomial coefficients

Specification
Alias: none
Argument(s): INTEGER
Default: 100

Description
When using an iterative polynomial coefficient estimation approach, e.g., cross-validation-based solvers, limits the maximum iterations in the coefficient solver.

expansion_samples_sequence
• Keywords Area
• method
• polynomial_chaos
• expansion_order_sequence
• expansion_samples_sequence

Number of simulation samples to estimate the PCE coefficients

Specification
Alias: none
Argument(s): INTEGERLIST

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>reuse_points</td>
<td>This describes the behavior of reuse of points in constructing polynomial chaos expansion models.</td>
</tr>
</tbody>
</table>
### Description

In this case, the expansion order p cannot be inferred from the numerical integration specification and it is necessary to provide an expansion order to specify p for a total-order expansion.

**Usage Tips**

For most use cases, this keyword will specify a single integer number of samples. In more advanced UQ studies with hierarchical models, the list of integers can apply to different models and/or model levels.

- `reuse_points`

  - **Keywords Area**
  - **method**
  - **polynomial_chaos**
  - **expansion_order_sequence**
  - **expansion_samples_sequence**
  - **reuse_points**

  This describes the behavior of reuse of points in constructing polynomial chaos expansion models.

### Specification

**Alias:** `reuse_samples`

**Argument(s):** none

**Default:** no sample reuse in coefficient estimation

### Description

The `reuse_points` option controls the reuse behavior of points for various types of polynomial chaos expansions, including: `collocation_points`, `collocation_ratio`, `expansion_samples`, or `orthogonal_least_interpolation`. If any of these approaches are specified to create a set of points for the polynomial chaos expansion, one can specify `reuse_points` so that any points that have been previously generated (for example, from the `import_points` file) can be reused.
incremental_lhs

- Keywords Area
- method
- polynomial_chaos
- expansion_order_sequence
- expansion_samples_sequence
- incremental_lhs

(Deprecated keyword) Augments an existing Latin Hypercube Sampling (LHS) study

**Specification**

Alias: none

Argument(s): none

Default: no sample reuse in coefficient estimation

**Description**

This keyword is deprecated. Instead specify `sample_type lhs` with `refinement_samples`.

An incremental random sampling approach will augment an existing random sampling study with refinement_samples to get better estimates of mean, variance, and percentiles. The number of refinement_samples in each refinement level must result in twice the number of previous samples.

Typically, this approach is used when you have an initial study with sample size N1 and you want to perform an additional N1 samples. Ideally, a Dakota restart file containing the initial N1 samples, so only N1 (instead of 2 x N1) potentially expensive function evaluations will be performed.

This process can be extended by repeatedly doubling the `refinement_samples`:

```plaintext
method
sampling
  seed = 1337
  samples = 50
  refinement_samples = 50 100 200 400 800
```

**Usage Tips**

The incremental approach is useful if it is uncertain how many simulations can be completed within available time.

See the examples below and the Usage and Restarting Dakota Studies pages.

**Examples**

Suppose an initial study is conducted using `sample_type lhs` with `samples = 50`. A follow-on study uses a new input file where `samples = 50`, and `refinement_samples = 50`, resulting in 50 reused samples (from restart) and 50 new random samples. The 50 new samples will be combined with the 50 previous samples to generate a combined sample of size 100 for the analysis.

One way to ensure the restart file is saved is to specify a non-default name, via a command line option:

```plaintext
dakota -input LHS_50.in -write_restart LHS_50.rst
```

which uses the input file:
6.2. METHOD

# LHS_50.in

environment
tabular_data
  tabular_data_file = ‘LHS_50.dat’

method
  sampling
    seed = 1337
    sample_type lhs
    samples = 50

model
  single

variables
  uniform_uncertain = 2
  descriptors = ‘input1’ ‘input2’
  lower_bounds = -2.0 -2.0
  upper_bounds = 2.0 2.0

interface
  analysis_drivers ‘text_book’
  fork

responses
  response_functions = 1
  no_gradients
  no_hessians

and the restart file is written to LHS_50.rst.

Then an incremental LHS study can be run with:

dakota -input LHS_100.in -read_restart LHS_50.rst -write_restart LHS_100.rst

where LHS_100.in is shown below, and LHS_50.rst is the restart file containing the results of the previous LHS study. In the example input files for the initial and incremental studies, the values for seed match. This ensures that the initial 50 samples generated in both runs are the same.

# LHS_100.in

environment
tabular_data
  tabular_data_file = ‘LHS_100.dat’

method
  sampling
    seed = 1337
    sample_type incremental_lhs
    samples = 50
    refinement_samples = 50

model
  single

variables
  uniform_uncertain = 2
  descriptors = ‘input1’ ‘input2’
  lower_bounds = -2.0 -2.0
  upper_bounds = 2.0 2.0

interface
  analysis_drivers ‘text_book’
The user will get 50 new LHS samples which maintain both the correlation and stratification of the original LHS sample. The new samples will be combined with the original samples to generate a combined sample of size 100.

**import_build_points_file**
- **Keywords Area**
- **method**
- **polynomial_chaos**
- **expansion_order_sequence**
- **import_build_points_file**

File containing points you wish to use to build a surrogate

### Specification

**Alias:** import_points_file  
**Argument(s):** STRING  
**Default:** no point import from a file

<table>
<thead>
<tr>
<th>Required/- Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional (Choose One)</td>
<td>Tabular Format (Group 1)</td>
<td>annotated</td>
<td>Selects annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>custom_annotated</td>
<td>Selects custom-annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>freeform</td>
<td>Selects freeform file format</td>
</tr>
<tr>
<td>Optional</td>
<td>active_only</td>
<td></td>
<td>Import only active variables from tabular data file</td>
</tr>
</tbody>
</table>

### Description

The `import_build_points_file` allows the user to specify a file that contains a list of points and truth model responses used to construct a surrogate model. These can be used by all methods that (explicitly, e.g. surrogate-based optimization, or implicitly, e.g. efficient global optimization) operate on a surrogate. In particular, these
points and responses are used in place of truth model evaluations to construct the initial surrogate. When used to construct surrogate models or emulators these are often called build points or training data.

**Default Behavior**
By default, methods do not import points from a file.

**Usage Tips**
Dakota parses input files without regard to whitespace, but the import_build_points_file must be in one of three formats:

- annotated (default)
- custom_annotated
- freeform

**Examples**

```dakota
method
  polynomial_chaos
    expansion_order = 4
    import_build_points_file = 'dakota_uq_rosenbrock_pce_import.annot.pts.dat'
```

**annotated**

- **Keywords Area**
- **method**
- **polynomial_chaos**
- **expansion_order_sequence**
- **import_build_points_file**
- **annotated**

Selects annotated tabular file format

**Topics**

This keyword is related to the topics:

- file_formats

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** annotated format
CHAPTER 6. KEYWORDS AREA

Description

An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior

By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips

• To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify custom_annotated header eval_id

• Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

• When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

• Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
annotated
```

Resulting tabular file:

```
%eval_id interface x1   x2    obj_fn nln_ineq_con_1 nln_ineq_con_2
1  NO_ID       0.9   1.1  0.0002  0.26      0.76
2  NO_ID       0.90009 1.1   0.000196404857 0.2601620081 0.759955
3  NO_ID       0.89991 1.1   0.0002003604863 0.2598380081 0.760045
...
```

custom_annotated

• Keywords Area

• method

• polynomial_chaos

• expansion_order_sequence

• import_build_points_file

• custom_annotated

Selects custom-annotated tabular file format
6.2. METHOD

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none

Argument(s): none

Default: annotated format

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>header</td>
<td>Enable header row in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>eval_id</td>
<td>Enable evaluation ID column in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>interface_id</td>
<td>Enable interface ID column in custom-annotated tabular file</td>
</tr>
</tbody>
</table>

Description

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

Default Behavior

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

Usage Tips

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:
environment
  tabular_data
  tabular_data_file = 'dakota_summary.dat'
  custom_annotated header eval_id

Resulting tabular file:

<table>
<thead>
<tr>
<th>eval_id</th>
<th>x1</th>
<th>x2</th>
<th>obj_fn</th>
<th>nln_ineq_con_1</th>
<th>nln_ineq_con_2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.9</td>
<td>1.1</td>
<td>0.0002</td>
<td>0.26</td>
<td>0.76</td>
</tr>
<tr>
<td>2</td>
<td>0.90009</td>
<td>1.1</td>
<td>0.0001996404857</td>
<td>0.2601620081</td>
<td>0.759955</td>
</tr>
<tr>
<td>3</td>
<td>0.89991</td>
<td>1.1</td>
<td>0.0002003604863</td>
<td>0.2598380081</td>
<td>0.760045</td>
</tr>
<tr>
<td>...</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

header
  - Keywords Area
  - method
  - polynomial_chaos
  - expansion_order_sequence
  - import_build_points_file
  - custom_annotated
  - header

Enable header row in custom-annotated tabular file

Specification

Alias: none
  Argument(s): none
  Default: no header

Description

See description of parent custom_annotated

eval_id
  - Keywords Area
  - method
  - polynomial_chaos
  - expansion_order_sequence
  - import_build_points_file
  - custom_annotated
  - eval_id

Enable evaluation ID column in custom-annotated tabular file
6.2. METHOD

Specification

Alias: none
  Argument(s): none
  Default: no eval_id column

Description

See description of parent custom.annotated

interface_id
  - Keywords Area
  - method
  - polynomial_chaos
  - expansion_order_sequence
  - import_build_points_file
  - custom.annotated
  - interface_id

Enable interface ID column in custom-annotated tabular file

Specification

Alias: none
  Argument(s): none
  Default: no interface_id column

Description

See description of parent custom.annotated

freeform
  - Keywords Area
  - method
  - polynomial_chaos
  - expansion_order_sequence
  - import_build_points_file
  - freeform

Selects freeform file format
Topics
This keyword is related to the topics:

- file_formats

Specification
Alias: none
Argument(s): none
Default: annotated format

Description
A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior
The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips

- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples
Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
freeform
```

Resulting tabular file:

```
0.9 1.1 0.0002 0.26 0.76
0.90009 1.1 0.0001996404857 0.2601620081 0.759955
0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...
```
6.2. METHOD

**active_only**

- Keywords Area
- method
- polynomial_chaos
- expansion_order_sequence
- import_build_points_file
- active_only

Import only active variables from tabular data file

**Topics**

This keyword is related to the topics:

- file_formats

**Specification**

Alias: none

Argument(s): none

**Description**

By default, files for tabular data imports are expected to contain columns for all variables, active and inactive. The keyword `active_only` indicates that the file to import contains only the active variables.

This option should only be used in contexts where the inactive variables have no influence, for example, building a surrogate over active variables, with the state variables held at nominal. It should not be used in more complex nested contexts, where the values of inactive variables are relevant to the function evaluations used to build the surrogate.

**orthogonal_least_interpolation**

- Keywords Area
- method
- polynomial_chaos
- orthogonal_least_interpolation

Build a polynomial chaos expansion from simulation samples using orthogonal least interpolation.

**Specification**

Alias: least_interpolation_oli

Argument(s): none
### Description

Build a polynomial chaos expansion from simulation samples using orthogonal least interpolation. Unlike the other regression methods `expansion_order` cannot be set. OLI will produce the lowest degree polynomial that interpolates the data

**collocation_points_sequence**

- **Keywords Area**
- **method**
- **polynomial_chaos**
- **orthogonal_least_interpolation**
- **collocation_points_sequence**

 Specify the number of collocation points used to estimate PCE coefficients using orthogonal least interpolation

### Specification

**Alias:** none  
**Argument(s):** INTEGERLIST
6.2. METHOD

Description
Specify the number of collocation points used to estimate PCE coefficients using orthogonal least interpolation

tensor_grid
- Keywords Area
- method
- polynomial_chaos
- orthogonal_least_interpolation
- tensor_grid

Use sub-sampled tensor-product quadrature points to build a polynomial chaos expansion.

Specification
Alias: none
Argument(s): INTEGERLIST
Default: regression with LHS sample set (point collocation)

Description
The collocation grid is defined using a subset of tensor-product quadrature points: the order of the tensor-product grid is selected as one more than the expansion order in each dimension (to avoid sampling at roots of the basis polynomials) and then the tensor multi-index is uniformly sampled to generate a non-repeated subset of tensor quadrature points.

reuse_points
- Keywords Area
- method
- polynomial_chaos
- orthogonal_least_interpolation
- reuse_points

This describes the behavior of reuse of points in constructing polynomial chaos expansion models.

Specification
Alias: reuse_samples
Argument(s): none
Default: no sample reuse in coefficient estimation
CHAPTER 6. KEYWORDS AREA

Description

The `reuse_points` option controls the reuse behavior of points for various types of polynomial chaos expansions, including: `collocation_points`, `collocation_ratio`, `expansion_samples`, or `orthogonal_least_interpolation`. If any of these approaches are specified to create a set of points for the polynomial chaos expansion, one can specify `reuse_points` so that any points that have been previously generated (for example, from the `import_points_file`) can be reused.

import_build_points_file

- **Keywords Area**
- **method**
- **polynomial_chaos**
- **orthogonal_least_interpolation**
- **import_build_points_file**

File containing points you wish to use to build a surrogate

Specification

**Alias:** `import_points_file`

**Argument(s):** STRING

**Default:** no point import from a file

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword annotated</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional (Choose One)</td>
<td>Tabular Format (Group 1)</td>
<td><code>custom_annotated</code></td>
<td>Selects custom-annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td><code>freeform</code></td>
<td>Selects freeform file format</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td><code>active_only</code></td>
<td>Import only active variables from tabular data file</td>
</tr>
</tbody>
</table>

Description

The `import_build_points_file` allows the user to specify a file that contains a list of points and truth model responses used to construct a surrogate model. These can be used by all methods that (explicitly, e.g. surrogate-based optimization, or implicitly, e.g. efficient global optimization) operate on a surrogate. In particular, these points and responses are used in place of truth model evaluations to construct the initial surrogate. When used to construct surrogate models or emulators these are often called build points or training data.

**Default Behavior**
6.2. METHOD

By default, methods do not import points from a file.

Usage Tips
Dakota parses input files without regard to whitespace, but the import_build_points_file must be in one of three formats:

- annotated (default)
- custom_annotated
- freeform

Examples

```plaintext
method
  polynomial_chaos
    expansion_order = 4
    import_build_points_file = 'dakota_uq_rosenbrock_pce_import.annot.pts.dat'
```

annotated

- Keywords Area
- method
- polynomial_chaos
- orthogonal_least_interpolation
- import_build_points_file
- annotated
  Selects annotated tabular file format

Topics
This keyword is related to the topics:

- file_formats

Specification

Alias: none

Argument(s): none

Default: annotated format

Description

An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior
By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips
• To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify `custom.annotated` header eval_id.

• Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

• When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

• Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

**Examples**

Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
  tabular_data_file = 'dakota_summary.dat'
  annotated

Resulting tabular file:

```
%eval_id interface x1 x2 obj_fn nln_ineq_con_1 nln_ineq_con_2
1   NO_ID   0.9 1.1  0.0002    0.26 0.76
2   NO_ID  0.90009 1.1  0.0001996404857 0.2601620081 0.759955
3   NO_ID  0.89991 1.1  0.0002003604863 0.2598380081 0.760045
...
```

**custom.annotated**

• **Keywords Area**

• **method**

• **polynomial.chaos**

• **orthogonal.least.interpolation**

• **import.build_points_file**

• **custom.annotated**

Selects custom-annotated tabular file format

**Topics**

This keyword is related to the topics:

• **file_formats**

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** annotated format
### Description

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether `header` row, `eval_id` column, and `interface_id` column appear in the tabular file, thus bridging freeform and (fully) annotated.

**Default Behavior**

The `annotated` format is the default for tabular export/import. To control which header row and columns are in the input/output, specify `custom_annotated`, followed by options, in the relevant export/import context.

**Usage Tips**

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to `annotated` format, though `freeform` remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the `freeform` option.

### Examples

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and `eval_id` (no `interface_id`), and data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
custom_annotated header eval_id
```

Resulting tabular file:

```plaintext
<table>
<thead>
<tr>
<th>eval_id</th>
<th>x1</th>
<th>x2</th>
<th>obj_fn</th>
<th>lnlncon1</th>
<th>lnlncon2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.9</td>
<td>1.1</td>
<td>0.0002</td>
<td>0.26</td>
<td>0.76</td>
</tr>
<tr>
<td>2</td>
<td>0.90009</td>
<td>1.1</td>
<td>0.0001996404857</td>
<td>0.2601620081</td>
<td>0.759955</td>
</tr>
<tr>
<td>3</td>
<td>0.89991</td>
<td>1.1</td>
<td>0.0002003604863</td>
<td>0.2598380081</td>
<td>0.760045</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
</tbody>
</table>
```
CHAPTER 6. KEYWORDS AREA

header

- Keywords Area
- method
- polynomial_chaos
- orthogonal_least_interpolation
- import_build_points_file
- custom_annotated
- header

Enable header row in custom-annotated tabular file

**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** no header

**Description**

See description of parent `custom_annotated`

**eval_id**

- Keywords Area
- method
- polynomial_chaos
- orthogonal_least_interpolation
- import_build_points_file
- custom_annotated
- eval_id

Enable evaluation ID column in custom-annotated tabular file

**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** no eval_id column

**Description**

See description of parent `custom_annotated`
interface_id

- Keywords Area
- method
- polynomial_chaos
- orthogonal_least_interpolation
- import_build_points_file
- custom_annotated
- interface_id

Enable interface ID column in custom-annotated tabular file

**Specification**

*Alias:* none

*Argument(s):* none

*Default:* no interface_id column

**Description**

See description of parent custom_annotated

**freeform**

- Keywords Area
- method
- polynomial_chaos
- orthogonal_least_interpolation
- import_build_points_file
- freeform

Selects freeform file format

**Topics**

This keyword is related to the topics:

- file_formats

**Specification**

*Alias:* none

*Argument(s):* none

*Default:* annotated format
CHAPTER 6. KEYWORDS AREA

Description

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior

The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips

- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```
environment
  tabular_data
    tabular_data_file = 'dakota_summary.dat'
    freeform
```

Resulting tabular file:

```
0.9 1.1 0.0002 0.26 0.76
0.90009 1.1 0.0001996404857 0.2601620081 0.759955
0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...
```

active_only

- Keywords Area
- method
- polynomial_chaos
- orthogonal_least_interpolation
- import_build_points_file
- active_only

Import only active variables from tabular data file

Topics

This keyword is related to the topics:

- file_formats
6.2. METHOD

Specification

Alias: none
Argument(s): none

Description

By default, files for tabular data imports are expected to contain columns for all variables, active and inactive. The keyword `active_only` indicates that the file to import contains only the active variables.

This option should only be used in contexts where the inactive variables have no influence, for example, building a surrogate over active variables, with the state variables held at nominal. It should not be used in more complex nested contexts, where the values of inactive variables are relevant to the function evaluations used to build the surrogate.

`import_expansion_file`

- Keywords Area
- method
- polynomial_chaos
- import_expansion_file

Build a Polynomial Chaos Expansion (PCE) by import coefficients and a multi-index from a file

Specification

Alias: none
Argument(s): STRING

Description

The coefficients can be specified in an arbitrary order. The multi-index provided is used to generate a sparse expansion that consists only of the indices corresponding to the non-zero coefficients provided in the file.

`variance_based_decomp`

- Keywords Area
- method
- polynomial_chaos
- variance_based_decomp

Activates global sensitivity analysis based on decomposition of response variance into main, interaction, and total effects

Specification

Alias: none
Argument(s): none
Default: no variance-based decomposition
**Description**

Dakota can calculate sensitivity indices through variance-based decomposition using the keyword `variance_based_decomp`. This approach decomposes main, interaction, and total effects in order to identify the most important variables and combinations of variables in contributing to the variance of output quantities of interest.

**Default Behavior**

Because of processing overhead and output volume, `variance_based_decomp` is inactive by default, unless required for dimension-adaptive refinement using Sobol’ indices.

**Expected Outputs**

When `variance_based_decomp` is specified, sensitivity indices for main effects, total effects, and any interaction effects will be reported. Each of these effects represents the percent contribution to the variance in the model response, where main effects include the aggregated set of univariate terms for each individual variable, interaction effects represent the set of mixed terms (the complement of the univariate set), and total effects represent the complete set of terms (univariate and mixed) that contain each individual variable. The aggregated set of main and interaction sensitivity indices will sum to one, whereas the sum of total effects sensitivity indices will be greater than one due to redundant counting of mixed terms.

**Usage Tips**

An important consideration is that the number of possible interaction terms grows exponentially with dimension and expansion order. To mitigate this, both in terms of compute time and output volume, possible interaction effects are suppressed whenever no contributions are present due to the particular form of an expansion. In addition, the `interaction_order` and `drop_tolerance` controls can further limit the computational and output requirements.

**Examples**

```
method,
  polynomial_chaos # or stoch_collocation
  sparse_grid_level = 3
  variance_based_decomp interaction_order = 2
```

**Theory**

In this context, we take sensitivity analysis to be global, not local as when calculating derivatives of output variables with respect to input variables. Our definition is similar to that of[73]: “The study of how uncertainty in the output of a model can be apportioned to different sources of uncertainty in the model input.”
6.2. METHOD

Variance based decomposition is a way of using sets of samples to understand how the variance of the output behaves, with respect to each input variable. A larger value of the sensitivity index, $S_i$, means that the uncertainty in the input variable $i$ has a larger effect on the variance of the output. More details on the calculations and interpretation of the sensitivity indices can be found in[87].

**interaction_order**
- Keywords Area
- method
- polynomial_chaos
- variance_based_decomp
- interaction_order

Specify the maximum number of variables allowed in an interaction when reporting interaction metrics.

**Specification**

Alias: none

Argument(s): INTEGER

Default: Unrestricted (VBD includes all interaction orders present in the expansion)

**Description**

The interaction_order option has been added to allow suppression of higher-order interactions, since the output volume (and memory and compute consumption) of these results could be extensive for high dimensional problems (note: the previous univariate_effects specification is equivalent to interaction_order = 1 in the current specification). Similar to suppression of interactions is the covariance control, which can be selected to be diagonal_covariance or full_covariance, with the former supporting suppression of the off-diagonal covariance terms (to again save compute and memory resources and reduce output volume).

**drop_tolerance**
- Keywords Area
- method
- polynomial_chaos
- variance_based_decomp
- drop_tolerance

Suppresses output of sensitivity indices with values lower than this tolerance.

**Specification**

Alias: none

Argument(s): REAL

Default: All VBD indices displayed
Description

The `drop_tolerance` keyword allows the user to specify a value below which sensitivity indices generated by `variance_based_decomp` are not displayed.

**Default Behavior**

By default, all sensitivity indices generated by `variance_based_decomp` are displayed.

**Usage Tips**

For `polynomial_chaos`, which outputs main, interaction, and total effects by default, the `univariate_effects` may be a more appropriate option. It allows suppression of the interaction effects since the output volume of these results can be prohibitive for high dimensional problems. Similar to suppression of these interactions is the covariance control, which can be selected to be `diagonal_covariance` or `full_covariance`, with the former supporting suppression of the off-diagonal covariance terms (to save compute and memory resources and reduce output volume).

**Examples**

```plaintext
method,
sampling
  sample_type lhs
  samples = 100
  variance_based_decomp
drop_tolerance = 0.001
```

diagonal_covariance

- **Keywords Area**
- **method**
- **polynomial_chaos**
- **diagonal_covariance**

Display only the diagonal terms of the covariance matrix

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** diagonal_covariance for response vector > 10; else full_covariance

**Description**

With a large number of responses, the covariance matrix can be very large. `diagonal_covariance` is used to suppress the off-diagonal covariance terms (to save compute and memory resources and reduce output volume).

**full_covariance**

- **Keywords Area**
- **method**
- **polynomial_chaos**
6.2. METHOD

- full_covariance

Display the full covariance matrix

Specification

Alias: none

Argument(s): none

Description

With a large number of responses, the covariance matrix can be very large. full_covariance is used to force Dakota to output the full covariance matrix.

normalized

- Keywords Area
- method
- polynomial_chaos
- normalized

The normalized specification requests output of PCE coefficients that correspond to normalized orthogonal basis polynomials

Specification

Alias: none

Argument(s): none

Default: PCE coefficients correspond to unnormalized basis polynomials

Description

The normalized specification requests output of PCE coefficients that correspond to normalized orthogonal basis polynomials

sample_type

- Keywords Area
- method
- polynomial_chaos
- sample_type

Selection of sampling strategy

Specification

Alias: none

Argument(s): none

Default: lhs
### Description

The `sample_type` keyword allows the user to select between two types of sampling: Monte Carlo (pure random) and Latin hypercube (stratified) sampling.

The incremental keywords are deprecated; instead use `samples` together with `refinement_samples`.

**Default Behavior**

If the `sample_type` keyword is present, it must be accompanied by `lhs` or `random`. In most contexts, `lhs` is the default (exception: multilevel_sampling uses Monte Carlo by default).

### Examples

```
method
  sampling
    sample_type lhs
    samples = 20
    seed = 83921
```

**lhs**

- **Keywords Area**
- **method**
- **polynomial_chaos**
- **sample_type**
- **lhs**

Uses Latin Hypercube Sampling (LHS) to sample variables

### Specification

**Alias:** none

**Argument(s):** none
6.2. METHOD

Description

The \texttt{lhs} keyword invokes Latin Hypercube Sampling as the means of drawing samples of uncertain variables according to their probability distributions. This is a stratified, space-filling approach that selects variable values from a set of equi-probable bins.

Default Behavior

Latin Hypercube Sampling is the default sampling mode in most contexts (exception: multilevel\_sampling). To explicitly specify LHS in the Dakota input file, the \texttt{lhs} keyword must appear in conjunction with the \texttt{sample\_type} keyword.

Usage Tips

Latin Hypercube Sampling is very robust and can be applied to any problem. It is fairly effective at estimating the mean of model responses and linear correlations with a reasonably small number of samples relative to the number of variables.

Examples

\begin{verbatim}
method sampling
  sample_type lhs
  samples = 20
\end{verbatim}

\textbf{random}

- Keywords Area
- method
- polynomial\_chaos
- sample\_type
- random

Uses purely random Monte Carlo sampling to sample variables.

Specification

Alias: none
Argument(s): none

Description

The \texttt{random} keyword invokes Monte Carlo sampling as the means of drawing samples of uncertain variables according to their probability distributions.

Default Behavior

In most contexts, Monte Carlo sampling is not the default sampling mode (exception: multilevel\_sampling). To change this behavior, the \texttt{random} keyword must be specified in conjunction with the \texttt{sample\_type} keyword.

Usage Tips

Monte Carlo sampling is more computationally expensive than Latin Hypercube Sampling as it requires a larger number of samples to accurately estimate statistics.
Examples

```plaintext
method
  sampling
    sample_type random
    samples = 200
```

**probability_refinement**

- **Keywords Area**
- **method**
- **polynomial_chaos**
- **probability_refinement**

Allow refinement of probability and generalized reliability results using importance sampling.

Topics

This keyword is related to the topics:

- **reliability_methods**

Specification

Alias: sample_refinement

**Argument(s):** none

**Default:** no refinement

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Required (Choose One)</strong></td>
<td>Group 1</td>
<td>import</td>
<td>Sampling option</td>
</tr>
<tr>
<td></td>
<td></td>
<td>adapt_import</td>
<td>Importance sampling option</td>
</tr>
<tr>
<td></td>
<td></td>
<td>mm_adapt_import</td>
<td>Sampling option</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>refinement_samples</td>
<td>Number of samples used to refine a probability estimate or sampling design.</td>
</tr>
</tbody>
</table>

Description

The `probability_refinement` allows refinement of probability and generalized reliability results using importance sampling. If one specifies `probability_refinement`, there are some additional options. One can specify which type of importance sampling to use (`import`, `adapt_import`, or `mm_adapt_import`). Additionally, one can specify the number of refinement samples to use with `refinement_samples` and the seed to use with `seed`.

The `probability_refinement` density reweighting accounts originally was developed based on Gaussian distributions. It now accounts for additional non-Gaussian cases.
import

- Keywords Area
- method
- polynomial_chaos
- probability_refinement
- import

Sampling option

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

*import* centers a sampling density at one of the initial LHS samples identified in the failure region. It then generates the importance samples, weights them by their probability of occurrence given the original density, and calculates the required probability (CDF or CCDF level).

*adapt_import*

- Keywords Area
- method
- polynomial_chaos
- probability_refinement
- adapt_import

Importance sampling option

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

*adapt_import* centers a sampling density at one of the initial LHS samples identified in the failure region. It then generates the importance samples, weights them by their probability of occurrence given the original density, and calculates the required probability (CDF or CCDF level). This continues iteratively until the failure probability estimate converges.
mm_adapt_import

- Keywords Area
- method
- polynomial_chaos
- probability_refinement
- mm_adapt_import

Sampling option

Specification

Alias: none
Argument(s): none

Description

mm_adapt_import starts with all of the samples located in the failure region to build a multimodal sampling density. First, it uses a small number of samples around each of the initial samples in the failure region. Note that these samples are allocated to the different points based on their relative probabilities of occurrence: more probable points get more samples. This early part of the approach is done to search for "representative" points. Once these are located, the multimodal sampling density is set and then mm_adapt_import proceeds similarly to adapt_import (sample until convergence).

refinement_samples

- Keywords Area
- method
- polynomial_chaos
- probability_refinement
- refinement_samples

Number of samples used to refine a probability estimate or sampling design.

Specification

Alias: none
Argument(s): INTEGERLIST

Description

Probability estimate: Specify the (scalar) number of samples used to improve a probability estimate. If using uni-modal sampling all samples are assigned to the sampling center. If using multi-modal sampling the samples are split between multiple samples according to some internally computed weights.

Sampling design: Specify one or a sequence of refinement samples to augment the initial_samples in a sampling design.
6.2. METHOD

import_approx_points_file

- Keywords Area
- method
- polynomial_chaos
- import_approx_points_file

Filename for points at which to evaluate the PCE/SC surrogate

**Specification**

**Alias:** none

**Argument(s):** STRING

**Default:** no point import from a file

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group (Tabular Format (Group 1))</th>
<th>Dakota Keyword annotated</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional (Choose One)</td>
<td></td>
<td></td>
<td>Selects annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
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<td>Selects custom-annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>freeform</td>
<td>Selects freeform file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>active_only</td>
<td>Import only active variables from tabular data file</td>
</tr>
</tbody>
</table>

**Description**

**Default Behavior** No import of points at which to evaluate the surrogate.

**Expected Output** The PCE/SC surrogate model will be evaluated at the list of points (input variable values) provided in the file and results tabulated and/or statistics computed at them, depending on the method context.

**Examples**

```plaintext
method polynomial_chaos
  expansion_order = 4
  import_approx_points_file = 'import.mcmc_annot.dat'
  annotated
```

**annotated**

- Keywords Area
- method
CHAPTER 6. KEYWORDS AREA

- polynomial_ chaos
- import_approx_points_file
- annotated

Selects annotated tabular file format

Topics
This keyword is related to the topics:
- file formats

Specification
Alias: none
Argument(s): none
Default: annotated format

Description
An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior
By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips
- To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify custom_ annotated header eval_id
- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples
Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```
environment
  tabular_data
    tabular_data_file = 'dakota_summary.dat'
    annotated

Resulting tabular file:
%eval_id interface x1 x2 obj_fn nln_ineq_con_1 nln_ineq_con_2
1 NO_ID   0.9 1.1   0.0002 0.26 0.76
2 NO_ID   0.90009 1.1 0.0001996404857 0.2601620081 0.759955
3 NO_ID   0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...```
6.2. METHOD

custom_annotated

- Keywords Area
- method
- polynomial_chaos
- import_approx_points_file
- custom_annotated

Selects custom-annotated tabular file format

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none
Argument(s): none
Default: annotated format

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>Group</td>
<td>header</td>
<td>Description</td>
</tr>
<tr>
<td>Optional</td>
<td>eval_id</td>
<td>Enable header row in custom-annotated tabular file</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>interface_id</td>
<td>Enable evaluation ID column in custom-annotated tabular file</td>
<td></td>
</tr>
</tbody>
</table>

Description

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

Default Behavior

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

Usage Tips
• Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

• When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

• Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples
Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
  tabular_data_file = 'dakota_summary.dat'
custom_annotated header eval_id

Resulting tabular file:

<table>
<thead>
<tr>
<th>eval_id</th>
<th>x1</th>
<th>x2</th>
<th>obj_fn</th>
<th>nln_ineq_con_1</th>
<th>nln_ineq_con_2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.9</td>
<td>1.1</td>
<td>0.0002</td>
<td>0.26</td>
<td>0.76</td>
</tr>
<tr>
<td>2</td>
<td>0.90009</td>
<td>1.1</td>
<td>0.0001996404857</td>
<td>0.2601620081</td>
<td>0.759955</td>
</tr>
<tr>
<td>3</td>
<td>0.89991</td>
<td>1.1</td>
<td>0.0002003604863</td>
<td>0.2598380081</td>
<td>0.760045</td>
</tr>
</tbody>
</table>
...
```

header

• Keywords Area

• method

• polynomial_chaos

• import_approx_points_file

• custom_annotated

• header

Enable header row in custom-annotated tabular file

Specification

Alias: none

Argument(s): none

Default: no header

Description

See description of parent custom_annotated
6.2. METHOD

eval_id

- Keywords Area
- method
- polynomial_choas
- import_approx_points_file
- custom_annotated
- eval_id

Enable evaluation ID column in custom-annotated tabular file

**Specification**

**Alias:** none

- **Argument(s):** none
- **Default:** no eval_id column

**Description**

See description of parent custom_annotated

interface_id

- Keywords Area
- method
- polynomial_choas
- import_approx_points_file
- custom_annotated
- interface_id

Enable interface ID column in custom-annotated tabular file

**Specification**

**Alias:** none

- **Argument(s):** none
- **Default:** no interface_id column

**Description**

See description of parent custom_annotated
freeform

- Keywords Area
- method
- polynomial_chaos
- import_approx_points_file
- freeform

Selects freeform file format

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none

Argument(s): none

Default: annotated format

Description

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior

The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips

- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.
6.2. METHOD

Examples

Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```python
environment
  tabular_data
    tabular_data_file = 'dakota_summary.dat'
    freeform
```

Resulting tabular file:

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>0.9</td>
<td>1.1</td>
<td>0.0002</td>
<td>0.26</td>
<td>0.76</td>
</tr>
<tr>
<td>0.90009</td>
<td>1.1</td>
<td>0.0001996404857</td>
<td>0.2601620081</td>
<td>0.759955</td>
</tr>
<tr>
<td>0.89991</td>
<td>1.1</td>
<td>0.0002003604863</td>
<td>0.2598380081</td>
<td>0.760045</td>
</tr>
</tbody>
</table>

... 

**active_only**

- Keywords Area
- method
- polynomial_chaos
- import_approx_points_file
- active_only

Import only active variables from tabular data file

Topics

This keyword is related to the topics:

- file_formats

Specification

**Alias:** none

**Argument(s):** none

Description

By default, files for tabular data imports are expected to contain columns for all variables, active and inactive. The keyword `active_only` indicates that the file to import contains only the active variables.

This option should only be used in contexts where the inactive variables have no influence, for example, building a surrogate over active variables, with the state variables held at nominal. It should not be used in more complex nested contexts, where the values of inactive variables are relevant to the function evaluations used to build the surrogate.
**export_approx_points_file**

- **Keywords Area**
- **method**
- **polynomial_chaos**
- **export_approx_points_file**

Output file for evaluations of a surrogate model

**Specification**

**Alias:** export_points_file  
**Argument(s):** STRING  
**Default:** no point export to a file

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional (Choose One)</td>
<td>Tabular Format (Group 1)</td>
<td>annotated</td>
<td>Selects annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>custom_annotated</td>
<td>Selects custom-annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>freeform</td>
<td>Selects freeform file format</td>
</tr>
</tbody>
</table>

**Description**

The `export_approx_points_file` keyword allows the user to specify a file in which the points (input variable values) at which the surrogate model is evaluated and corresponding response values computed by the surrogate model will be written. The response values are the surrogate’s predicted approximation to the truth model responses at those points.

**Usage Tips**

Dakota exports tabular data in one of three formats:

- `annotated` (default)
- `custom_annotated`
- `freeform`

**annotated**

- **Keywords Area**
- **method**
- **polynomial_chaos**
- **export_approx_points_file**
• annotated

Selects annotated tabular file format

Topics
This keyword is related to the topics:
• file formats

Specification
Alias: none
Argument(s): none
Default: annotated format

Description
An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior
By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips
• To specify pre-Dakota 6.1 tabular format, which did not include interface id, specify custom_annotated header eval_id

• Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

• When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

• Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples
Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```
environment
  tabular_data
    tabular_data_file = 'dakota_summary.dat'
      annotated

Resulting tabular file:

%eval_id interface x1   x2    obj_fn nln_ineq_con_1 nln_ineq_con_2   
1     NO_ID  0.9    1.1   0.0002   0.26   0.76
2     NO_ID  0.90009 1.1  0.0001996404857 0.2601620081 0.759955
3     NO_ID  0.89991 1.1  0.0002003604863 0.2598380081 0.760045
...```
custom_annotated

- Keywords Area
- method
- polynomial_chaos
- export_approx_points_file
- custom_annotated

Selects custom-annotated tabular file format

Topics
This keyword is related to the topics:

- file_formats

Specification
Alias: none
Argument(s): none
Default: annotated format

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>header</td>
<td></td>
<td>Enable header row in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td>eval_id</td>
<td></td>
<td>Enable evaluation ID column in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td>interface_id</td>
<td></td>
<td>Enable interface ID column in custom-annotated tabular file</td>
</tr>
</tbody>
</table>

Description
A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

Default Behavior
The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

Usage Tips
• Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

• When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

• Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:

```environment
  tabular_data
  tabular_data_file = 'dakota_summary.dat'
  custom_annotated header eval_id
```

Resulting tabular file:

```%
  eval_id x1    x2    obj_fn nln_ineq_con_1 nln_ineq_con_2
  1 0.9 1.1 0.0002 0.26 0.76
  2 0.90009 1.1 0.0001996404857 0.2601620081 0.759955
  3 0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...
```

header

• Keywords Area

• method

• polynomial_chaos

• export_approx_points_file

• custom_annotated

• header

Enable header row in custom-annotated tabular file

Specification

Alias: none

Argument(s): none

Default: no header

Description

See description of parent custom_annotated
eval_id

- Keywords Area
- method
- polynomial_chaos
- export_approx_points_file
- custom_annotated
- eval_id

Enable evaluation ID column in custom-annotated tabular file

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no eval_id column

**Description**

See description of parent `custom_annotated`

interface_id

- Keywords Area
- method
- polynomial_chaos
- export_approx_points_file
- custom_annotated
- interface_id

Enable interface ID column in custom-annotated tabular file

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no interface_id column

**Description**

See description of parent `custom_annotated`
freeform

- Keywords Area
- method
- polynomial_chaos
- export_approx_points_file
- freeform

Selects freeform file format

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none

Argument(s): none

Default: annotated format

Description

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports.imports as well.

Default Behavior

The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips

- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.
Examples

Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```python
environment
tabular_data
  tabular_data_file = 'dakota_summary.dat'
freeform

Resulting tabular file:

<table>
<thead>
<tr>
<th>0.9</th>
<th>1.1</th>
<th>0.0002</th>
<th>0.26</th>
<th>0.76</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.90009</td>
<td>1.1</td>
<td>0.001996404857</td>
<td>0.2601620081</td>
<td>0.759955</td>
</tr>
<tr>
<td>0.89991</td>
<td>1.1</td>
<td>0.0002003604863</td>
<td>0.2598380081</td>
<td>0.760045</td>
</tr>
</tbody>
</table>
...```

`export_expansion_file`

- **Keywords Area**
- **method**
- **polynomial_chaos**
- **export_expansion_file**

Export the coefficients and multi-index of a Polynomial Chaos Expansion (PCE) to a file

### Specification

**Alias:** none

**Argument(s):** STRING

### Description

Export the coefficients and multi-index of a Polynomial Chaos Expansion (PCE) to a file. The multi-index written will be sparse. Specifically the expansion will consists only of the indices corresponding to the non-zero coefficients of the PCE.

`reliability_levels`

- **Keywords Area**
- **method**
- **polynomial_chaos**
- **reliability_levels**

Specify reliability levels at which the response values will be estimated

### Specification

**Alias:** none

**Argument(s):** REALLIST

**Default:** No CDF/CCDF response levels to compute
6.2. METHOD

<table>
<thead>
<tr>
<th>Required/Optional Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>num_reliability_levels</td>
<td></td>
<td>Specify which reliability_levels correspond to which response</td>
</tr>
</tbody>
</table>

**Description**

Response levels are calculated for specified CDF/CCDF reliabilities by projecting out the prescribed number of sample standard deviations from the sample mean.

**Theory**

Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.

In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

An inverse mapping involves computing the belief and plausibility response level for either a specified probability level or a specified generalized reliability level (two results for each level mapping in the evidence-based epistemic case, instead of the one result for each level mapping in the aleatory case).

**num_reliability_levels**

- Keywords Area
- method
- polynomial_chaos
- reliability_levels
- num_reliability_levels

Specify which reliability_levels correspond to which response

**Specification**

Alias: none

Argument(s): INTEGERLIST

Default: reliability_levels evenly distributed among response functions

**Description**

See parent page
response_levels

- Keywords Area
- method
- polynomial_chaos
- response_levels

Values at which to estimate desired statistics for each response

### Specification

**Alias:** none

**Argument(s):** REALLIST

**Default:** No CDF/CCDF probabilities/reliabilities to compute

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>num_response_levels</td>
<td></td>
<td></td>
<td>Number of values at which to estimate desired statistics for each response</td>
</tr>
</tbody>
</table>

**Optional**

<table>
<thead>
<tr>
<th>compute</th>
</tr>
</thead>
</table>

**Description**

The `response_levels` specification provides the target response values for which to compute probabilities, reliabilities, or generalized reliabilities (forward mapping).

**Default Behavior**

If `response_levels` are not specified, no statistics will be computed. If they are, probabilities will be computed by default.

**Expected Outputs**

If `response_levels` are specified, Dakota will create two tables in the standard output: a Probability Density function (PDF) histogram and a Cumulative Distribution Function (CDF) table. The PDF histogram has the lower and upper endpoints of each bin and the corresponding density of that bin. Note that the PDF histogram has bins defined by the `probabilityLevels` and/or `response_levels` in the Dakota input file. If there are not very many levels, the histogram will be coarse. Dakota does not do anything to optimize the bin size or spacing. The CDF table has the list of response levels and the corresponding probability that the response value is less than or equal to each response level threshold.

**Usage Tips**

The `num_response_levels` is used to specify which arguments of the `response_level` correspond to which response.
6.2. METHOD

Examples

For example, specifying a response_level of 52.3 followed with compute probabilities will result in the calculation of the probability that the response value is less than or equal to 52.3, given the uncertain distributions on the inputs.

For an example with multiple responses, the following specification

response_levels = 1. 2. .1 .2 .3 .4 10. 20. 30.
num_response_levels = 2 4 3

would assign the first two response levels (1., 2.) to response function 1, the next four response levels (.1, .2, .3, .4) to response function 2, and the final three response levels (10., 20., 30.) to response function 3. If the num_response_levels key were omitted from this example, then the response levels would be evenly distributed among the response functions (three levels each in this case).

The Dakota input file below specifies a sampling method with response levels of interest.

method,
sampling,
samples = 100 seed = 1
complementary distribution
response_levels = 3.6e+11 4.0e+11 4.4e+11
6.0e+04 6.5e+04 7.0e+04
3.5e+05 4.0e+05 4.5e+05

variables,
normal_uncertain = 2
means = 248.89, 593.33
std_deviations = 12.4, 29.7
descriptors = ‘TF1n’ ‘TF2n’
uniform_uncertain = 2
lower_bounds = 199.3, 474.63
upper_bounds = 298.5, 712.
descriptors = ‘TF1u’ ‘TF2u’
weibull_uncertain = 2
alphas = 12., 30.
betas = 250., 590.
descriptors = ‘TF1w’ ‘TF2w’
histogram_bin_uncertain = 2
num_pairs = 3 4
abscissas = 5 8 10 .1 .2 .3 .4
counts = 17 21 0 12 24 12 0
descriptors = ‘TF1h’ ‘TF2h’
histogram_point_uncertain
real = 1
num_pairs = 2
abscissas = 3 4
counts = 1 1
descriptors = ‘TF3h’

interface,
system asynch evaluation_concurrency = 5
analysis_driver = ‘text_book’

responses,
response_functions = 3
no_gradients
no_hessians

Given the above Dakota input file, the following excerpt from the output shows the PDF and CCDF generated. Note that the bounds on the bins of the PDF are the response values specified in the input file. The probability levels corresponding to those response values are shown in the CCDF.
Probability Density Function (PDF) histograms for each response function:

PDF for response_fn_1:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.7604749078e+11</td>
<td>3.6000000000e+11</td>
<td>5.3601733194e-12</td>
</tr>
<tr>
<td>3.6000000000e+11</td>
<td>4.0000000000e+11</td>
<td>4.2500000000e-12</td>
</tr>
<tr>
<td>4.0000000000e+11</td>
<td>4.4000000000e+11</td>
<td>3.7500000000e-12</td>
</tr>
<tr>
<td>4.4000000000e+11</td>
<td>4.5196114379e+11</td>
<td>2.2557612778e-12</td>
</tr>
</tbody>
</table>

PDF for response_fn_2:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.6431154744e+04</td>
<td>6.0000000000e+04</td>
<td>2.8742313192e-05</td>
</tr>
<tr>
<td>6.0000000000e+04</td>
<td>6.5000000000e+04</td>
<td>6.4000000000e-05</td>
</tr>
<tr>
<td>6.5000000000e+04</td>
<td>7.0000000000e+04</td>
<td>4.0000000000e-05</td>
</tr>
<tr>
<td>7.0000000000e+04</td>
<td>7.8702465755e+04</td>
<td>1.0341896485e-05</td>
</tr>
</tbody>
</table>

PDF for response_fn_3:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.379637090e+05</td>
<td>3.5000000000e+05</td>
<td>4.284460868e-06</td>
</tr>
<tr>
<td>3.5000000000e+05</td>
<td>4.0000000000e+05</td>
<td>8.6000000000e-06</td>
</tr>
<tr>
<td>4.0000000000e+05</td>
<td>4.5000000000e+05</td>
<td>1.8000000000e-06</td>
</tr>
</tbody>
</table>

Level mappings for each response function:

Complementary Cumulative Distribution Function (CCDF) for response_fn_1:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.6000000000e+11</td>
<td>5.5000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.0000000000e+11</td>
<td>3.8000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.4000000000e+11</td>
<td>2.3000000000e-01</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Complementary Cumulative Distribution Function (CCDF) for response_fn_2:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.0000000000e+04</td>
<td>6.1000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6.5000000000e+04</td>
<td>2.9000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7.0000000000e+04</td>
<td>9.0000000000e-02</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Complementary Cumulative Distribution Function (CCDF) for response_fn_3:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.5000000000e+05</td>
<td>5.2000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.0000000000e+05</td>
<td>9.0000000000e-02</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.5000000000e+05</td>
<td>0.0000000000e+00</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Theory

Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function. In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

A forward mapping involves computing the belief and plausibility probability level for a specified response level.

**num_response_levels**

- Keywords Area
- method
- polynomial_chaos
6.2. METHOD

- response_levels
- num_response_levels

Number of values at which to estimate desired statistics for each response

Specification

Alias: none
Argument(s): INTEGERLIST
Default: response_levels evenly distributed among response functions

Description

The num_response_levels keyword allows the user to specify the number of response values, for each response, at which estimated statistics are of interest. Statistics that can be computed are probabilities and reliabilities, both according to either a cumulative distribution function or a complementary cumulative distribution function.

Default Behavior

If num_response_levels is not specified, the response_levels will be evenly distributed among the responses.

Expected Outputs

The specific output will be determined by the type of statistics that are specified. In a general sense, the output will be a list of response level-statistic pairs that show the estimated value of the desired statistic for each response level specified.

Examples

```
method
    sampling
        samples = 100
        seed = 34785
        num_response_levels = 1 1 1
        response_levels = 0.5 0.5 0.5
    compute
```

compute

- Keywords Area
- method
- polynomial_chaos
- response_levels
- compute

Selection of statistics to compute at each response level

Specification

Alias: none
Argument(s): none
Default: probabilities
**CHAPTER 6. KEYWORDS AREA**

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword Description</th>
<th>Dakota Keyword</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required <strong>(Choose One)</strong></td>
<td></td>
<td><strong>probabilities</strong></td>
<td>Computes probabilities associated with response levels</td>
</tr>
<tr>
<td></td>
<td></td>
<td><strong>reliabilities</strong></td>
<td>Computes reliabilities associated with response levels</td>
</tr>
<tr>
<td></td>
<td></td>
<td><strong>gen_reliabilities</strong></td>
<td>Computes generalized reliabilities associated with response levels</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td><strong>system</strong></td>
<td>Compute system reliability (series or parallel)</td>
</tr>
</tbody>
</table>

**Description**

The `compute` keyword is used to select which forward statistical mapping is calculated at each response level.

**Default Behavior**

If `response_levels` is not specified, no statistics are computed. If `response_levels` is specified but `compute` is not, probabilities will be computed by default. If both `response_levels` and `compute` are specified, then one of the following must be specified: `probabilities`, `reliabilities`, or `gen_reliabilities`.

**Expected Output**

The type of statistics specified by `compute` will be reported for each response level.

**Usage Tips**

CDF/CCDF probabilities are calculated for specified response levels using a simple binning approach.

CDF/CCDF reliabilities are calculated for specified response levels by computing the number of sample standard deviations separating the sample mean from the response level.

**Examples**

```plaintext
method
  sampling
    sample_type random
    samples = 100 seed = 1
    complementary distribution
    response_levels = 3.6e+11 4.0e+11 4.4e+11
                   6.0e+04 6.5e+04 7.0e+04
                   3.5e+05 4.0e+05 4.5e+05
    compute reliabilities
    probabilities
```
6.2. METHOD

- Keywords Area
- method
- polynomial_chaos
- response_levels
- compute
- probabilities

Computes probabilities associated with response levels

Specification

Alias: none
Argument(s): none

Description

The probabilities keyword directs Dakota to compute the probability that the model response will be below (cumulative) or above (complementary cumulative) a specified response value. This is done for every response level designated for each response.

Default Behavior

If response_levels is specified, the probabilities are computed by default. To explicitly specify it in the Dakota input file, though, the probabilities keyword should be specified in conjunction with the compute keyword.

Expected Outputs

The Dakota output is a set of response level-probability pairs that give the probability that the model response will be below or above the corresponding response level, depending on the distribution defined.

Examples

method
sampling
  sample_type random
  samples = 100 seed = 1
  complementary_distribution
  response_levels = 3.6e+11 4.0e+11 4.4e+11
  6.0e+04 6.5e+04 7.0e+04
  3.5e+05 4.0e+05 4.5e+05
  compute probabilities

reliabilities
• **reliabilities**

Computes reliabilities associated with response levels

**Specification**

Alias: none  
Argument(s): none

**Description**

The `reliabilities` keyword directs Dakota to compute reliabilities according to the specified distribution for a specified response value. This is done for every response level designated for each response.

**Default Behavior**

If `response_levels` is specified, the reliabilities are not computed by default. To change this behavior, the `reliabilities` keyword should be specified in conjunction with the `compute` keyword.

**Expected Outputs**

The Dakota output is a set of response level-reliability pairs according to the distribution defined.

**Examples**

```plaintext
method  
sampling  
sample_type random  
samples = 100 seed = 1  
complementary distribution  
response_levels = 3.6e+11 4.0e+11 4.4e+11  
6.0e+04 6.5e+04 7.0e+04  
3.5e+05 4.0e+05 4.5e+05  
compute  
reliabilities
```

**gen_reliabilities**

• **Keywords Area**

• **method**

• **polynomial_chaos**

• **response_levels**

• **compute**

• **gen_reliabilities**

Computes generalized reliabilities associated with response levels

**Specification**

Alias: none  
Argument(s): none
Description

The `gen_reliabilities` keyword directs Dakota to compute generalized reliabilities according to the specified distribution for a specified response value. This is done for every response level designated for each response.

Default Behavior

If `response_levels` is specified, the generalized reliabilities are not computed by default. To change this behavior, the `gen_reliabilities` keyword should be specified in conjunction with the `compute` keyword.

Expected Outputs

The Dakota output is a set of response level-generalized reliability pairs according to the distribution defined.

Examples

```plaintext
method
  sampling
    sample_type random
    samples = 100 seed = 1
  complementary distribution
  response_levels = 3.6e+11 4.0e+11 4.4e+11
    6.0e+04 6.5e+04 7.0e+04
    3.5e+05 4.0e+05 4.5e+05
  compute gen_reliabilities

system
  • Keywords Area
  • method
  • polynomial_chaos
  • response_levels
  • compute
  • system

Compute system reliability (series or parallel)
```

Specification

Alias: none

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>Required (Choose One)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>series</td>
<td>Aggregate response statistics assuming a series system</td>
</tr>
</tbody>
</table>
Description

With the system probability/reliability option, statistics for specified response levels are calculated and reported assuming the response functions combine either in series or parallel to produce a total system response.

For a series system, the system fails when any one component (response) fails. The probability of failure is the complement of the product of the individual response success probabilities.

For a parallel system, the system fails only when all components (responses) fail. The probability of failure is the product of the individual response failure probabilities.

series

• Keywords Area
• method
• polynomial_chaos
• response_levels
• compute
• system
• series

Aggregate response statistics assuming a series system

Specification

Alias: none
Argument(s): none

Description

See parent keyword system for description.

parallel

• Keywords Area
• method
• polynomial_chaos
• response_levels
• compute
• system
6.2. METHOD

- parallel

Aggregate response statistics assuming a parallel system

**Specification**

**Alias:** none  
**Argument(s):** none

**Description**

See parent keyword `system` for description.

**distribution**

- **Keywords Area**
- **method**
- **polynomial_chaos**
- **distribution**

Selection of cumulative or complementary cumulative functions

**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** cumulative (CDF)

<p>| Required/- | Description of | Dakota Keyword | Dakota Keyword |</p>
<table>
<thead>
<tr>
<th>Optional Required</th>
<th>Group Group 1</th>
<th>cumulative</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Choose One</td>
<td></td>
<td></td>
<td>Computes statistics according to cumulative functions</td>
</tr>
<tr>
<td></td>
<td>complement</td>
<td>complementarily</td>
<td>Computes statistics according to complementary cumulative functions</td>
</tr>
</tbody>
</table>

**Description**

The `distribution` keyword allows the user to select between a cumulative distribution/belief/plausibility function and a complementary cumulative distribution/belief/plausibility function. This choice affects how probabilities and reliability indices are reported.

**Default Behavior**

If the `distribution` keyword is present, it must be accompanied by either `cumulative` or `complementary`. Otherwise, a cumulative distribution will be used by default.
Expected Outputs
Output will be a set of model response-probability pairs determined according to the choice of distribution. The choice of distribution also defines the sign of the reliability or generalized reliability indices.

Examples

```
method
  sampling
    sample_type lhs
    samples = 10
    distribution cumulative
```

`cumulative`

- Keywords Area
- method
- polynomial_chaos
- distribution
- cumulative

Computes statistics according to cumulative functions

Specification

Alias: none
Argument(s): none

Description
Statistics on model responses will be computed according to a cumulative distribution/belief/plausibility function.

Default Behavior
By default, a cumulative distribution/belief/plausibility function will be used. To explicitly specify it in the Dakota input file, however, the `cumulative` keyword must be appear in conjunction with the `distribution` keyword.

Expected Outputs
Output will be a set of model response-probability pairs determined according to a cumulative distribution/belief/plausibility function. The probabilities reported are the probabilities that the model response falls below given response thresholds.

Examples

```
method
  sampling
    sample_type lhs
    samples = 10
    distribution cumulative
```
6.2. METHOD

complementary

- Keywords Area
- method
- polynomial_chaos
- distribution
- complementary

Computes statistics according to complementary cumulative functions

Specification

Alias: none

Argument(s): none

Description

Statistics on model responses will be computed according to a complementary cumulative distribution/belief/plausibility function.

Default Behavior

By default, a complementary cumulative distribution/belief/plausibility function will not be used. To change that behavior, the complementary keyword must be appear in conjunction with the distribution keyword.

Expected Outputs

Output will be a set of model response-probability pairs determined according to a complementary cumulative distribution/belief/plausibility function. The probabilities reported are the probabilities that the model response falls above given response thresholds.

Examples

method
  sampling
    sample_type lhs
    samples = 10
    distribution complementary

probability_levels

- Keywords Area
- method
- polynomial_chaos
- probability_levels

Specify probability levels at which to estimate the corresponding response value

Specification

Alias: none

Argument(s): REALLIST

Default: No CDF/CCDF response levels to compute
CHAPTER 6. KEYWORDS AREA

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional Optional</td>
<td>Group</td>
<td>num_probability_-levels</td>
<td>Specify which probability_-levels correspond to which response</td>
</tr>
</tbody>
</table>

**Description**

Response levels are calculated for specified CDF/CCDF probabilities by indexing into a sorted samples array (the response levels computed are not interpolated and will correspond to one of the sampled values).

**Expected Output**

If `probability_levels` are specified, Dakota will create two tables in the standard output: a Probability Density function (PDF) histogram and a Cumulative Distribution Function (CDF) table. The PDF histogram has the lower and upper endpoints of each bin and the corresponding density of that bin. Note that the PDF histogram has bins defined by the `probability_levels` and/or `response_levels` in the Dakota input file. If there are not very many levels, the histogram will be coarse. Dakota does not do anything to optimize the bin size or spacing. The CDF table has the list of response levels and the corresponding probability that the response value is less than or equal to each response level threshold.

**Examples**

The Dakota input file below specifies a sampling method with probability levels of interest.

```plaintext
method,
  sampling,
  samples = 100 seed = 1
  complementary distribution
  probability_levels = 1. .66 .33 0.
  1. .8 .5 0.
  1. .3 .2 0.

variables,
  normal_uncertain = 2
  means = 248.89, 593.33
  std_deviations = 12.4, 29.7
  descriptors = 'TF1n' 'TF2n'
  uniform_uncertain = 2
  lower_bounds = 199.3, 474.63
  upper_bounds = 298.5, 712.
  descriptors = 'TF1u' 'TF2u'
  weibull_uncertain = 2
  alphas = 12., 30.
  betas = 250., 590.
  descriptors = 'TF1w' 'TF2w'
  histogram_bin_uncertain = 2
  num_pairs = 3 4
  abscissas = 5 8 10 .1 .2 .3 .4
  counts = 17 21 0 12 24 12 0
  descriptors = 'TF1h' 'TF2h'
  histogram_point_uncertain
  real = 1
  num_pairs = 2
  abscissas = 3 4
  counts = 1 1
  descriptors = 'TF3h'
```
6.2. METHOD

interface,

    system asynch evaluation_concurrency = 5
    analysis_driver = 'text_book'

responses,

    response_functions = 3
    no_gradients
    no_hessians

Given the above Dakota input file, the following excerpt from the output shows the PDF and CCDF generated. Note that the bounds on the bins of the PDF are the response values that correspond the probability levels specified in the input file. Those response values are also shown in the CCDF.

Probability Density Function (PDF) histograms for each response function:

PDF for response_fn_1:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.7604749078e+11</td>
<td>3.4221494996e+11</td>
<td>5.1384774972e-12</td>
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</table>

PDF for response_fn_2:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.6431154744e+04</td>
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<td>5.8916108390e-05</td>
</tr>
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PDF for response_fn_3:

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<td>9.0600555634e-06</td>
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<td>3.8100966235e+05</td>
<td>4.411498127e+05</td>
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Complementary Cumulative Distribution Function (CCDF) for each response function:

Complementary Cumulative Distribution Function (CCDF) for response_fn_1:

<table>
<thead>
<tr>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.7604749078e+11</td>
<td>1.000000000000e+00</td>
<td></td>
</tr>
<tr>
<td>3.4221494996e+11</td>
<td>6.600000000000e-01</td>
<td></td>
</tr>
<tr>
<td>4.0634975300e+11</td>
<td>3.000000000000e-01</td>
<td></td>
</tr>
</tbody>
</table>

Complementary Cumulative Distribution Function (CCDF) for response_fn_2:

<table>
<thead>
<tr>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.6431154744e+04</td>
<td>1.000000000000e+00</td>
<td></td>
</tr>
<tr>
<td>5.6511827775e+04</td>
<td>8.000000000000e-01</td>
<td></td>
</tr>
<tr>
<td>6.1603813790e+04</td>
<td>5.000000000000e-01</td>
<td></td>
</tr>
</tbody>
</table>

Complementary Cumulative Distribution Function (CCDF) for response_fn_3:

<table>
<thead>
<tr>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.3796737090e+05</td>
<td>1.000000000000e+00</td>
<td></td>
</tr>
<tr>
<td>3.6997214153e+05</td>
<td>3.000000000000e-01</td>
<td></td>
</tr>
<tr>
<td>3.8100966235e+05</td>
<td>2.000000000000e-01</td>
<td></td>
</tr>
</tbody>
</table>

Theory

Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.
In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

An inverse mapping involves computing the belief and plausibility response level for either a specified probability level or a specified generalized reliability level (two results for each level mapping in the evidence-based epistemic case, instead of the one result for each level mapping in the aleatory case).

**num_probability_levels**

- **Keywords Area**
- **method**
- **polynomial_choas**
- **probability_levels**
- **num_probability_levels**

Specify which *probability_levels* correspond to which response

**Specification**

**Alias:** none

**Argument(s):** INTEGERLIST

**Default:** probability_levels evenly distributed among response functions

**Description**

See parent page

**gen_reliability_levels**

- **Keywords Area**
- **method**
- **polynomial_choas**
- **gen_reliability_levels**

Specify generalized reliability levels at which to estimate the corresponding response value

**Specification**

**Alias:** none

**Argument(s):** REALLIST

**Default:** No CDF/CCDF response levels to compute
6.2. METHOD

<table>
<thead>
<tr>
<th>Optional</th>
<th>num_gen_reliability_levels</th>
<th>Specify which gen_reliability_levels correspond to which response</th>
</tr>
</thead>
</table>

**Description**

Response levels are calculated for specified generalized reliabilities by indexing into a sorted samples array (the response levels computed are not interpolated and will correspond to one of the sampled values).

**Theory**

Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.

In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

An inverse mapping involves computing the belief and plausibility response level for either a specified probability level or a specified generalized reliability level (two results for each level mapping in the evidence-based epistemic case, instead of the one result for each level mapping in the aleatory case).

**num_gen_reliability_levels**

- **Keywords** Area
- method
- polynomial_chaos
- gen_reliability_levels
- num_gen_reliability_levels

Specify which gen_reliability_levels correspond to which response

**Specification**

**Alias:** none

**Argument(s):** INTEGERLIST

**Default:** gen_reliability_levels evenly distributed among response functions

**Description**

See parent page
**rng**

- **Keywords Area**
- **method**
- **polynomial_ chaos**
- **rng**

Selection of a random number generator

**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** Mersenne twister (mt19937)

<table>
<thead>
<tr>
<th>Required/-Optional Required (Choose One)</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
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<tbody>
<tr>
<td></td>
<td></td>
<td>mt19937</td>
<td>Generates random numbers using the Mersenne twister</td>
</tr>
<tr>
<td></td>
<td></td>
<td>rnum2</td>
<td>Generates pseudo-random numbers using the Pecos package</td>
</tr>
</tbody>
</table>

**Description**

The **rng** keyword is used to indicate a choice of random number generator.

**Default Behavior**

If specified, the **rng** keyword must be accompanied by either **rnum2** (pseudo-random numbers) or **mt19937** (random numbers generated by the Mersenne twister). Otherwise, **mt19937**, the Mersenne twister is used by default.

**Usage Tips**

The default is recommended, as the Mersenne twister is a higher quality random number generator.

**Examples**

```plaintext
method
  sampling
    sample_type lhs
    samples = 10
    seed = 98765
    rng rnum2
```

**mt19937**

- **Keywords Area**
- **method**
6.2. METHOD

- polynomial_chaos
- rng
- mt19937

Generates random numbers using the Mersenne twister

Specification

Alias: none
Argument(s): none

Description

The mt19937 keyword directs Dakota to use the Mersenne twister to generate random numbers. Additional information can be found on wikipedia: http://en.wikipedia.org/wiki/Mersenne_twister.

Default Behavior

mt19937 is the default random number generator. To specify it explicitly in the Dakota input file, however, it must be specified in conjunction with the rng keyword.

Usage Tips

Use of the Mersenne twister random number generator (mt19937) is recommended.

Examples

```
method sampling
  sample_type lhs
  samples = 10
  seed = 98765
  rng mt19937
```

rnum2

- Keywords Area
- method
- polynomial_chaos
- rng
- rnum2

Generates pseudo-random numbers using the Pecos package

Specification

Alias: none
Argument(s): none
CHAPTER 6. KEYWORDS AREA

Description

The `rnum2` keyword directs Dakota to use pseudo-random numbers generated by the Pecos package.

Default Behavior

`rnum2` is not used by default. To change this behavior, it must be specified in conjunction with the `rng` keyword.

Usage Tips

Use of the Mersenne twister random number generator (`mt19937`) is recommended over `rnum2`.

Examples

```
method
  sampling
    sample_type lhs
    samples = 10
    seed = 98765
  rng rnum2
```

`model_pointer`

- Keywords Area
- method
- polynomial_chaos
- model_pointer

Identifier for model block to be used by a method

Topics

This keyword is related to the topics:

- block_pointer

Specification

Alias: none

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)

Description

The `model_pointer` is used to specify which `model` block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a `model` block in the Dakota input file that has a corresponding `id_model` with the same name.

Usage Tips

When doing advanced analyses that involve using multiple methods and multiple models, defining a `model_pointer` for each method is imperative.

See `block_pointer` for details about pointers.
6.2. METHOD

Examples

environment
tabular_graphics_data
method_pointer = 'UQ'

method
id_method = 'UQ'
model_pointer = 'SURR'
sampling,
samples = 10
seed = 98765 rng rnum2
response_levels = 0.1 0.2 0.6
0.1 0.2 0.6
0.1 0.2 0.6
sample_type lhs
distribution cumulative

model
id_model = 'SURR'
surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
id_method = 'DACE'
model_pointer = 'DACE_M'
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = 'DACE_M'
single
interface_pointer = 'I1'

variables
uniform_uncertain = 2
lower_bounds = 0. 0.
upper_bounds = 1. 1.
descriptors = 'x1' 'x2'

interface
id_interface = 'I1'
system asynch evaluation_concurrency = 5
analysis_driver = 'text_book'

responses
response_functions = 3
no_gradients
no_hessians

6.2.49 stoch_collocation

• Keywords Area

• method

• stoch_collocation

Uncertainty quantification with stochastic collocation
### Specification

**Alias:** nond_stoch_collocation  
**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>samples_on_emulator</td>
<td></td>
<td>Number of samples at which to evaluate an emulator (surrogate)</td>
</tr>
<tr>
<td>Optional</td>
<td>seed</td>
<td></td>
<td>Seed of the random number generator</td>
</tr>
<tr>
<td>Optional</td>
<td>fixed_seed</td>
<td></td>
<td>Reuses the same seed value for multiple random sampling sets</td>
</tr>
<tr>
<td>Optional</td>
<td>max_refinement_iterations</td>
<td></td>
<td>Maximum number of expansion refinement iterations</td>
</tr>
<tr>
<td>Optional</td>
<td>convergence_tolerance</td>
<td></td>
<td>Stopping criterion based on convergence of the objective function or statistics</td>
</tr>
<tr>
<td>Optional</td>
<td>final_moments</td>
<td></td>
<td>Output moments of the specified type and include them within the set of final statistics.</td>
</tr>
</tbody>
</table>

Optional (Choose One)

<table>
<thead>
<tr>
<th>Automated refinement type (Group 1)</th>
<th>p_refinement</th>
<th>Automated polynomial order refinement</th>
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<tbody>
<tr>
<td></td>
<td>h_refinement</td>
<td>Employ h-refinement to refine the grid</td>
</tr>
<tr>
<td>Optional (Choose One)</td>
<td>Basis polynomial family (Group 2)</td>
<td>piecewise</td>
</tr>
<tr>
<td>-----------------------</td>
<td>-----------------------------------</td>
<td>-----------</td>
</tr>
<tr>
<td>askey</td>
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<td></td>
</tr>
<tr>
<td>wiener</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Required (Choose One)</td>
<td>Interpolation grid type (Group 3)</td>
<td>quadrature_order_sequence</td>
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<td></td>
<td></td>
<td>sparse_grid_level_sequence</td>
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<tr>
<td>Optional</td>
<td></td>
<td>dimension_preference</td>
</tr>
<tr>
<td>Optional</td>
<td>Nesting of quadrature rules (Group 4)</td>
<td>Use derivative data to construct surrogate models</td>
</tr>
<tr>
<td>----------</td>
<td>--------------------------------------</td>
<td>-----------------------------------------------</td>
</tr>
<tr>
<td>Optional (Choose One)</td>
<td>nested</td>
<td>Enforce use of nested quadrature rules if available</td>
</tr>
<tr>
<td></td>
<td>non_nested</td>
<td>Enforce use of non-nested quadrature rules</td>
</tr>
<tr>
<td>Optional</td>
<td>Covariance type (Group 5)</td>
<td>Activates global sensitivity analysis based on decomposition of response variance into main, interaction, and total effects</td>
</tr>
<tr>
<td>Optional (Choose One)</td>
<td>diagonal_covariance</td>
<td>Display only the diagonal terms of the covariance matrix</td>
</tr>
<tr>
<td></td>
<td>full_covariance</td>
<td>Display the full covariance matrix</td>
</tr>
<tr>
<td>Optional</td>
<td>sample_type</td>
<td>Selection of sampling strategy</td>
</tr>
<tr>
<td>Optional</td>
<td>probability_refinement</td>
<td>Allow refinement of probability and generalized reliability results using importance sampling</td>
</tr>
<tr>
<td>Optional</td>
<td>import_approx_points_file</td>
<td>Filename for points at which to evaluate the PCE/SC surrogate</td>
</tr>
<tr>
<td>Optional</td>
<td>export_approx_points_file</td>
<td>Output file for evaluations of a surrogate model</td>
</tr>
</tbody>
</table>
### Description

Stochastic collocation is a general framework for approximate representation of random response functions in terms of finite-dimensional interpolation bases.

The stochastic collocation (SC) method is very similar to polynomial chaos, with the key difference that the orthogonal polynomial basis functions are replaced with interpolation polynomial bases. The interpolation polynomials may be either local or global and either value-based or gradient-enhanced. In the local case, value-based are piecewise linear splines and gradient-enhanced are piecewise cubic splines, and in the global case, value-based are Lagrange interpolants and gradient-enhanced are Hermite interpolants. A value-based expansion takes the form

$$R = \sum_{i=1}^{N_p} r_i L_i(\xi)$$

where $N_p$ is the total number of collocation points, $r_i$ is a response value at the $i^{th}$ collocation point, $L_i$ is the...
Thus, in PCE, one forms coefficients for known orthogonal polynomial basis functions, whereas SC forms multidimensional interpolation functions for known coefficients.

**Basis polynomial family (Group 2)**

In addition to the askey and wiener basis types also supported by polynomial_chaos, SC supports the option of piecewise local basis functions. These are piecewise linear splines, or in the case of gradient-enhanced interpolation via the use_derivatives specification, piecewise cubic Hermite splines. Both of these basis options provide local support only over the range from the interpolated point to its nearest 1D neighbors (within a tensor grid or within each of the tensor grids underlying a sparse grid), which exchanges the fast convergence of global bases for smooth functions for robustness in the representation of nonsmooth response functions (that can induce Gibbs oscillations when using high-order global basis functions). When local basis functions are used, the usage of nonequidistant collocation points (e.g., the Gauss point selections described above) is not well motivated, so equidistant Newton-Cotes points are employed in this case, and all random variable types are transformed to standard uniform probability space. The global gradient-enhanced interpolants (Hermite interpolation polynomials) are also restricted to uniform or transformed uniform random variables (due to the need to compute collocation weights by integration of the basis polynomials) and share the variable support shown in variable_support for Piecewise SE. Due to numerical instability in these high-order basis polynomials, they are deactivated by default but can be activated by developers using a compile-time switch.

**Interpolation grid type (Group 3)**

To form the multidimensional interpolants \( L_i \) of the expansion, two options are provided.

1. interpolation on a tensor-product of Gaussian quadrature points (specified with quadrature_order and, optionally, dimension_preference for anisotropic tensor grids). As for PCE, non-nested Gauss rules are employed by default, although the presence of p_refinement or h_refinement will result in default usage of nested rules for normal or uniform variables after any variable transformations have been applied (both defaults can be overridden using explicit nested or non_nested specifications).

2. interpolation on a Smolyak sparse grid (specified with sparse_grid_level and, optionally, dimension_preference for anisotropic sparse grids) defined from Gaussian rules. As for sparse PCE, nested rules are employed unless overridden with the non_nested option, and the growth rules are restricted unless overridden by the unrestricted keyword.

Another distinguishing characteristic of stochastic collocation relative to polynomial_chaos is the ability to reformulate the interpolation problem from a nodal interpolation approach into a hierarchical formulation in which each new level of interpolation defines a set of incremental refinements (known as hierarchical surpluses) layered on top of the interpolants from previous levels. This formulation lends itself naturally to uniform or adaptive refinement strategies, since the hierarchical surpluses can be interpreted as error estimates for the interpolant. Either global or local/piecewise interpolants in either value-based or gradient-enhanced approaches can be formulated using hierarchical interpolation. The primary restriction for the hierarchical case is that it currently requires a sparse grid approach using nested quadrature rules (Genz-Keister, Gauss-Patterson, or Newton-Cotes for standard normals and standard uniforms in a transformed space: Askey, Wiener, or Piecewise settings may be required), although this restriction can be relaxed in the future. A selection of hierarchical interpolation will provide greater precision in the increments to mean, standard deviation, covariance, and reliability-based level mappings induced by a grid change within uniform or goal-oriented adaptive refinement approaches (see following section).

It is important to note that, while quadrature_order and sparse_grid_level are array inputs, only one scalar from these arrays is active at a time for a particular expansion estimation. These scalars can be augmented with a dimension_preference to support anisotropy across the random dimension set. The array inputs are present to support advanced use cases such as multifidelity UQ, where multiple grid resolutions can be employed.
6.2. METHOD

Automated refinement type (Group 1)
Automated expansion refinement can be selected as either p_refinement or h_refinement, and either refinement specification can be either uniform or dimension_adaptive. The dimension_adaptive case can be further specified as either sobol or generalized (decay not supported). Each of these automated refinement approaches makes use of the max_iterations and convergence_tolerance iteration controls. The h_refinement specification involves use of the same piecewise interpolants (linear or cubic Hermite splines) described above for the piecewise specification option (it is not necessary to redundantly specify piecewise in the case of h_refinement). In future releases, the hierarchical interpolation approach will enable local refinement in addition to the current uniform and dimension_adaptive options.

Covariance type (Group 5)
These two keywords are used to specify how this method computes, stores, and outputs the covariance of the responses. In particular, the diagonal covariance option is provided for reducing post-processing overhead and output volume in high dimensional applications.

Active Variables
The default behavior is to form expansions over aleatory uncertain continuous variables. To form expansions over a broader set of variables, one needs to specify active followed by state, epistemic, design, or all in the variables specification block.
For continuous design, continuous state, and continuous epistemic uncertain variables included in the expansion, interpolation points for these dimensions are based on Gauss-Legendre rules if non-nested, Gauss-Patterson rules if nested, and Newton-Cotes points in the case of piecewise bases. Again, when probability integrals are evaluated, only the aleatory random variable domain is integrated, leaving behind a polynomial relationship between the statistics and the remaining design/state/epistemic variables.

Optional Keywords regarding method outputs
Each of these sampling specifications refer to sampling on the SC approximation for the purposes of generating approximate statistics.

- sample_type
- samples
- seed
- fixed_seed
- rng
- probability_refinement
- distribution
- reliability_levels
- response_levels
- probability_levels
- gen_reliability_levels

Since SC approximations are formed on structured grids, there should be no ambiguity with simulation sampling for generating the SC expansion.

When using the probability_refinement control, the number of refinement samples is not under the user’s control (these evaluations are approximation-based, so management of this expense is less critical). This option allows for refinement of probability and generalized reliability results using importance sampling.

Multi-fidelity UQ
When using multifidelity UQ, the high fidelity expansion generated from combining the low fidelity and discrepancy expansions retains the polynomial form of the low fidelity expansion (only the coefficients are updated). Refer to `polynomial_chaos` for information on the multifidelity interpretation of array inputs for `quadrature_order` and `sparse_grid_level`.

**Usage Tips**

If $n$ is small, then tensor-product Gaussian quadrature is again the preferred choice. For larger $n$, tensor-product quadrature quickly becomes too expensive and the sparse grid approach is preferred. For self-consistency in growth rates, nested rules employ restricted exponential growth (with the exception of the `dimension_adaptive_p_refinement generalized case`) for consistency with the linear growth used for non-nested Gauss rules (integrand precision $i = 4l + 1$ for sparse grid level $l$ and $i = 2m - 1$ for tensor grid order $m$).

**Additional Resources**


**Examples**

```plaintext
method, stoch_collocation
  sparse_grid_level = 2
  samples = 10000 seed = 12347 rng rnum2
  response_levels = .1 1. 50. 100. 500. 1000.
  variance_based_decomp
```

**Theory**

As mentioned above, a value-based expansion takes the form

$$ R = \sum_{i=1}^{N_p} r_i L_i(\xi) $$

The $i^{th}$ interpolation polynomial assumes the value of 1 at the $i^{th}$ collocation point and 0 at all other collocation points, involving either a global Lagrange polynomial basis or local piecewise splines. It is easy to see that the approximation reproduces the response values at the collocation points and interpolates between these values at other points. A gradient-enhanced expansion (selected via the `use_derivatives` keyword) involves both type 1 and type 2 basis functions as follows:

$$ R = \sum_{i=1}^{N_p} [r_i H_i^{(1)}(\xi) + \sum_{j=1}^{n} \frac{dr_i}{d\xi_j} H_{ij}^{(2)}(\xi)] $$

where the $i^{th}$ type 1 interpolant produces 1 for the value at the $i^{th}$ collocation point, 0 for values at all other collocation points, and 0 for derivatives (when differentiated) at all collocation points, and the $ij^{th}$ type 2 interpolant produces 0 for values at all collocation points, 1 for the $j^{th}$ derivative component at the $i^{th}$ collocation point, and 0 for the $j^{th}$ derivative component at all other collocation points. Again, this expansion reproduces the response values at each of the collocation points, and when differentiated, also reproduces each component of the gradient at each of the collocation points. Since this technique includes the derivative interpolation explicitly, it eliminates issues with matrix ill-conditioning that can occur in the gradient-enhanced PCE approach based on regression. However, the calculation of high-order global polynomials with the desired interpolation properties can be similarly numerically challenging such that the use of local cubic splines is recommended due to numerical stability.
6.2. METHOD

See Also

These keywords may also be of interest:

- adaptive_sampling
- gpais
- local_reliability
- global_reliability
- sampling
- importance_sampling
- polynomial_chaos

samples_on_emulator

- Keywords Area
- method
- stoch_collocation
- samples_on_emulator

Number of samples at which to evaluate an emulator (surrogate)

Specification

Alias: samples

Argument(s): INTEGER

Description

How many approximate function evaluations to perform on the emulator model, e.g., to compute statistics

Default Behavior

The default number of samples is method-dependent.

Examples

Perform 10000 samples on the PCE approximation of the true model:

```
method
  polynomial_chaos
  quadrature_order = 2
  samples_on_emulator = 10000
```
seed

• Keywords Area

• method

• stoch_collocation

• seed

Seed of the random number generator

Specification

Alias: none

Argument(s): INTEGER

Default: system-generated (non-repeatable)

Description

The random seed control provides a mechanism for making a stochastic method repeatable. That is, the use of the same random seed in identical studies will generate identical results.

Default Behavior

If not specified, the seed is randomly generated.

Expected Output

If seed is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

Usage Tips

If a stochastic study was run without seed specified, and the user later wishes to repeat the study using the same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen. That value can then be added to the Dakota input file.

Examples

method
  sampling
    sample_type lhs
    samples = 10
    seed = 15347

fixed_seed

• Keywords Area

• method

• stoch_collocation

• fixed_seed

Reuses the same seed value for multiple random sampling sets
6.2. METHOD

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** not fixed; pattern varies run-to-run

**Description**

The *fixed_seed* flag is relevant if multiple sampling sets will be generated over the course of a Dakota analysis. This occurs when using advance methods (e.g., surrogate-based optimization, optimization under uncertainty). The same seed value is reused for each of these multiple sampling sets, which can be important for reducing variability in the sampling results.

**Default Behavior**

The default behavior is to not use a fixed seed, as the repetition of the same sampling pattern can result in a modeling weakness that an optimizer could potentially exploit (resulting in actual reliabilities that are lower than the estimated reliabilities). For repeatable studies, the *seed* must also be specified.

**Examples**

```plaintext
method
  sampling
    sample_type lhs
    samples = 10
    fixed_seed
```

**max_refinement_iterations**

- **Keywords Area**

- **method**

- **stoch_collocation**

- **max_refinement_iterations**

  Maximum number of expansion refinement iterations

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** 100

**Description**

Limits the number of times the expansion can be refined under various refinement strategies.
Examples

method,
polynomial_chaos
dimension_adaptive generalized
p_refinement
  max_refinement_iterations = 20
corvergence_tol = 1.e-4
sparse_grid_level = 1

convergence_tolerance

- Keywords Area
- method
- stoch_collocation
- convergence_tolerance

Stopping criterion based on convergence of the objective function or statistics

Topics

This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none

Argument(s): REAL

Default: 1.e-4

Description

The convergence_tolerance specification provides a real value for controlling the termination of iteration. For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by convergence_tolerance, then this convergence criterion is satisfied on the current iteration.

Therefore, permissible values are between 0 and 1, non-inclusive.

Behavior Varies by Package/Library

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- DOT: must be satisfied for two consecutive iterations
6.2. METHOD

- NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of `convergence_tolerance` approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., `convergence_tolerance = 1.e-6` will result in approximately six digits of accuracy in the final objective function).

- NL2SOL: See nl2sol

**final_moments**

- **Keywords Area**
- **method**
- **stoch_collocation**
- **final_moments**

Output moments of the specified type and include them within the set of final statistics.

**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** standard

<table>
<thead>
<tr>
<th>Required/-Optional Required(Choose One)</th>
<th>Description of Group objective formulation (Group 1)</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>none</td>
<td></td>
<td>none</td>
<td>Omit moments from the set of final statistics.</td>
</tr>
<tr>
<td>standard</td>
<td></td>
<td>standard</td>
<td>Output standardized moments and include them within the set of final statistics.</td>
</tr>
<tr>
<td>central</td>
<td></td>
<td>central</td>
<td>Output central moments and include them within the set of final statistics.</td>
</tr>
</tbody>
</table>

**Description**

When performing a nested study that may employ moment statistics on the inner loop, it can be desirable to control the type of these moments. The `final_moments` specification supports options of `none`, `standard` (default), or `central`, corresponding to omission of moments, standardized moments (mean, standard deviation, skewness, and excess kurtosis), or central moments (mean, variance, 3rd central, and 4th central).
The presence or omission of moment results in the final statistics influences the outer level mappings in the case of a nested study. For example, `final_moments none` can allow for a more compact specification of primary and/or secondary response mappings.

**Examples**

The following method specification overrides the default to print central moments and include them in the set of final statistics.

```plaintext
method,
  sampling
    samples = 50 seed = 1234
    response_levels = 3.6e+11 1.2e+05 3.5e+05
    final_moments central

Overriding the default to `none` as follows:

```plaintext
method,
  sampling
    samples = 50 seed = 1234
    response_levels = 3.6e+11 1.2e+05 3.5e+05
    final_moments none
```

allows associated nested model mappings to be simplified from:

```plaintext
model
  nested
    sub_method_pointer = 'UQ'
    primary_response_mapping = 0. 0. 1. 0. 0. 1. 0. 0. 0.
    secondary_response_mapping = 0. 0. 0. 0. 0. 0. 0. 0. 1.
```

to a more compact version focused only on the response level mappings (two leading zeros per response function for moment mappings have been removed):

```plaintext
model
  nested
    sub_method_pointer = 'UQ'
    primary_response_mapping = 1. 1. 0.
    secondary_response_mapping = 0. 0. 1.
```

- **Keywords Area**
- method
- **stoch_collocation**
- **final_moments**
- none

Omit moments from the set of final statistics.

**Specification**

*Alias: none*

*Argument(s): none*
6.2. METHOD

Description

The omission of moment results from the final statistics can allow for a more compact definition of primary and/or secondary response mappings within a nested model specification.

Examples

method,
sampling
    samples = 50 seed = 1234
    response_levels = 3.6e+11 1.2e+05 3.5e+05
    final_moments none

standard

- Keywords Area
- method
- stoch_collocation
- final_moments
- standard

Output standardized moments and include them within the set of final statistics.

Specification

Alias: none

Argument(s): none

Description

Output standardized moments (mean, standard deviation, skewness, and excess kurtosis) and include the first two within the set of final statistics to be used at a higher level (e.g., optimization under uncertainty, mixed aleatory-epistemic UQ). This inclusion of moment results affects the primary and/or secondary response mappings in a nested model specification.

Examples

The following method specification overrides the default to print central moments and include them in the set of final statistics.

method,
sampling
    samples = 50 seed = 1234
    response_levels = 3.6e+11 1.2e+05 3.5e+05
    final_moments standard
central

- Keywords Area
- method
- stoch_collocation
- final_moments
- central

Output central moments and include them within the set of final statistics.

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

Output central moments (mean, variance, 3rd central, and 4th central) and include the first two within the set of final statistics to be used at a higher level (e.g., optimization under uncertainty, mixed aleatory-epistemic U-Q). This inclusion of moment results affects the primary and/or secondary response mappings in a nested model specification.

**Examples**

The following method specification overrides the default to print central moments and include them in the set of final statistics.

```plaintext
method,
sampling
    samples = 50 seed = 1234
    response_levels = 3.6e+11 1.2e+05 3.5e+05
    final_moments central
```

**p_refinement**

- Keywords Area
- method
- stoch_collocation
- p_refinement

Automatic polynomial order refinement

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no refinement
### Description

The p-refinement keyword specifies the usage of automated polynomial order refinement, which can be either uniform or dimension adaptive.

The dimension adaptive option is supported for the tensor-product quadrature and Smolyak sparse grid options and uniform is supported for tensor and sparse grids as well as regression approaches (collocation-points or collocation-ratio).

Each of these refinement cases makes use of the max_iterations and convergence_tolerance method independent controls. The former control limits the number of refinement iterations, and the latter control terminates refinement when the two-norm of the change in the response covariance matrix (or, in goal-oriented approaches, the two-norm of change in the statistical quantities of interest (QOI)) falls below the tolerance.

The dimension adaptive case can be further specified to utilize sobol, decay, or generalized refinement controls. The former two cases employ anisotropic tensor/sparse grids in which the anisotropic dimension preference (leading to anisotropic integrations/expansions with differing refinement levels for different random dimensions) is determined using either total Sobol’ indices from variance-based decomposition (sobol case: high indices result in high dimension preference) or using spectral coefficient decay rates from a rate estimation technique similar to Richardson extrapolation (decay case: low decay rates result in high dimension preference). In these two cases as well as the uniform refinement case, the quadrature_order or sparse_grid_level are ramped by one on each refinement iteration until either of the two convergence controls is satisfied. For the uniform refinement case with regression approaches, the expansion_order is ramped by one on each iteration while the oversampling ratio (either defined by collocation_ratio or inferred from collocation_points based on the initial expansion) is held fixed. Finally, the generalized dimension adaptive case is the default adaptive approach; it refers to the generalized sparse grid algorithm, a greedy approach in which candidate index sets are evaluated for their impact on the statistical QOI, the most influential sets are selected and used to generate additional candidates, and the index set frontier of a sparse grid is evolved in an unstructured and goal-oriented manner (refer to User’s Manual PCE descriptions for additional specifics).

For the case of p-refinement or the case of an explicit nested override, Gauss-Hermite rules are replaced with Genz-Keister nested rules and Gauss-Legendre rules are replaced with Gauss-Patterson nested rules, both of which exchange lower integrand precision for greater point reuse.

<table>
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<tr>
<th>Required/-Optional Required (Choose One)</th>
<th>Description of Group p-refinement type (Group 1)</th>
<th>Dakota Keyword: uniform</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
</table>
|                                          |                                                | dimension_adaptive      | Perform anisotropic expansion refinement by preferentially adapting in dimensions that are detected to have higher ‘importance’.

### uniform

The uniform refinement keyword specifies the usage of automated polynomial order refinement, which can be either uniform or dimension adaptive.

The dimension adaptive option is supported for the tensor-product quadrature and Smolyak sparse grid options and uniform is supported for tensor and sparse grids as well as regression approaches (collocation-points or collocation-ratio).

Each of these refinement cases makes use of the max_iterations and convergence_tolerance method independent controls. The former control limits the number of refinement iterations, and the latter control terminates refinement when the two-norm of the change in the response covariance matrix (or, in goal-oriented approaches, the two-norm of change in the statistical quantities of interest (QOI)) falls below the tolerance.

The dimension adaptive case can be further specified to utilize sobol, decay, or generalized refinement controls. The former two cases employ anisotropic tensor/sparse grids in which the anisotropic dimension preference (leading to anisotropic integrations/expansions with differing refinement levels for different random dimensions) is determined using either total Sobol’ indices from variance-based decomposition (sobol case: high indices result in high dimension preference) or using spectral coefficient decay rates from a rate estimation technique similar to Richardson extrapolation (decay case: low decay rates result in high dimension preference). In these two cases as well as the uniform refinement case, the quadrature_order or sparse_grid_level are ramped by one on each refinement iteration until either of the two convergence controls is satisfied. For the uniform refinement case with regression approaches, the expansion_order is ramped by one on each iteration while the oversampling ratio (either defined by collocation_ratio or inferred from collocation_points based on the initial expansion) is held fixed. Finally, the generalized dimension adaptive case is the default adaptive approach; it refers to the generalized sparse grid algorithm, a greedy approach in which candidate index sets are evaluated for their impact on the statistical QOI, the most influential sets are selected and used to generate additional candidates, and the index set frontier of a sparse grid is evolved in an unstructured and goal-oriented manner (refer to User’s Manual PCE descriptions for additional specifics).

For the case of p-refinement or the case of an explicit nested override, Gauss-Hermite rules are replaced with Genz-Keister nested rules and Gauss-Legendre rules are replaced with Gauss-Patterson nested rules, both of which exchange lower integrand precision for greater point reuse.
Refine an expansion uniformly in all dimensions.

**Specification**

**Alias:** none  
**Argument(s):** none

**Description**

The quadrature order or sparse_grid_level are ramped by one on each refinement iteration until either of the two convergence controls is satisfied. For the uniform refinement case with regression approaches, the expansion_order is ramped by one on each iteration while the oversampling ratio (either defined by collocation_ratio or inferred from collocation_points based on the initial expansion) is held fixed.

**dimension_adaptive**

Perform anisotropic expansion refinement by preferentially adapting in dimensions that are detected to have higher ‘importance’.

**Specification**

**Alias:** none  
**Argument(s):** none
### Description

Perform anisotropic expansion refinement by preferentially adapting in dimensions that are detected to hold higher ‘importance’ in resolving statistical quantities of interest.

Dimension importance must be estimated as part of the refinement process. Techniques include either sobol or generalized for stochastic collocation and either sobol, decay, or generalized for polynomial chaos. Each of these automated refinement approaches makes use of the max_iterations and convergence_tolerance iteration controls.

**sobol**

- Keywords Area
- method
- stoch_collocation
- p_refinement
- dimension_adaptive
- sobol

Estimate dimension preference for automated refinement of stochastic expansion using total Sobol’ sensitivity indices.

### Specification

**Alias:** none

**Argument(s):** none

**Default:** generalized
Description

Determine dimension preference for refinement of a stochastic expansion from the total Sobol’ sensitivity indices obtained from global sensitivity analysis. High indices indicate high importance for resolving statistical quantities of interest and therefore result in high dimension preference.

Examples

```plaintext
method,
    polynomial_chaos
    sparse_grid_level = 3
    dimension_adaptive p_refinement sobol
    max_iterations = 20
    convergence_tol = 1.e-4

generalized

• Keywords Area
• method
• stoch_collocation
• p_refinement
• dimension_adaptive
• generalized

Use the generalized sparse grid dimension adaptive algorithm to refine a sparse grid approximation of stochastic expansion.

Specification

Alias: none
Argument(s): none

Description

The generalized sparse grid algorithm is a greedy approach in which candidate index sets are evaluated for their impact on the statistical QOI, the most influential sets are selected and used to generate additional candidates, and the index set frontier of a sparse grid is evolved in an unstructured and goal-oriented manner (refer to User’s Manual PCE descriptions for additional specifics).

Examples

```plaintext
method,
    polynomial_chaos
    sparse_grid_level = 3
    dimension_adaptive p_refinement generalized
    max_iterations = 20
    convergence_tol = 1.e-4
```
6.2. METHOD

**h_refinement**

- **Keywords Area**
- **method**
- **stoch_collocation**
- **h_refinement**

Employ h-refinement to refine the grid

### Specification

**Alias:** none  
**Argument(s):** none  
**Default:** no refinement

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Required (Choose One)</strong></td>
<td>h-refinement type (Group 1)</td>
<td><strong>uniform</strong></td>
<td>Refine an expansion uniformly in all dimensions.</td>
</tr>
<tr>
<td></td>
<td></td>
<td><strong>dimension_adaptive</strong></td>
<td>Perform anisotropic expansion refinement by preferentially adapting in dimensions that are detected to have higher ‘importance’.</td>
</tr>
<tr>
<td></td>
<td></td>
<td><strong>local_adaptive</strong></td>
<td>Planned future capability for local pointwise refinement within a generalized sparse grid.</td>
</tr>
</tbody>
</table>

### Description

Automated expansion refinement can be selected as either p_refinement or h_refinement, and either refinement specification can be either uniform or dimension_adaptive. The dimension_adaptive case can be further specified as either sobol or generalized (decay not supported). Each of these automated refinement approaches makes use of the max_iterations and convergence_tolerance iteration controls. The h_refinement specification involves use of the same piecewise interpolants (linear or cubic Hermite splines) described above for the piecewise specification option (it is not necessary to redundantly specify piecewise in the case of h_refinement). In future releases, the hierarchical interpolation approach will enable local refinement in addition to the current uniform and dimension_adaptive options.
uniform

- Keywords Area
- method
- stoch_collocation
- h_refinement
- uniform

Refine an expansion uniformly in all dimensions.

**Specification**

*Alias:* none
*Argument(s):* none

**Description**

The quadrature_order or sparse_grid_level are ramped by one on each refinement iteration until either of the two convergence controls is satisfied. For the uniform refinement case with regression approaches, the expansion_order is ramped by one on each iteration while the oversampling ratio (either defined by collocation_ratio or inferred from collocation_points based on the initial expansion) is held fixed.

dimension_adaptive

- Keywords Area
- method
- stoch_collocation
- h_refinement
- dimension_adaptive

Perform anisotropic expansion refinement by preferentially adapting in dimensions that are detected to have higher ‘importance’.

**Specification**

*Alias:* none
*Argument(s):* none
### Description

Perform anisotropic expansion refinement by preferentially adapting in dimensions that are detected to hold higher ‘importance’ in resolving statistical quantities of interest.

Dimension importance must be estimated as part of the refinement process. Techniques include either sobol or generalized for stochastic collocation and either sobol, decay, or generalized for polynomial chaos. Each of these automated refinement approaches makes use of the max_iterations and convergence_tolerance iteration controls.

- **sobol**
  - Keywords Area
  - method
  - stoch_collocation
  - h_refinement
  - dimension_adaptive
  - sobol

Estimate dimension preference for automated refinement of stochastic expansion using total Sobol’ sensitivity indices.

### Specification

**Alias:** none

**Argument(s):** none

**Default:** generalized
CHAPTER 6. KEYWORDS AREA

Description
Determine dimension preference for refinement of a stochastic expansion from the total Sobol’ sensitivity indices obtained from global sensitivity analysis. High indices indicate high importance for resolving statistical quantities of interest and therefore result in high dimension preference.

Examples

```
method, polynomial_chaos
  sparse_grid_level = 3
  dimension_adaptive p_refinement sobol
  max_iterations = 20
  convergence_tol = 1.e-4
```

generalized

- Keywords Area
- method
- stoch_collocation
- h_refinement
- dimension_adaptive
- generalized

Use the generalized sparse grid dimension adaptive algorithm to refine a sparse grid approximation of stochastic expansion.

Specification

Alias: none
Argument(s): none

Description
The generalized sparse grid algorithm is a greedy approach in which candidate index sets are evaluated for their impact on the statistical QOI, the most influential sets are selected and used to generate additional candidates, and the index set frontier of a sparse grid is evolved in an unstructured and goal-oriented manner (refer to User’s Manual PCE descriptions for additional specifics).

Examples

```
method, polynomial_chaos
  sparse_grid_level = 3
  dimension_adaptive p_refinement generalized
  max_iterations = 20
  convergence_tol = 1.e-4
```
6.2. **METHOD**

**local_adaptive**

- **Keywords Area**
- **method**
- **stoch_collocation**
- **h_refinement**
- **local_adaptive**

Planned future capability for local pointwise refinement within a generalized sparse grid.

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

Sparse grid interpolation admits approaches for pointwise local refinement within the general framework of generalized sparse grids. This algorithmic capability is currently in a partial prototype stage.

**piecewise**

- **Keywords Area**
- **method**
- **stoch_collocation**
- **piecewise**

Use piecewise local basis functions

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** extended (Askey + numerically-generated)

**Description**

SC also supports the option of piecewise local basis functions. These are piecewise linear splines, or in the case of gradient-enhanced interpolation via the use_derivatives specification, piecewise cubic Hermite splines. Both of these basis selections provide local support only over the range from the interpolated point to its nearest 1D neighbors (within a tensor grid or within each of the tensor grids underlying a sparse grid), which exchanges the fast convergence of global bases for smooth functions for robustness in the representation of nonsmooth response functions (that can induce Gibbs oscillations when using high-order global basis functions). When local basis functions are used, the usage of nonequidistant collocation points (e.g., the Gauss point selections described above) is not well motivated, so equidistant Newton-Cotes points are employed in this case, and all random variable types are transformed to standard uniform probability space.
askey

- Keywords Area
- method
- stoch_collocation
- askey

Select the standardized random variables (and associated basis polynomials) from the Askey family that best match the user-specified random variables.

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** extended (Askey + numerically-generated)

**Description**

The Askey option employs standard normal, standard uniform, standard exponential, standard beta, and standard gamma random variables in a transformed probability space. These selections correspond to Hermite, Legendre, Laguerre, Jacobi, and generalized Laguerre orthogonal polynomials, respectively.

Specific mappings for the basis polynomials are based on a closest match criterion, and include Hermite for normal (optimal) as well as bounded normal, lognormal, bounded lognormal, gumbel, frechet, and weibull (sub-optimal); Legendre for uniform (optimal) as well as loguniform, triangular, and bin-based histogram (sub-optimal); Laguerre for exponential (optimal); Jacobi for beta (optimal); and generalized Laguerre for gamma (optimal).

**See Also**

These keywords may also be of interest:

- polynomial_chaos
- wiener

**wiener**

- Keywords Area
- method
- stoch_collocation
- wiener

Use standard normal random variables (along with Hermite orthogonal basis polynomials) when transforming to a standardized probability space.
6.2. METHOD

Specification

Alias: none
Argument(s): none
Default: extended (Askey + numerically-generated)

Description

The Wiener option employs standard normal random variables in a transformed probability space, corresponding to a Hermite orthogonal polynomial basis. This is the same nonlinear variable transformation used by local and global reliability methods (and therefore has the same variable support).

See Also

These keywords may also be of interest:

- polynomial_chaos
- askey

quadrature_order_sequence

- Keywords Area
- method
- stoch_collocation
- quadrature_order_sequence

Order for tensor-products of Gaussian quadrature rules

Specification

Alias: none
Argument(s): INTEGERLIST

Description

Multidimensional integration by a tensor-product of Gaussian quadrature rules (specified with quadrature_order, and, optionally, dimension_preference). The default rule selection is to employ non_nested Gauss rules including Gauss-Hermite (for normals or transformed normals), Gauss-Legendre (for uniforms or transformed uniforms), Gauss-Jacobi (for betas), Gauss-Laguerre (for exponentials), generalized Gauss-Laguerre (for gammas), and numerically-generated Gauss rules (for other distributions when using an Extended basis). For the case of p_refinement or the case of an explicit nested override, Gauss-Hermite rules are replaced with Genz-Keister nested rules and Gauss-Legendre rules are replaced with Gauss-Patterson nested rules, both of which exchange lower integrand precision for greater point reuse. By specifying a dimension_preference, where higher preference leads to higher order polynomial resolution, the tensor grid may be rendered anisotropic. The dimension specified to have highest preference will be set to the specified quadrature_order and all other dimensions will be reduced in proportion to their reduced preference; any non-integral portion is truncated. To synchronize with tensor-product integration, a tensor-product expansion is used, where the order \( p_i \) of the expansion in each dimension is selected to be half of the integrand precision available from the rule in use,
rounded down. In the case of non-nested Gauss rules with integrand precision $2m_i - 1$, $p_i$ is one less than the quadrature order $m_i$ in each dimension (a one-dimensional expansion contains the same number of terms, $p + 1$, as the number of Gauss points). The total number of terms, $N$, in a tensor-product expansion involving $n$ uncertain input variables is

$$N = 1 + P = \prod_{i=1}^{n} (p_i + 1)$$

In some advanced use cases (e.g., multifidelity UQ), multiple grid resolutions can be employed; for this reason, the `quadrature_order` specification supports an array input.

**Usage Tips**

For most use cases, this keyword will specify a single integer order. In more advanced UQ studies with hierarchical models, the list of integers can apply to different models and/or model levels

**sparse_grid_level_sequence**

- **Keywords Area**
- **method**
- **stoch_collocation**
- **sparse_grid_level_sequence**

Level to use in sparse grid integration or interpolation

**Specification**

**Alias:** none

**Argument(s):** INTEGERLIST

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional (Choose One)</td>
<td></td>
<td>restricted</td>
<td>Level to use in sparse grid integration or interpolation</td>
</tr>
<tr>
<td>unrestricted</td>
<td></td>
<td>restricted</td>
<td>Override the default restriction of growth rates for nested and non-nested rules that are by default synchronized for consistency.</td>
</tr>
</tbody>
</table>
6.2. METHOD

<table>
<thead>
<tr>
<th>Optional (Choose One)</th>
<th>Group 2</th>
<th>nodal</th>
<th>Level to use in sparse grid integration or interpolation</th>
</tr>
</thead>
<tbody>
<tr>
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<td>hierarchical</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Level to use in sparse grid integration or interpolation</td>
</tr>
</tbody>
</table>

**Description**

Multi-dimensional integration by the Smolyak sparse grid method (specified with `sparse_grid_level` and, optionally, `dimension_preference`). The underlying one-dimensional integration rules are the same as for the tensor-product quadrature case; however, the default rule selection is nested for sparse grids (Genz-Keister for normals/transformed normals and Gauss-Patterson for uniforms/transformed uniforms). This default can be overridden with an explicit non_nested specification (resulting in Gauss-Hermite for normals/transformed normals and Gauss-Legendre for uniforms/transformed uniforms). As for tensor quadrature, the `dimension_preference` specification enables the use of anisotropic sparse grids (refer to the PCE description in the User’s Manual for the anisotropic index set constraint definition). Similar to anisotropic tensor grids, the dimension with greatest preference will have resolution at the full `sparse_grid_level` and all other dimension resolutions will be reduced in proportion to their reduced preference. For PCE with either isotropic or anisotropic sparse grids, a summation of tensor-product expansions is used, where each anisotropic tensor-product quadrature rule underlying the sparse grid construction results in its own anisotropic tensor-product expansion as described in case 1. These anisotropic tensor-product expansions are summed into a sparse PCE using the standard Smolyak summation (again, refer to the User’s Manual for additional details). As for quadrature order, the `sparse_grid_level` specification admits an array input for enabling specification of multiple grid resolutions used by certain advanced solution methodologies.

**Usage Tips**

This keyword can be used when using sparse grid integration to calculate PCE coefficients or when generating samples for sparse grid collocation.

For most use cases, this keyword will specify a single integer level. In more advanced UQ studies with hierarchical models, the list of integers can apply to different models and/or model levels

---

**restricted**

- Keywords Area
- method
- stoch_collocation
- `sparse_grid_level_sequence`
- restricted

Level to use in sparse grid integration or interpolation
Specification

Alias: none

Argument(s): none

Default: restricted (except for generalized sparse grids)

Description

Multi-dimensional integration by the Smolyak sparse grid method (specified with sparse_grid_level and, optionally, dimension_preference). The underlying one-dimensional integration rules are the same as for the tensor-product quadrature case; however, the default rule selection is nested for sparse grids (Genz-Keister for normals/transformed normals and Gauss-Patterson for uniforms/transformed uniforms). This default can be overridden with an explicit non_nested specification (resulting in Gauss-Hermite for normals/transformed normals and Gauss-Legendre for uniforms/transformed uniforms). As for tensor quadrature, the dimension_preference specification enables the use of anisotropic sparse grids (refer to the PCE description in the User’s Manual for the anisotropic index set constraint definition). Similar to anisotropic tensor grids, the dimension with greatest preference will have resolution at the full sparse_grid_level and all other dimension resolutions will be reduced in proportion to their reduced preference. For PCE with either isotropic or anisotropic sparse grids, a summation of tensor-product expansions is used, where each anisotropic tensor-product quadrature rule underlying the sparse grid construction results in its own anisotropic tensor-product expansion as described in case 1. These anisotropic tensor-product expansions are summed into a sparse PCE using the standard Smolyak summation (again, refer to the User’s Manual for additional details). As for quadrature_order, the sparse_grid_level specification admits an array input for enabling specification of multiple grid resolutions used by certain advanced solution methodologies.

Usage Tips

This keyword can be used when using sparse grid integration to calculate PCE coefficients or when generating samples for sparse grid collocation.

For most use cases, this keyword will specify a single integer level. In more advanced UQ studies with hierarchical models, the list of integers can apply to different models and/or model levels

unrestricted

- Keywords Area
- method
- stoch_collocation
- sparse_grid_level_sequence
- unrestricted

Override the default restriction of growth rates for nested and non-nested rules that are by default synchronized for consistency.

Specification

Alias: none

Argument(s): none
6.2. METHOD

Description

In the quadrature and sparse grid cases, growth rates for nested and non-nested rules can be synchronized for consistency. For a non-nested Gauss rule used within a sparse grid, linear one-dimensional growth rules of \( m = 2l + 1 \) are used to enforce odd quadrature orders, where \( l \) is the grid level and \( m \) is the number of points in the rule. The precision of this Gauss rule is then \( i = 2m - 1 = 4l + 1 \). For nested rules, order growth with level is typically exponential; however, the default behavior is to restrict the number of points to be the lowest order rule that is available that meets the one-dimensional precision requirement implied by either a level \( l \) for a sparse grid (\( i = 4l + 1 \)) or an order \( m \) for a tensor grid (\( i = 2m - 1 \)). This behavior is known as "restricted growth" or "delayed sequences." To override this default behavior in the case of sparse grids, the unrestricted keyword can be used; it cannot be overridden for tensor grids using nested rules since it also provides a mapping to the available nested rule quadrature orders. An exception to the default usage of restricted growth is the dimension_adaptive p_refinement generalized sparse grid case described previously, since the ability to evolve the index sets of a sparse grid in an unstructured manner eliminates the motivation for restricting the exponential growth of nested rules.

nodal

- Keywords Area
- method
- stoch_collocation
- sparse_grid_level_sequence
- nodal

Level to use in sparse grid integration or interpolation

Specification

Alias: none

Argument(s): none

Default: nodal

Description

Multi-dimensional integration by the Smolyak sparse grid method (specified with sparse_grid_level and, optionally, dimension_preference). The underlying one-dimensional integration rules are the same as for the tensor-product quadrature case; however, the default rule selection is nested for sparse grids (Genz-Keister for normals/transformed normals and Gauss-Patterson for uniforms/transformed uniforms). This default can be overridden with an explicit non_nested specification (resulting in Gauss-Hermite for normals/transformed normals and Gauss-Legendre for uniforms/transformed uniforms). As for tensor quadrature, the dimension_preference specification enables the use of anisotropic sparse grids (refer to the PCE description in the User’s Manual for the anisotropic index set constraint definition). Similar to anisotropic tensor grids, the dimension with greatest preference will have resolution at the full sparse_grid_level and all other dimension resolutions will be reduced in proportion to their reduced preference. For PCE with either isotropic or anisotropic sparse grids, a summation of tensor-product expansions is used, where each anisotropic tensor-product quadrature rule underlying the sparse grid construction results in its own anisotropic tensor-product expansion as described in case 1. These anisotropic tensor-product expansions are summed into a sparse PCE using the standard Smolyak summation (again, refer to the User’s Manual for additional details). As for quadrature_order, the sparse_grid_level specification admits an
array input for enabling specification of multiple grid resolutions used by certain advanced solution methodologies.

Usage Tips
This keyword can be used when using sparse grid integration to calculate PCE coefficients or when generating samples for sparse grid collocation.

For most use cases, this keyword will specify a single integer level. In more advanced UQ studies with hierarchical models, the list of integers can apply to different models and/or model levels.

**hierarchical**

- Keywords Area
- method
- stoch_collocation
- sparse_grid_level_sequence
- hierarchical

Level to use in sparse grid integration or interpolation

**Specification**

**Alias**: none

**Argument(s)**: none

**Description**
Multi-dimensional integration by the Smolyak sparse grid method (specified with `sparse_grid_level` and, optionally, `dimension_preference`). The underlying one-dimensional integration rules are the same as for the tensor-product quadrature case; however, the default rule selection is nested for sparse grids (Genz-Keister for normals-transformed normals and Gauss-Patterson for uniforms-transformed uniforms). This default can be overridden with an explicit non_nested specification (resulting in Gauss-Hermite for normals-transformed normals and Gauss-Legendre for uniforms-transformed uniforms). As for tensor quadrature, the `dimension_preference` specification enables the use of anisotropic sparse grids (refer to the PCE description in the User’s Manual for the anisotropic index set constraint definition). Similar to anisotropic tensor grids, the dimension with greatest preference will have resolution at the full `sparse_grid_level` and all other dimension resolutions will be reduced in proportion to their reduced preference. For PCE with either isotropic or anisotropic sparse grids, a summation of tensor-product expansions is used, where each anisotropic tensor-product quadrature rule underlying the sparse grid construction results in its own anisotropic tensor-product expansion as described in case 1. These anisotropic tensor-product expansions are summed into a sparse PCE using the standard Smolyak summation (again, refer to the User’s Manual for additional details). As for quadrature order, the `sparse_grid_level` specification admits an array input for enabling specification of multiple grid resolutions used by certain advanced solution methodologies.

Usage Tips
This keyword can be used when using sparse grid integration to calculate PCE coefficients or when generating samples for sparse grid collocation.

For most use cases, this keyword will specify a single integer level. In more advanced UQ studies with hierarchical models, the list of integers can apply to different models and/or model levels.
6.2. METHOD

**dimension_preference**
- Keywords Area
- method
- stoch_collocation
- dimension_preference

A set of weights specifying the relative importance of each uncertain variable (dimension)

**Specification**
- **Alias:** none
- **Argument(s):** REALLIST
- **Default:** isotropic grids

**Description**
A set of weights specifying the relative importance of each uncertain variable (dimension). Using this specification leads to anisotropic integrations with differing refinement levels for different random dimensions.

**See Also**
These keywords may also be of interest:
- sobol
- decay

**use_derivatives**
- Keywords Area
- method
- stoch_collocation
- use_derivatives

Use derivative data to construct surrogate models

**Specification**
- **Alias:** none
- **Argument(s):** none
- **Default:** use function values only

**Description**
The `use_derivatives` flag specifies that any available derivative information should be used in global approximation builds, for those global surrogate types that support it (currently, polynomial regression and the Surfpack Gaussian process).
- However, its use with Surfpack Gaussian process is not recommended.
nested

- Keywords Area
- method
- stoch_collocation
- nested

Enforce use of nested quadrature rules if available

**Specification**

Alias: none

Argument(s): none

Default: quadrature: non_nested unless automated refinement; sparse grids: nested

**Description**

Enforce use of nested quadrature rules if available. For instance if the aleatory variables are Gaussian use the Nested Genz-Keister rule instead of the default non-nested Gauss-Hermite rule variables are non_nested

non_nested

- Keywords Area
- method
- stoch_collocation
- non_nested

Enforce use of non-nested quadrature rules

**Specification**

Alias: none

Argument(s): none

**Description**

Enforce use of non-nested quadrature rules if available. For instance if the aleatory variables are Gaussian use the non-nested Gauss-Hermite rule

**variance_based_decomp**

- Keywords Area
- method
- stoch_collocation
- variance_based_decomp

Activates global sensitivity analysis based on decomposition of response variance into main, interaction, and total effects
Specification

Alias: none

Argument(s): none

Default: no variance-based decomposition

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>interaction_order</td>
<td>Specify the maximum number of variables allowed in an interaction when reporting interaction metrics. Suppressed output of sensitivity indices with values lower than this tolerance</td>
</tr>
<tr>
<td></td>
<td></td>
<td>drop_tolerance</td>
<td></td>
</tr>
</tbody>
</table>

Description

Dakota can calculate sensitivity indices through variance-based decomposition using the keyword `variance_based_decomp`. This approach decomposes main, interaction, and total effects in order to identify the most important variables and combinations of variables in contributing to the variance of output quantities of interest.

Default Behavior

Because of processing overhead and output volume, `variance_based_decomp` is inactive by default, unless required for dimension-adaptive refinement using Sobol' indices.

Expected Outputs

When `variance_based_decomp` is specified, sensitivity indices for main effects, total effects, and any interaction effects will be reported. Each of these effects represents the percent contribution to the variance in the model response, where main effects include the aggregated set of univariate terms for each individual variable, interaction effects represent the set of mixed terms (the complement of the univariate set), and total effects represent the complete set of terms (univariate and mixed) that contain each individual variable. The aggregated set of main and interaction sensitivity indices will sum to one, whereas the sum of total effects sensitivity indices will be greater than one due to redundant counting of mixed terms.

Usage Tips

An important consideration is that the number of possible interaction terms grows exponentially with dimension and expansion order. To mitigate this, both in terms of compute time and output volume, possible interaction effects are suppressed whenever no contributions are present due to the particular form of an expansion. In addition, the `interaction_order` and `drop_tolerance` controls can further limit the computational and output requirements.

Examples

```plaintext
method,
  polynomial_chaos # or stoch_collocation
  sparse_grid_level = 3
  variance_based_decomp interaction_order = 2
```
Theory

In this context, we take sensitivity analysis to be global, not local as when calculating derivatives of output variables with respect to input variables. Our definition is similar to that of [73]: “The study of how uncertainty in the output of a model can be apportioned to different sources of uncertainty in the model input.”

Variance based decomposition is a way of using sets of samples to understand how the variance of the output behaves, with respect to each input variable. A larger value of the sensitivity index, $S_i$, means that the uncertainty in the input variable $i$ has a larger effect on the variance of the output. More details on the calculations and interpretation of the sensitivity indices can be found in [87].

interaction_order

- Keywords Area
- method
- stoch_collocation
- variance_based_decomp
- interaction_order

Specify the maximum number of variables allowed in an interaction when reporting interaction metrics.

Specification

Alias: none

Argument(s): INTEGER

Default: Unrestricted (VBD includes all interaction orders present in the expansion)

Description

The interaction_order option has been added to allow suppression of higher-order interactions, since the output volume (and memory and compute consumption) of these results could be extensive for high dimensional problems (note: the previous univariate_effects specification is equivalent to interaction_order = 1 in the current specification). Similar to suppression of interactions is the covariance control, which can be selected to be diagonal_covariance or full_covariance, with the former supporting suppression of the off-diagonal covariance terms (to again save compute and memory resources and reduce output volume)

drop_tolerance

- Keywords Area
- method
- stoch_collocation
- variance_based_decomp
- drop_tolerance

Suppresses output of sensitivity indices with values lower than this tolerance
6.2. METHOD

Specification

Alias: none

Argument(s): REAL
Default: All VBD indices displayed

Description

The drop_tolerance keyword allows the user to specify a value below which sensitivity indices generated by variance_based_decomp are not displayed.

Default Behavior
By default, all sensitivity indices generated by variance_based_decomp are displayed.

Usage Tips
For polynomial_chaos, which outputs main, interaction, and total effects by default, the univariate-effects may be a more appropriate option. It allows suppression of the interaction effects since the output volume of these results can be prohibitive for high dimensional problems. Similar to suppression of these interactions is the covariance control, which can be selected to be diagonal_covariance or full_covariance, with the former supporting suppression of the off-diagonal covariance terms (to save compute and memory resources and reduce output volume).

Examples

```plaintext
def method, sampling
    sample_type lhs
    samples = 100
    variance_based_decomp
    drop_tolerance = 0.001
```

diagonal_covariance

- Keywords Area
- method
- stoch_collocation
- diagonal_covariance

Display only the diagonal terms of the covariance matrix

Specification

Alias: none

Argument(s): none
Default: diagonal_covariance for response vector > 10; else full_covariance

Description

With a large number of responses, the covariance matrix can be very large. diagonal_covariance is used to suppress the off-diagonal covariance terms (to save compute and memory resources and reduce output volume).
full_covariance

- Keywords Area
- method
- stoch_collocation
- full_covariance

Display the full covariance matrix

Specification

Alias: none
Argument(s): none

Description

With a large number of responses, the covariance matrix can be very large. full_covariance is used to force Dakota to output the full covariance matrix.

sample_type

- Keywords Area
- method
- stoch_collocation
- sample_type

Selection of sampling strategy

Specification

Alias: none
Argument(s): none
Default: lhs

<table>
<thead>
<tr>
<th>Required/Optional Required</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Choose One</td>
<td>Group 1</td>
<td>lhs</td>
<td>Uses Latin Hypercube Sampling (LHS) to sample variables</td>
</tr>
</tbody>
</table>
6.2. **METHOD**

| random | Uses purely random Monte Carlo sampling to sample variables |

**Description**

The `sample_type` keyword allows the user to select between two types of sampling: Monte Carlo (pure random) and Latin hypercube (stratified) sampling.

The incremental keywords are deprecated; instead use `samples` together with `refinement_samples`.

**Default Behavior**

If the `sample_type` keyword is present, it must be accompanied by `lhs` or `random`. In most contexts, `lhs` is the default (exception: multilevel_sampling uses Monte Carlo by default).

**Examples**

```
method
   sampling
      sample_type lhs
      samples = 20
      seed = 83921
```

**lhs**

- **Keywords Area**
- **method**
- **stoch_collocation**
- **sample_type**
- **lhs**

Uses Latin Hypercube Sampling (LHS) to sample variables

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

The `lhs` keyword invokes Latin Hypercube Sampling as the means of drawing samples of uncertain variables according to their probability distributions. This is a stratified, space-filling approach that selects variable values from a set of equi-probable bins.

**Default Behavior**

Latin Hypercube Sampling is the default sampling mode in most contexts (exception: multilevel_sampling). To explicitly specify LHS in the Dakota input file, the `lhs` keyword must appear in conjunction with the `sample_type` keyword.

**Usage Tips**
Latin Hypercube Sampling is very robust and can be applied to any problem. It is fairly effective at estimating the mean of model responses and linear correlations with a reasonably small number of samples relative to the number of variables.

Examples

```
method
  sampling
    sample_type lhs
    samples = 20
```

random

- Keywords Area
- method
- stoch_collocation
- sample_type
- random

Uses purely random Monte Carlo sampling to sample variables

Specification

Alias: none

Argument(s): none

Description

The random keyword invokes Monte Carlo sampling as the means of drawing samples of uncertain variables according to their probability distributions.

Default Behavior

In most contexts, Monte Carlo sampling is not the default sampling mode (exception: multilevel_sampling). To change this behavior, the random keyword must be specified in conjunction with the sample_type keyword.

Usage Tips

Monte Carlo sampling is more computationally expensive than Latin Hypercube Sampling as it requires a larger number of samples to accurately estimate statistics.

Examples

```
method
  sampling
    sample_type random
    samples = 200
```
6.2. METHOD

probability_refinement

- Keywords Area
- method
- stoch_collocation
- probability_refinement

Allow refinement of probability and generalized reliability results using importance sampling

Topics

This keyword is related to the topics:
- reliability_methods

Specification

Alias: sample_refinement
Argument(s): none

<table>
<thead>
<tr>
<th>Required/ Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required (Choose One)</td>
<td>Group 1</td>
<td>import</td>
<td>Sampling option</td>
</tr>
<tr>
<td></td>
<td></td>
<td>adapt_import</td>
<td>Importance sampling option</td>
</tr>
<tr>
<td></td>
<td></td>
<td>mm_adapt_import</td>
<td>Sampling option</td>
</tr>
</tbody>
</table>

| Optional | | refinement_samples | | |
| Number of samples used to refine a probability estimate or sampling design. |

Description

The probability_refinement allows refinement of probability and generalized reliability results using importance sampling. If one specifies probability_refinement, there are some additional options. One can specify which type of importance sampling to use (import, adapt_import, or mm_adapt_import). Additionally, one can specify the number of refinement samples to use with refinement_samples and the seed to use with seed.

The probability_refinement density reweighting accounts originally was developed based on Gaussian distributions. It now accounts for additional non-Gaussian cases.

import

- Keywords Area
- method
- stoch_collocation
CHAPTER 6. KEYWORDS AREA

- probability_refinement
- import

Sampling option

Specification

Alias: none
Argument(s): none

Description

import centers a sampling density at one of the initial LHS samples identified in the failure region. It then generates the importance samples, weights them by their probability of occurrence given the original density, and calculates the required probability (CDF or CCDF level).

adapt_import

- Keywords Area
- method
- stoch_collocation
- probability_refinement
- adapt_import

Importance sampling option

Specification

Alias: none
Argument(s): none

Description

adapt_import centers a sampling density at one of the initial LHS samples identified in the failure region. It then generates the importance samples, weights them by their probability of occurrence given the original density, and calculates the required probability (CDF or CCDF level). This continues iteratively until the failure probability estimate converges.

mm_adapt_import

- Keywords Area
- method
- stoch_collocation
- probability_refinement
- mm_adapt_import

Sampling option
6.2. METHOD

Specification

Alias: none
Argument(s): none

Description

**mm_adapt_import** starts with all of the samples located in the failure region to build a multimodal sampling density. First, it uses a small number of samples around each of the initial samples in the failure region. Note that these samples are allocated to the different points based on their relative probabilities of occurrence: more probable points get more samples. This early part of the approach is done to search for "representative" points. Once these are located, the multimodal sampling density is set and then **mm_adapt_import** proceeds similarly to **adapt_import** (sample until convergence).

**refinement_samples**
- Keywords Area
- method
- stoch_collocation
- probability_refinement
- refinement_samples

Number of samples used to refine a probability estimate or sampling design.

Specification

Alias: none
Argument(s): INTEGERLIST

Description

Probability estimate: Specify the (scalar) number of samples used to improve a probability estimate. If using uni-modal sampling all samples are assigned to the sampling center. If using multi-modal sampling the samples are split between multiple samples according to some internally computed weights.

Sampling design: Specify one or a sequence of refinement samples to augment the initial_samples in a sampling design.

**import_approx_points_file**
- Keywords Area
- method
- stoch_collocation
- import_approx_points_file

Filename for points at which to evaluate the PCE/SC surrogate
CHAPTER 6. KEYWORDS AREA

**Specification**

**Alias:** none

**Argument(s):** STRING

**Default:** no point import from a file

| Required/- | Description of Group Tabular Format (Group 1) | Dakota Keyword | Dakota Keyword Description |
| Optional | | annotated | Selects annotated tabular file format |
| custom.annotated | | custom.annotated | Selects custom-annotated tabular file format |
| freeform | | freeform | Selects freeform file format |
| active_only | | active_only | Import only active variables from tabular data file |

**Description**

**Default Behavior** No import of points at which to evaluate the surrogate.

**Expected Output** The PCE/SC surrogate model will be evaluated at the list of points (input variable values) provided in the file and results tabulated and/or statistics computed at them, depending on the method context.

**Examples**

```plaintext
method
   polynomial_chaos
       expansion_order = 4
       import_approx_points_file = 'import.mcmc_annot.dat'
       annotated
```

annotated

- Keywords Area
- method
- stoch_collocation
- import_approx_points_file
- annotated

Selects annotated tabular file format

**Topics**

This keyword is related to the topics:

- file_formats
6.2. METHOD

Specification

Alias: none
Argument(s): none
Default: annotated format

Description

An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior

By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips

• To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify custom_annotated
header eval_id

• Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to
annotated format, though freeform remains an option.

• When importing tabular data, a warning will be generated if a specific number of data are expected, but
extra is found and an error generated when there is insufficient data.

• Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

environment
  tabular_data
    tabular_data_file = 'dakota_summary.dat'
    annotated

Resulting tabular file:

<table>
<thead>
<tr>
<th>eval_id</th>
<th>interface</th>
<th>x1</th>
<th>x2</th>
<th>obj_fn</th>
<th>nln_ineq_con_1</th>
<th>nln_ineq_con_2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>NO_ID</td>
<td>0.9</td>
<td>1.1</td>
<td>0.0002</td>
<td>0.26</td>
<td>0.76</td>
</tr>
<tr>
<td>2</td>
<td>NO_ID</td>
<td>0.90009</td>
<td>1.1</td>
<td>0.0001996404857</td>
<td>0.2601620081</td>
<td>0.759955</td>
</tr>
<tr>
<td>3</td>
<td>NO_ID</td>
<td>0.89991</td>
<td>1.1</td>
<td>0.0002003604863</td>
<td>0.2598380081</td>
<td>0.760045</td>
</tr>
<tr>
<td>...</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

custom_annotated

• Keywords Area

• method

• stoch_collocation

• import_approx_points_file

• custom_annotated

Selects custom-annotated tabular file format
Topics

This keyword is related to the topics:

- file formats

Specification

Alias: none
Argument(s): none
Default: annotated format

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>header</td>
<td>Enable header row in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>eval_id</td>
<td>Enable evaluation ID column in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>interface_id</td>
<td>Enable interface ID column in custom-annotated tabular file</td>
</tr>
</tbody>
</table>

Description

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

Default Behavior

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom.annotated, followed by options, in the relevant export/import context.

Usage Tips

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:
6.2. METHOD

environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
custom_annotated header eval_id

Resulting tabular file:

<table>
<thead>
<tr>
<th>eval_id</th>
<th>x1</th>
<th>x2</th>
<th>obj_fn</th>
<th>nln_ineq_con_1</th>
<th>nln_ineq_con_2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.9</td>
<td>1.1</td>
<td>0.0002</td>
<td>0.26</td>
<td>0.76</td>
</tr>
<tr>
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<td>1.1</td>
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<td>0.759955</td>
</tr>
<tr>
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<td>0.89991</td>
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<td>0.0002003604863</td>
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<td>0.760045</td>
</tr>
<tr>
<td>...</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

header

- Keywords Area
- method
- stoch_collocation
- import_approx_points_file
- custom_annotated
- header

Enable header row in custom-annotated tabular file

Specification

Alias: none
  Argument(s): none
  Default: no header

Description

See description of parent custom_annotated

eval_id

- Keywords Area
- method
- stoch_collocation
- import_approx_points_file
- custom_annotated
- eval_id

Enable evaluation ID column in custom-annotated tabular file
**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no eval_id column

**Description**

See description of parent `custom_annotated`

`interface_id`

- Keywords Area
- method
- stoch_collocation
- import_approx_points_file
- custom_annotated
- interface_id

Enable interface ID column in custom-annotated tabular file

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no interface_id column

**Description**

See description of parent `custom_annotated`

`freeform`

- Keywords Area
- method
- stoch_collocation
- import_approx_points_file
- freeform

Selects freeform file format

**Topics**

This keyword is related to the topics:

- file_formats
6.2. METHOD

Specification

Alias: none
Argument(s): none
Default: annotated format

Description

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior

The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips

- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```plaintext
environment
  tabular_data
  tabular_data_file = 'dakota_summary.dat'
  freeform

Resulting tabular file:

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>0.9</td>
<td>1.1</td>
<td>0.0002</td>
<td>0.26</td>
<td>0.76</td>
</tr>
<tr>
<td>0.90009</td>
<td>1.1</td>
<td>0.0001996404857</td>
<td>0.2601620081</td>
<td>0.759955</td>
</tr>
<tr>
<td>0.89991</td>
<td>1.1</td>
<td>0.0002003604863</td>
<td>0.2598380081</td>
<td>0.760045</td>
</tr>
</tbody>
</table>
```

active_only

- Keywords Area
- method
- stoch_collocation
- import_approx_points_file
- active_only

Import only active variables from tabular data file
Topics
This keyword is related to the topics:

- file formats

Specification
Alias: none
Argument(s): none

Description
By default, files for tabular data imports are expected to contain columns for all variables, active and inactive. The keyword `active_only` indicates that the file to import contains only the active variables.

This option should only be used in contexts where the inactive variables have no influence, for example, building a surrogate over active variables, with the state variables held at nominal. It should not be used in more complex nested contexts, where the values of inactive variables are relevant to the function evaluations used to build the surrogate.

**export_approx_points_file**

- Keywords Area
- method
- stoch_collocation
- export_approx_points_file

Output file for evaluations of a surrogate model

Specification
Alias: export_points_file
Argument(s): STRING
Default: no point export to a file

<table>
<thead>
<tr>
<th>Required-/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional(Choose One)</td>
<td>Tabular Format (Group 1)</td>
<td>annotated</td>
<td>Selects annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>custom_annotated</td>
<td>Selects custom-annotated tabular file format</td>
</tr>
</tbody>
</table>
6.2. METHOD

|          |          |          | freeform | Selects freeform file format |

**Description**

The `export_approx_points_file` keyword allows the user to specify a file in which the points (input variable values) at which the surrogate model is evaluated and corresponding response values computed by the surrogate model will be written. The response values are the surrogate’s predicted approximation to the truth model responses at those points.

**Usage Tips**

Dakota exports tabular data in one of three formats:

- annotated (default)
- custom_annotated
- freeform

**annotated**

- Keywords Area
- method
- stoch_collocation
- `export_approx_points_file`
- annotated
  
  Selects annotated tabular file format

**Topics**

This keyword is related to the topics:

- `file_formats`

**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** annotated format

**Description**

An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

**Default Behavior**

By default, Dakota imports and exports tabular files in annotated format. The `annotated` keyword can be used to explicitly specify this.

**Usage Tips**
To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify `custom_annotated`.

Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to `annotated` format, though `freeform` remains an option.

When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the `freeform` option.

**Examples**

Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```plaintext
environment
  tabular_data
    tabular_data_file = 'dakota_summary.dat'
    annotated

Resulting tabular file:

```
%eval_id interface x1  x2  obj_fn nln_ineq_con_1 nln_ineq_con_2
1   NO_ID   0.9  1.1  0.0002     0.26    0.76
2   NO_ID  0.90009 1.1  0.0001996404857  0.2601620081  0.759955
3   NO_ID  0.89991 1.1  0.0002003604863  0.2598380081  0.760045
...```

**Keywords Area**

- **method**
- **stoch_collocation**
- **export_approx_points_file**
- **custom_annotated**

Selects custom-annotated tabular file format

**Topics**

This keyword is related to the topics:

- **file_formats**

**Specification**

*Alias:* none

*Argument(s):* none

*Default:* annotated format
6.2. METHOD

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>header</td>
<td>Enable header row in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>eval_id</td>
<td>Enable evaluation ID column in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>interface_id</td>
<td>Enable interface ID column in custom-annotated tabular file</td>
</tr>
</tbody>
</table>

**Description**

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

**Default Behavior**

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

**Usage Tips**

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

**Examples**

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:

```plaintext
environment
  tabular_data
  tabular_data_file = 'dakota_summary.dat'
  custom_annotated header eval_id
```

Resulting tabular file:

```plaintext
%eval_id  x1  x2  obj_fn  nln_ineq_con_1  nln_ineq_con_2
1  0.9  1.1  0.0002  0.26  0.76
2  0.90009  1.1  0.0001996404857  0.2601620081  0.759955
3  0.89991  1.1  0.0002003604863  0.2598380081  0.760045
...
```
header

• Keywords Area

• method

• stoch_collocation

• export_approx_points_file

• custom_annotated

• header

Enable header row in custom-annotated tabular file

**Specification**

Alias: none

Argument(s): none

Default: no header

**Description**

See description of parent `custom_annotated`

eval_id

• Keywords Area

• method

• stoch_collocation

• export_approx_points_file

• custom_annotated

• eval_id

Enable evaluation ID column in custom-annotated tabular file

**Specification**

Alias: none

Argument(s): none

Default: no eval_id column

**Description**

See description of parent `custom_annotated`
interface_id

- Keywords Area
- method
- stoch_collocation
- export_approx_points_file
- custom.annotated
- interface_id

Enable interface ID column in custom-annotated tabular file

**Specification**

Alias: none

Argument(s): none

Default: no interface_id column

**Description**

See description of parent custom.annotated

freeform

- Keywords Area
- method
- stoch_collocation
- export_approx_points_file
- freeform

Selects freeform file format

**Topics**

This keyword is related to the topics:

- fileFormats

**Specification**

Alias: none

Argument(s): none

Default: annotated format
CHAPTER 6. KEYWORDS AREA

Description
A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior
The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips
- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples
Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
freeform
```

Resulting tabular file:

```
0.9 1.1 0.0002 0.26 0.76
0.90009 1.1 0.0001996404857 0.2601620081 0.759955
0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...
```

reliability_levels

- Keywords Area
- method
- stoch_collocation
- reliability_levels

Specify reliability levels at which the response values will be estimated

Specification
Alias: none

Argument(s): REALLIST
Default: No CDF/CCDF response levels to compute
Description
Response levels are calculated for specified CDF/CCDF reliabilities by projecting out the prescribed number of sample standard deviations from the sample mean.

Theory
Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.

In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

An inverse mapping involves computing the belief and plausibility response level for either a specified probability level or a specified generalized reliability level (two results for each level mapping in the evidence-based epistemic case, instead of the one result for each level mapping in the aleatory case).

num_reliability_levels
- Keywords Area
- method
- stoch_collocation
- reliability_levels
- num_reliability_levels

Specify which reliability_levels correspond to which response

Specification
Alias: none
Argument(s): INTEGERLIST
Default: reliability_levels evenly distributed among response functions

Description
See parent page
CHAPTER 6. KEYWORDS AREA

response_levels

- Keywords Area
- method
- stoch_collocation
- response_levels

Values at which to estimate desired statistics for each response

**Specification**

**Alias:** none

**Argument(s):** REALLIST

**Default:** No CDF/CCDF probabilities/reliabilities to compute

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>num_response_levels</td>
<td>Number of values at which to estimate desired statistics for each response</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>compute</td>
<td>Selection of statistics to compute at each response level</td>
</tr>
</tbody>
</table>

**Description**

The `response_levels` specification provides the target response values for which to compute probabilities, reliabilities, or generalized reliabilities (forward mapping).

**Default Behavior**

If `response_levels` are not specified, no statistics will be computed. If they are, probabilities will be computed by default.

**Expected Outputs**

If `response_levels` are specified, Dakota will create two tables in the standard output: a Probability Density function (PDF) histogram and a Cumulative Distribution Function (CDF) table. The PDF histogram has the lower and upper endpoints of each bin and the corresponding density of that bin. Note that the PDF histogram has bins defined by the `probability_levels` and/or `response_levels` in the Dakota input file. If there are not many levels, the histogram will be coarse. Dakota does not do anything to optimize the bin size or spacing. The CDF table has the list of response levels and the corresponding probability that the response value is less than or equal to each response level threshold.

**Usage Tips**

The `num_response_levels` is used to specify which arguments of the `response_level` correspond to which response.
6.2. **METHOD**

Examples

For example, specifying a `response_level` of 52.3 followed with `compute probabilities` will result in the calculation of the probability that the response value is less than or equal to 52.3, given the uncertain distributions on the inputs.

For an example with multiple responses, the following specification

```plaintext
response_levels = 1. 2. 3.4 10. 20. 30.
num_response_levels = 2 4 3
```

would assign the first two response levels (1., 2.) to response function 1, the next four response levels (1., 2., 3., .4) to response function 2, and the final three response levels (10., 20., 30.) to response function 3. If the `num_response_levels` key were omitted from this example, then the response levels would be evenly distributed among the response functions (three levels each in this case).

The Dakota input file below specifies a sampling method with response levels of interest.

```plaintext
method, 
  sampling, 
  samples = 100 seed = 1 
  complementary distribution
  response_levels = 3.6e+11 4.0e+11 4.4e+11
  6.0e+04 6.5e+04 7.0e+04
  3.5e+05 4.0e+05 4.5e+05

variables,
  normal_uncertain = 2 
  means = 248.89, 593.33 
  std_deviations = 12.4, 29.7 
  descriptors = 'TF1n' 'TF2n'
  uniform_uncertain = 2 
  lower_bounds = 199.3, 474.63 
  upper_bounds = 298.5, 712. 
  descriptors = 'TF1u' 'TF2u'
  weibull_uncertain = 2 
  alphas = 12., 30. 
  betas = 250., 590. 
  descriptors = 'TF1w' 'TF2w'
  histogram_bin_uncertain = 2 
  num_pairs = 3 4 
  abscissas = 5 8 10 .1 .2 .3 .4 
  counts = 17 21 0 12 24 12 0 
  descriptors = 'TF1h' 'TF2h'
  histogram_point_uncertain
  real = 1 
  num_pairs = 2 
  abscissas = 3 4 
  counts = 1 1 
  descriptors = 'TF3h'

interface,
  system asynch evaluation_concurrency = 5
  analysis_driver = 'text_book'

responses,
  response_functions = 3 
  no_gradients
  no_hessians

Given the above Dakota input file, the following excerpt from the output shows the PDF and CCDF generated. Note that the bounds on the bins of the PDF are the response values specified in the input file. The probability levels corresponding to those response values are shown in the CCDF.
Probability Density Function (PDF) histograms for each response function:

PDF for response_fn_1:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.7604749078e+11</td>
<td>3.6000000000e+11</td>
<td>5.3601733194e-12</td>
</tr>
<tr>
<td>3.6000000000e+11</td>
<td>4.0000000000e+11</td>
<td>4.2500000000e-12</td>
</tr>
<tr>
<td>4.0000000000e+11</td>
<td>4.4000000000e+11</td>
<td>3.7500000000e-12</td>
</tr>
<tr>
<td>4.4000000000e+11</td>
<td>5.4196114379e+11</td>
<td>2.2557612778e-12</td>
</tr>
</tbody>
</table>

PDF for response_fn_2:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.631154744e+04</td>
<td>6.0000000000e+04</td>
<td>2.8742313192e-05</td>
</tr>
<tr>
<td>6.0000000000e+04</td>
<td>6.5000000000e+04</td>
<td>6.4000000000e-05</td>
</tr>
<tr>
<td>6.5000000000e+04</td>
<td>7.0000000000e+04</td>
<td>4.0000000000e-05</td>
</tr>
<tr>
<td>7.0000000000e+04</td>
<td>7.8702465755e+04</td>
<td>1.0341896485e-05</td>
</tr>
</tbody>
</table>

PDF for response_fn_3:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.379673709e+05</td>
<td>3.5000000000e+05</td>
<td>4.2844660868e-06</td>
</tr>
<tr>
<td>3.5000000000e+05</td>
<td>4.0000000000e+05</td>
<td>8.6000000000e-06</td>
</tr>
<tr>
<td>4.0000000000e+05</td>
<td>4.5000000000e+05</td>
<td>1.8000000000e-06</td>
</tr>
</tbody>
</table>

Level mappings for each response function:

Complementary Cumulative Distribution Function (CCDF) for response_fn_1:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.6000000000e+11</td>
<td>5.5000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.0000000000e+11</td>
<td>3.8000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.4000000000e+11</td>
<td>2.3000000000e-01</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Complementary Cumulative Distribution Function (CCDF) for response_fn_2:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.0000000000e+04</td>
<td>6.1000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6.5000000000e+04</td>
<td>2.9000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7.0000000000e+04</td>
<td>9.0000000000e-02</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Complementary Cumulative Distribution Function (CCDF) for response_fn_3:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.5000000000e+05</td>
<td>5.2000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.0000000000e+05</td>
<td>9.0000000000e-02</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.5000000000e+05</td>
<td>0.0000000000e+00</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Theory**

Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.

In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

A forward mapping involves computing the belief and plausibility probability level for a specified response level.

**num_response_levels**

- **Keywords Area**
- **method**
- **stoch_collocation**
6.2. METHOD

- response_levels
- num_response_levels

Number of values at which to estimate desired statistics for each response

Specification

Alias: none
Argument(s): INTEGERLIST
Default: response_levels evenly distributed among response functions

Description

The num_response_levels keyword allows the user to specify the number of response values, for each response, at which estimated statistics are of interest. Statistics that can be computed are probabilities and reliabilities, both according to either a cumulative distribution function or a complementary cumulative distribution function.

Default Behavior
If num_response_levels is not specified, the response_levels will be evenly distributed among the responses.

Expected Outputs
The specific output will be determined by the type of statistics that are specified. In a general sense, the output will be a list of response level-statistic pairs that show the estimated value of the desired statistic for each response level specified.

Examples

```
method
  sampling
    samples = 100
    seed = 34785
  num_response_levels = 1 1 1
  response_levels = 0.5 0.5 0.5

compute
```

Selection of statistics to compute at each response level

Specification

Alias: none
Argument(s): none
Default: probabilities
CHAPTER 6. KEYWORDS AREA

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Group 1</strong></td>
<td></td>
<td>probabilities</td>
<td>Computes probabilities associated with response levels</td>
</tr>
<tr>
<td></td>
<td></td>
<td>reliabilities</td>
<td>Computes reliabilities associated with response levels</td>
</tr>
<tr>
<td></td>
<td></td>
<td>gen_reliabilities</td>
<td>Computes generalized reliabilities associated with response levels</td>
</tr>
<tr>
<td>Optional</td>
<td>system</td>
<td></td>
<td>Compute system reliability (series or parallel)</td>
</tr>
</tbody>
</table>

**Description**

The `compute` keyword is used to select which forward stastical mapping is calculated at each response level.

**Default Behavior**

If `response_levels` is not specified, no statistics are computed. If `response_levels` is specified but `compute` is not, probabilities will be computed by default. If both `response_levels` and `compute` are specified, then one of the following must be specified: `probabilities`, `reliabilities`, or `gen_reliabilities`.

**Expected Output**

The type of statistics specified by `compute` will be reported for each response level.

**Usage Tips**

CDF/CCDF probabilities are calculated for specified response levels using a simple binning approach. CDF/CCDF reliabilities are calculated for specified response levels by computing the number of sample standard deviations separating the sample mean from the response level.

**Examples**

```
method
  sampling
    sample_type random
    samples = 100 seed = 1
    complementary distribution
    response_levels = 3.6e+11 4.0e+11 4.4e+11
                      6.0e+04 6.5e+04 7.0e+04
                      3.5e+05 4.0e+05 4.5e+05
    compute reliabilities

  probabilities
```
6.2. METHOD

- Keywords Area
- method
- stoch_collocation
- response_levels
- compute
- probabilities

Computes probabilities associated with response levels

Specification

Alias: none
Argument(s): none

Description

The `probabilities` keyword directs Dakota to compute the probability that the model response will be below (cumulative) or above (complementary cumulative) a specified response value. This is done for every response level designated for each response.

Default Behavior

If `response_levels` is specified, the probabilities are computed by default. To explicitly specify it in the Dakota input file, though, the `probabilities` keyword should be specified in conjunction with the `compute` keyword.

Expected Outputs

The Dakota output is a set of response level-probability pairs that give the probability that the model response will be below or above the corresponding response level, depending on the distribution defined.

Examples

```dakota
method
  sampling
    sample_type random
    samples = 100 seed = 1
  complementary distribution
    response_levels = 3.6e+11 4.0e+11 4.4e+11
                      6.0e+04 6.5e+04 7.0e+04
                      3.5e+05 4.0e+05 4.5e+05
  compute probabilities
```

reliabilities

- Keywords Area
- method
- stoch_collocation
- response_levels
- compute
CHAPTER 6.  KEYWORDS AREA

- reliabilities

Computes reliabilities associated with response levels

**Specification**

Alias: none

Argument(s): none

**Description**

The `reliabilities` keyword directs Dakota to compute reliabilities according to the specified distribution for a specified response value. This is done for every response level designated for each response.

**Default Behavior**

If `response_levels` is specified, the reliabilities are not computed by default. To change this behavior, the `reliabilities` keyword should be specified in conjunction with the `compute` keyword.

**Expected Outputs**

The Dakota output is a set of response level-reliability pairs according to the distribution defined.

**Examples**

```plaintext
method
  sampling
    sample_type random
    samples = 100 seed = 1
  complementary distribution
    response_levels = 3.6e+11 4.0e+11 4.4e+11
    6.0e+04 6.5e+04 7.0e+04
    3.5e+05 4.0e+05 4.5e+05
  compute reliabilities

gen_reliabilities

- Keywords Area
- method
- stoch_collocation
- response_levels
- compute
- gen_reliabilities

Computes generalized reliabilities associated with response levels

**Specification**

Alias: none

Argument(s): none
6.2. METHOD

Description

The gen_reliabilities keyword directs Dakota to compute generalized reliabilities according to the specified distribution for a specified response value. This is done for every response level designated for each response.

Default Behavior

If response_levels is specified, the generalized reliabilities are not computed by default. To change this behavior, the gen_reliabilities keyword should be specified in conjunction with the compute keyword.

Expected Outputs

The Dakota output is a set of response level-generalized reliability pairs according to the distribution defined.

Examples

method
sampling
  sample_type random
  samples = 100 seed = 1
complementary distribution
  response_levels = 3.6e+11 4.0e+11 4.4e+11
                  6.0e+04 6.5e+04 7.0e+04
                  3.5e+05 4.0e+05 4.5e+05
  compute gen_reliabilities

system

• Keywords Area
• method
• stoch_collocation
• response_levels
• compute
• system

Compute system reliability (series or parallel)

Specification

Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/Optional Required (Choose One)</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>series</td>
<td>Aggregate response statistics assuming a series system</td>
</tr>
</tbody>
</table>
aggregate response statistics assuming a parallel system

### Description

With the system probability/reliability option, statistics for specified `response_levels` are calculated and reported assuming the response functions combine either in series or parallel to produce a total system response.

For a series system, the system fails when any one component (response) fails. The probability of failure is the complement of the product of the individual response success probabilities.

For a parallel system, the system fails only when all components (responses) fail. The probability of failure is the product of the individual response failure probabilities.

- **series**
  - `Keywords Area`
  - `method`
  - `stoch_collocation`
  - `response_levels`
  - `compute`
  - `system`
  - `series`

Aggregate response statistics assuming a series system

### Specification

**Alias:** none

**Argument(s):** none

### Description

See parent keyword `system` for description.

- **parallel**
  - `Keywords Area`
  - `method`
  - `stoch_collocation`
  - `response_levels`
  - `compute`
  - `system`
• parallel

Aggregate response statistics assuming a parallel system

Specification

Alias: none

Argument(s): none

Description

See parent keyword system for description.

distribution

• Keywords Area

• method

• stoch_collocation

• distribution

Selection of cumulative or complementary cumulative functions

Specification

Alias: none

Argument(s): none

Default: cumulative (CDF)

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>cumulative</td>
<td>Computes statistics according to cumulative functions</td>
</tr>
<tr>
<td></td>
<td></td>
<td>complementary</td>
<td>Computes statistics according to complementary cumulative functions</td>
</tr>
</tbody>
</table>

Description

The distribution keyword allows the user to select between a cumulative distribution/belief/plausibility function and a complementary cumulative distribution/belief/plausibility function. This choice affects how probabilities and reliability indices are reported.

Default Behavior

If the distribution keyword is present, it must be accompanied by either cumulative or complementary. Otherwise, a cumulative distribution will be used by default.
CHAPTER 6. KEYWORDS AREA

Expected Outputs
Output will be a set of model response-probability pairs determined according to the choice of distribution. The choice of distribution also defines the sign of the reliability or generalized reliability indices.

Examples

method
sampling
  sample_type lhs
  samples = 10
distribution cumulative

cumulative
  • Keywords Area
  • method
  • stoch_collocation
  • distribution
  • cumulative

Computes statistics according to cumulative functions

Specification
Alias: none
  Argument(s): none

Description
Statistics on model responses will be computed according to a cumulative distribution/belief/plausibility function.

Default Behavior
By default, a cumulative distribution/belief/plausibility function will be used. To explicitly specify it in the Dakota input file, however, the cumulative keyword must be appear in conjunction with the distribution keyword.

Expected Outputs
Output will be a set of model response-probability pairs determined according to a cumulative distribution/belief/plausibility function. The probabilities reported are the probabilities that the model response falls below given response thresholds.

Examples

method
  sampling
    sample_type lhs
    samples = 10
distribution cumulative
6.2. METHOD

complementary

- Keywords Area
- method
- stoch_collocation
- distribution
- complementary

Computes statistics according to complementary cumulative functions

Specification

Alias: none

Argument(s): none

Description

Statistics on model responses will be computed according to a complementary cumulative distribution/belief/plausibility function.

Default Behavior

By default, a complementary cumulative distribution/belief/plausibility function will not be used. To change that behavior, the complementary keyword must be appear in conjunction with the distribution keyword.

Expected Outputs

Output will be a set of model response-probability pairs determined according to a complementary cumulative distribution/belief/plausibility function. The probabilities reported are the probabilities that the model response falls above given response thresholds.

Examples

```
method
  sampling
    sample_type lhs
    samples = 10
    distribution complementary
```

probability_levels

- Keywords Area
- method
- stoch_collocation
- probability_levels

Specify probability levels at which to estimate the corresponding response value

Specification

Alias: none

Argument(s): REALLIST

Default: No CDF/CCDF response levels to compute
### Description

Response levels are calculated for specified CDF/CCDF probabilities by indexing into a sorted samples array (the response levels computed are not interpolated and will correspond to one of the sampled values).

**Expected Output**

If `probability_levels` are specified, Dakota will create two tables in the standard output: a Probability Density function (PDF) histogram and a Cumulative Distribution Function (CDF) table. The PDF histogram has the lower and upper endpoints of each bin and the corresponding density of that bin. Note that the PDF histogram has bins defined by the `probability_levels` and/or `response_levels` in the Dakota input file. If there are not very many levels, the histogram will be coarse. Dakota does not do anything to optimize the bin size or spacing. The CDF table has the list of response levels and the corresponding probability that the response value is less than or equal to each response level threshold.

### Examples

The Dakota input file below specifies a sampling method with probability levels of interest.

```plaintext
method,
  sampling,
  samples = 100 seed = 1
  complementary distribution
  probability_levels = 1. .66 .33 0.
    1.8 .5 0.
    1.3 .2 0.
variables,
  normal_uncertain = 2
    means = 248.89, 593.33
    std_deviations = 12.4, 29.7
    descriptors = 'TF1n' 'TF2n'
  uniform_uncertain = 2
    lower_bounds = 199.3, 474.63
    upper_bounds = 298.5, 712.
    descriptors = 'TF1u' 'TF2u'
  weibull_uncertain = 2
    alphas = 12., 30.
    betas = 250., 590.
    descriptors = 'TF1w' 'TF2w'
histogram_bin_uncertain = 2
  num_pairs = 3 4
  abscissas = 5 8 10 .1 .2 .3 .4
  counts = 17 21 0 12 24 12 0
  descriptors = 'TF1h' 'TF2h'
histogram_point_uncertain
  real = 1
  num_pairs = 2
  abscissas = 3 4
  counts = 1 1
  descriptors = 'TF3h'
```

<p>| Required/- | Description of | Dakota Keyword | Dakota Keyword |</p>
<table>
<thead>
<tr>
<th>Optional</th>
<th>Optional Group</th>
<th>num_probability_-</th>
<th>Description</th>
</tr>
</thead>
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<tr>
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<td>levels</td>
<td>specify which</td>
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<td></td>
<td></td>
<td></td>
<td>probability_-</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>levels</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>correspond to</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>which response</td>
</tr>
</tbody>
</table>
6.2. METHOD

interface,
    system asynch evaluation_concurrency = 5
    analysis_driver = 'text_book'

responses,
    response_functions = 3
    no_gradients
    no_hessians

Given the above Dakota input file, the following excerpt from the output shows the PDF and CCDF generated. Note that the bounds on the bins of the PDF are the response values that correspond to the probability levels specified in the input file. Those response values are also shown in the CCDF.

Probability Density Function (PDF) histograms for each response function:

PDF for response_fn_1:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.7604749078e+11</td>
<td>3.4221494996e+11</td>
<td>5.1384774972e-12</td>
</tr>
<tr>
<td>3.4221494996e+11</td>
<td>4.0634975300e+11</td>
<td>5.145122311e-12</td>
</tr>
<tr>
<td>4.0634975300e+11</td>
<td>5.4196114379e+11</td>
<td>2.4334239039e-12</td>
</tr>
</tbody>
</table>

PDF for response_fn_2:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.643154744e+04</td>
<td>5.6511827775e+04</td>
<td>1.983945149e-05</td>
</tr>
<tr>
<td>5.6511827775e+04</td>
<td>6.1603813790e+04</td>
<td>5.8916108390e-05</td>
</tr>
<tr>
<td>6.1603813790e+04</td>
<td>7.8702465755e+04</td>
<td>2.9242071306e-05</td>
</tr>
</tbody>
</table>

PDF for response_fn_3:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.3796737090e+05</td>
<td>3.6997214153e+05</td>
<td>5.3028386523e-06</td>
</tr>
<tr>
<td>3.6997214153e+05</td>
<td>3.8100966235e+05</td>
<td>9.0600055634e-06</td>
</tr>
<tr>
<td>3.8100966235e+05</td>
<td>4.4111498127e+05</td>
<td>3.274925348e-06</td>
</tr>
</tbody>
</table>

Level mappings for each response function:

Complementary Cumulative Distribution Function (CCDF) for response_fn_1:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.7604749078e+11</td>
<td>1.0000000000e+00</td>
<td>0.0000000000e+00</td>
<td>0.0000000000e+00</td>
</tr>
<tr>
<td>3.4221494996e+11</td>
<td>6.0000000000e-01</td>
<td>4.0000000000e-01</td>
<td>2.0000000000e-01</td>
</tr>
<tr>
<td>4.0634975300e+11</td>
<td>3.0000000000e-01</td>
<td>1.0000000000e+00</td>
<td>1.0000000000e+00</td>
</tr>
</tbody>
</table>

Complementary Cumulative Distribution Function (CCDF) for response_fn_2:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.643154744e+04</td>
<td>1.0000000000e+00</td>
<td>0.0000000000e+00</td>
<td>0.0000000000e+00</td>
</tr>
<tr>
<td>5.6511827775e+04</td>
<td>8.0000000000e-01</td>
<td>2.0000000000e+00</td>
<td>2.0000000000e+00</td>
</tr>
<tr>
<td>6.1603813790e+04</td>
<td>5.0000000000e-01</td>
<td>1.0000000000e+00</td>
<td>1.0000000000e+00</td>
</tr>
<tr>
<td>7.8702465755e+04</td>
<td>0.0000000000e+00</td>
<td>0.0000000000e+00</td>
<td>0.0000000000e+00</td>
</tr>
</tbody>
</table>

Complementary Cumulative Distribution Function (CCDF) for response_fn_3:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.3796737090e+05</td>
<td>1.0000000000e+00</td>
<td>0.0000000000e+00</td>
<td>0.0000000000e+00</td>
</tr>
<tr>
<td>3.6997214153e+05</td>
<td>3.0000000000e-01</td>
<td>2.0000000000e+00</td>
<td>2.0000000000e+00</td>
</tr>
<tr>
<td>3.8100966235e+05</td>
<td>2.0000000000e-01</td>
<td>1.0000000000e+00</td>
<td>1.0000000000e+00</td>
</tr>
<tr>
<td>4.4111498127e+05</td>
<td>0.0000000000e+00</td>
<td>0.0000000000e+00</td>
<td>0.0000000000e+00</td>
</tr>
</tbody>
</table>

Theory

Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.
In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

An inverse mapping involves computing the belief and plausibility response level for either a specified probability level or a specified generalized reliability level (two results for each level mapping in the evidence-based epistemic case, instead of the one result for each level mapping in the aleatory case).

num_probability_levels
- Keywords Area
- method
- stoch_collocation
- probability_levels
- num_probability_levels

Specify which probability_levels correspond to which response

Specification
Alias: none
Argument(s): INTEGERLIST
Default: probability_levels evenly distributed among response functions

Description
See parent page

gen_reliability_levels
- Keywords Area
- method
- stoch_collocation
- gen_reliability_levels

Specify generalized reliability levels at which to estimate the corresponding response value

Specification
Alias: none
Argument(s): REALLIST
Default: No CDF/CCDF response levels to compute
### Description

Response levels are calculated for specified generalized reliabilities by indexing into a sorted samples array (the response levels computed are not interpolated and will correspond to one of the sampled values).

### Theory

Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.

In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

An inverse mapping involves computing the belief and plausibility response level for either a specified probability level or a specified generalized reliability level (two results for each level mapping in the evidence-based epistemic case, instead of the one result for each level mapping in the aleatory case).

### num_gen_reliability_levels

- **Keywords Area**
- **method**
- **stoch_collocation**
- **gen_reliability_levels**
- **num_gen_reliability_levels**

Specify which `gen_reliability_levels` correspond to which response.

### Specification

**Alias:** none

**Argument(s):** INTEGERLIST

**Default:** `gen_reliability_levels` evenly distributed among response functions

### Description

See parent page
**rng**

- **Keywords Area**
- **method**
- **stoch_collocation**
- **rng**

Selection of a random number generator

**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** Mersenne twister (mt19937)

<table>
<thead>
<tr>
<th>Required/-Optional Required (Choose One)</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>mt19937</td>
<td>Generates random numbers using the Mersenne twister</td>
</tr>
<tr>
<td></td>
<td></td>
<td>rnum2</td>
<td>Generates pseudo-random numbers using the Pecos package</td>
</tr>
</tbody>
</table>

**Description**

The `rng` keyword is used to indicate a choice of random number generator.

**Default Behavior**

If specified, the `rng` keyword must be accompanied by either `rnum2` (pseudo-random numbers) or `mt19937` (random numbers generated by the Mersenne twister). Otherwise, `mt19937`, the Mersenne twister is used by default.

**Usage Tips**

The default is recommended, as the Mersenne twister is a higher quality random number generator.

**Examples**

```plaintext
method
  sampling
    sample_type lhs
    samples = 10
    seed = 98765
    rng rnum2

mt19937
  - **Keywords Area**
  - **method**
```
6.2. METHOD

- stoch_collocation
- rng
- mt19937

Generates random numbers using the Mersenne twister

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

The `mt19937` keyword directs Dakota to use the Mersenne twister to generate random numbers. Additional information can be found on wikipedia: [http://en.wikipedia.org/wiki/Mersenne_twister](http://en.wikipedia.org/wiki/Mersenne_twister).

**Default Behavior**

`mt19937` is the default random number generator. To specify it explicitly in the Dakota input file, however, it must be specified in conjunction with the `rng` keyword.

**Usage Tips**

Use of the Mersenne twister random number generator (`mt19937`) is recommended.

**Examples**

```plaintext
method sampling
    sample_type lhs
    samples = 10
    seed = 98765
    rng mt19937
```

**rnum2**

- **Keywords Area**
- **method**
- **stoch_collocation**
- **rng**
- **rnum2**

Generates pseudo-random numbers using the Pecos package

**Specification**

**Alias:** none

**Argument(s):** none
Description

The `rnum2` keyword directs Dakota to use pseudo-random numbers generated by the Pecos package.

**Default Behavior**

`rnum2` is not used by default. To change this behavior, it must be specified in conjunction with the `rng` keyword.

**Usage Tips**

Use of the Mersenne twister random number generator (mt19937) is recommended over `rnum2`.

Examples

```
method
  sampling
    sample_type lhs
    samples = 10
    seed = 98765
  rng rnum2
```

**model_pointer**

- Keywords Area
- method
- stoch_collocation
- model_pointer

Identifier for model block to be used by a method

Topics

This keyword is related to the topics:

- block_pointer

Specification

Alias: none

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)

Description

The `model_pointer` is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

**Default Behavior**

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding `id_model` with the same name.

**Usage Tips**

When doing advanced analyses that involve using multiple methods and multiple models, defining a `model_pointer` for each method is imperative.

See `block_pointer` for details about pointers.
6.2. METHOD

Examples

```plaintext
environment
  tabular_graphics_data
  method_pointer = 'UQ'

method
  id_method = 'UQ'
  model_pointer = 'SURR'
  sampling,
    samples = 10
    seed = 98765 rng rnum2
    response_levels = 0.1 0.2 0.6
      0.1 0.2 0.6
      0.1 0.2 0.6
  sample_type lhs
distribution cumulative

model
  id_model = 'SURR'
  surrogate global,
    dace_method_pointer = 'DACE'
    polynomial quadratic

method
  id_method = 'DACE'
  model_pointer = 'DACE_M'
  sampling sample_type lhs
    samples = 121 seed = 5034 rng rnum2

model
  id_model = 'DACE_M'
  single
  interface_pointer = 'I1'

variables
  uniform_uncertain = 2
  lower_bounds = 0. 0.
  upper_bounds = 1. 1.
  descriptors = 'x1' 'x2'

interface
  id_interface = 'I1'
  system asynch evaluation_concurrency = 5
    analysis_driver = 'text_book'

responses
  response_functions = 3
  no_gradients
  no_hessians
```

6.2.50 sampling

- Keywords Area
- method
- sampling

Randomly samples variables according to their distributions
This keyword is related to the topics:

- uncertainty\_quantification
- sampling

**Specification**

**Alias:** nond\_sampling

**Argument(s):** none
<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>samples</td>
<td>Number of samples for sampling-based methods</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>seed</td>
<td>Seed of the random number generator</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>fixed_seed</td>
<td>Reuses the same seed value for multiple random sampling sets</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>sample_type</td>
<td>Selection of sampling strategy</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>refinement_-samples</td>
<td>Number of samples used to refine a probability estimate or sampling design.</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>d_optimal</td>
<td>Generate a D-optimal sampling design</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>variance_based_-decomp</td>
<td>Activates global sensitivity analysis based on decomposition of response variance into contributions from variables</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>backfill</td>
<td>Ensures that the samples of discrete variables with finite support are unique</td>
</tr>
<tr>
<td>Optional</td>
<td>principal_components</td>
<td>Activates principal components analysis of the response matrix of N samples * L responses.</td>
<td></td>
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<tr>
<td>----------</td>
<td>----------------------</td>
<td>-----------------------------------------------------------------------------------------</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>wilks</td>
<td>Number of samples for random sampling using Wilks statistics</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>final_moments</td>
<td>Output moments of the specified type and include them within the set of final statistics.</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>reliability_levels</td>
<td>Specify reliability levels at which the response values will be estimated</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>response_levels</td>
<td>Values at which to estimate desired statistics for each response</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>distribution</td>
<td>Selection of cumulative or complementary cumulative functions</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>probability_levels</td>
<td>Specify probability levels at which to estimate the corresponding response value</td>
<td></td>
</tr>
</tbody>
</table>
**6.2. METHOD**

| Optional | gen_reliability_levels | Specify generalized reliability levels at which to estimate the corresponding response value |
| Optional | rng | Selection of a random number generator |
| Optional | model_pointer | Identifier for model block to be used by a method |

**Description**

This method generates parameter values by drawing samples from the specified uncertain variable probability distributions. The computational model is executed over all generated parameter values to compute the responses for which statistics are computed. The statistics support sensitivity analysis and uncertainty quantification.

**Default Behavior**

By default, sampling methods operate on aleatory and epistemic uncertain variables. The types of variables can be restricted or expanded (to include design or state variables) through use of the `active` keyword in the `variables` block in the Dakota input file. If continuous design and/or state variables are designated as active, the sampling algorithm will treat them as parameters with uniform probability distributions between their upper and lower bounds. Refer to `variable_support` for additional information on supported variable types, with and without correlation.

The following keywords change how the samples are selected:

- `sample_type`
- `fixed_seed`
- `rng`
- `samples`
- `seed`
- `variance_based_decomp`

**Expected Outputs**

As a default, Dakota provides correlation analyses when running LHS. Correlation tables are printed with the simple, partial, and rank correlations between inputs and outputs. These can be useful to get a quick sense of how correlated the inputs are to each other, and how correlated various outputs are to inputs. `variance_based_decomp` is used to request more sensitivity information, with additional cost.

Additional statistics can be computed from the samples using the following keywords:

- `response_levels`
- `reliability_levels`
- `probability_levels`
• gen_reliability_levels

response_levels computes statistics at the specified response value. The other three allow the specification of the statistic value, and will estimate the corresponding response value.

distribution is used to specify whether the statistic values are from cumulative or complementary cumulative functions.

Usage Tips
	sampling is a robust approach to doing sensitivity analysis and uncertainty quantification that can be applied to any problem. It requires more simulations than newer, advanced methods. Thus, an alternative may be preferable if the simulation is computationally expensive.

Examples

# tested on Dakota 6.0 on 140501

environment
tabular_data
tabular_data_file = 'Sampling_basic.dat'

method
sampling
sample_type lhs
samples = 20

model
single

variables
active uncertain
uniform_uncertain = 2
descriptors = 'input1' 'input2'
lower_bounds = -2.0 -2.0
upper_bounds = 2.0 2.0
continuous_state = 1
descriptors = 'constant1'
initial_state = 100

interface
analysis_drivers 'text_book'
fork

responses
response_functions = 1
no_gradients
no_hessians

This example illustrates a basic sampling Dakota input file.

• LHS is used instead of purely random sampling.

• The default random number generator is used.

• Without a seed specified, this will not be reproducible

• In the variables block, two types of variables are used

• Only the uncertain variables are varied, this is the default behavior, and is also specified by the active keyword, w/ the uncertain option
6.2. METHOD

See Also
These keywords may also be of interest:

- active

FAQ
Q: Do I need to keep the LHS* and S4 files? A: No

samples

- Keywords Area
- method
- sampling
- samples

Number of samples for sampling-based methods

Specification

Alias: initial_samples
- Argument(s): INTEGER
- Default: 0

Description
The samples keyword is used to define the number of samples (i.e., randomly chosen sets of variable values) at which to execute a model.

- Default Behavior
  - By default, Dakota will use the minimum number of samples required by the chosen method.

- Usage Tips
  - To obtain linear sensitivities or to construct a linear response surface, at least dim+1 samples should be used, where "dim" is the number of variables. For sensitivities to quadratic terms or quadratic response surfaces, at least (dim+1)(dim+2)/2 samples are needed. For uncertainty quantification, we recommend at least 10*dim samples. For variance_based_decomp, we recommend hundreds to thousands of samples. Note that for variance_based_decomp, the number of simulations performed will be N*(dim+2).

Examples

```plaintext
method
  sampling
    sample_type lhs
    samples = 20
```
seed

- Keywords Area
- method
- sampling
- seed

Seed of the random number generator

**Specification**

Alias: none
Argument(s): INTEGER
Default: system-generated (non-repeatable)

**Description**

The random seed control provides a mechanism for making a stochastic method repeatable. That is, the use of the same random seed in identical studies will generate identical results.

**Default Behavior**

If not specified, the seed is randomly generated.

**Expected Output**

If seed is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

**Usage Tips**

If a stochastic study was run without seed specified, and the user later wishes to repeat the study using the same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen. That value can then be added to the Dakota input file.

**Examples**

```dakota
method
  sampling
    sample_type lhs
    samples = 10
    seed = 15347
```

fixed_seed

- Keywords Area
- method
- sampling
- fixed_seed

Reuses the same seed value for multiple random sampling sets
6.2. METHOD

Specification

**Alias:** none

**Argument(s):** none

**Default:** not fixed; pattern varies run-to-run

Description

The `fixed_seed` flag is relevant if multiple sampling sets will be generated over the course of a Dakota analysis. This occurs when using advance methods (e.g., surrogate-based optimization, optimization under uncertainty). The same seed value is reused for each of these multiple sampling sets, which can be important for reducing variability in the sampling results.

**Default Behavior**

The default behavior is to not use a fixed seed, as the repetition of the same sampling pattern can result in a modeling weakness that an optimizer could potentially exploit (resulting in actual reliabilities that are lower than the estimated reliabilities). For repeatable studies, the `seed` must also be specified.

Examples

```
method
  sampling
    sample_type lhs
    samples = 10
    fixed_seed
```

**sample_type**

- **Keywords Area**
- **method**
- **sampling**
- **sample_type**

Selection of sampling strategy

Specification

**Alias:** none

**Argument(s):** none

**Default:** lhs

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required <em>(Choose One)</em></td>
<td>Group 1</td>
<td><code>lhs</code></td>
</tr>
<tr>
<td>Uses Latin Hypercube Sampling (LHS) to sample variables</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
CHAPTER 6. KEYWORDS AREA

<table>
<thead>
<tr>
<th>random</th>
<th>Uses purely random Monte Carlo sampling to sample variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>incremental_lhs</td>
<td>(Deprecated keyword) Augments an existing Latin Hypercube Sampling (LHS) study</td>
</tr>
<tr>
<td>incremental_random</td>
<td>(Deprecated keyword) Augments an existing random sampling study</td>
</tr>
</tbody>
</table>

**Description**

The `sample_type` keyword allows the user to select between two types of sampling: Monte Carlo (pure random) and Latin hypercube (stratified) sampling.

The incremental keywords are deprecated; instead use `samples` together with `refinement_samples`.

**Default Behavior**

If the `sample_type` keyword is present, it must be accompanied by `lhs` or `random`. In most contexts, `lhs` is the default (exception: multilevel_sampling uses Monte Carlo by default).

**Examples**

```plaintext
method
  sampling
    sample_type lhs
    samples = 20
    seed = 83921
```

**lhs**

- Keywords Area
- method
- sampling
- sample_type
- lhs

Uses Latin Hypercube Sampling (LHS) to sample variables
6.2. METHOD

**Specification**

**Alias:** none  
**Argument(s):** none

**Description**

The lhs keyword invokes Latin Hypercube Sampling as the means of drawing samples of uncertain variables according to their probability distributions. This is a stratified, space-filling approach that selects variable values from a set of equi-probable bins.

**Default Behavior**

Latin Hypercube Sampling is the default sampling mode in most contexts (exception: multilevel_sampling). To explicitly specify LHS in the Dakota input file, the lhs keyword must appear in conjunction with the sample_type keyword.

**Usage Tips**

Latin Hypercube Sampling is very robust and can be applied to any problem. It is fairly effective at estimating the mean of model responses and linear correlations with a reasonably small number of samples relative to the number of variables.

**Examples**

```plaintext
method sampling
   sample_type lhs
   samples = 20
```

**random**

- **Keywords Area**
- **method**
- **sampling**
- **sample_type**
- **random**

Uses purely random Monte Carlo sampling to sample variables

**Specification**

**Alias:** none  
**Argument(s):** none

**Description**

The random keyword invokes Monte Carlo sampling as the means of drawing samples of uncertain variables according to their probability distributions.

**Default Behavior**

In most contexts, Monte Carlo sampling is not the default sampling mode (exception: multilevel_sampling). To change this behavior, the random keyword must be specified in conjunction with the sample_type keyword.

**Usage Tips**
Monte Carlo sampling is more computationally expensive than Latin Hypercube Sampling as it requires a larger number of samples to accurately estimate statistics.

Examples

```dakota
method
  sampling
    sample_type random
    samples = 200
```

incremental_lhs

- **Keywords Area**
- **method**
- **sampling**
- **sample_type**
- **incremental_lhs**

(Deprecated keyword) Augments an existing Latin Hypercube Sampling (LHS) study

Specification

**Alias:** none

**Argument(s):** none

**Default:** no sample reuse in coefficient estimation

Description

This keyword is deprecated. Instead specify `sample_type lhs` with `refinement_samples`.

An incremental random sampling approach will augment an existing random sampling study with refinement_samples to get better estimates of mean, variance, and percentiles. The number of refinement_samples in each refinement level must result in twice the number of previous samples.

Typically, this approach is used when you have an initial study with sample size N1 and you want to perform an additional N1 samples. Ideally, a Dakota restart file containing the initial N1 samples, so only N1 (instead of 2 x N1) potentially expensive function evaluations will be performed.

This process can be extended by repeatedly doubling the `refinement_samples`:

```dakota
method
  sampling
    seed = 1337
    samples = 50
    refinement_samples = 50 100 200 400 800
```

Usage Tips

The incremental approach is useful if it is uncertain how many simulations can be completed within available time.

See the examples below and the Usage and Restarting Dakota Studies pages.
6.2. METHOD

Examples

Suppose an initial study is conducted using sample_type lhs with samples = 50. A follow-on study uses a new input file where samples = 50, and refinement_samples = 50, resulting in 50 reused samples (from restart) and 50 new random samples. The 50 new samples will be combined with the 50 previous samples to generate a combined sample of size 100 for the analysis.

One way to ensure the restart file is saved is to specify a non-default name, via a command line option:

dakota -input LHS_50.in -write_restart LHS_50.rst

which uses the input file:

```
# LHS_50.in
environment
  tabular_data
    tabular_data_file = 'LHS_50.dat'

method
  sampling
    seed = 1337
    sample_type lhs
    samples = 50

model
  single

variables
  uniform_uncertain = 2
  descriptors = ‘input1’ ‘input2’
  lower_bounds = -2.0 -2.0
  upper_bounds = 2.0 2.0

interface
  analysis_drivers ‘text_book’
  fork

responses
  response_functions = 1
  no_gradients
  no_hessians

and the restart file is written to LHS_50.rst.

Then an incremental LHS study can be run with:

dakota -input LHS_100.in -read_restart LHS_50.rst -write_restart LHS_100.rst

where LHS_100.in is shown below, and LHS_50.rst is the restart file containing the results of the previous LHS study. In the example input files for the initial and incremental studies, the values for seed match. This ensures that the initial 50 samples generated in both runs are the same.

```
# LHS_100.in
environment
  tabular_data
    tabular_data_file = 'LHS_100.dat'

method
  sampling
    seed = 1337
    sample_type incremental_lhs
    samples = 50
```
refinement_samples = 50

model
  single
variables
  uniform_uncertain = 2
  descriptors = 'input1' 'input2'
  lower_bounds = -2.0 -2.0
  upper_bounds =  2.0  2.0

interface
  analysis_drivers 'text_book'
  fork

responses
  response_functions = 1
  no_gradients
  no_hessians

The user will get 50 new LHS samples which maintain both the correlation and stratification of the original LHS sample. The new samples will be combined with the original samples to generate a combined sample of size 100.

**incremental_random**

- **Keywords Area**
- **method**
- **sampling**
- **sample_type**
- **incremental_random**

(Deprecated keyword) Augments an existing random sampling study

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

This keyword is deprecated. Instead specify **sample_type random** with **refinement_samples**.

An incremental random sampling approach will augment an existing random sampling study with refinement_samples to get better estimates of mean, variance, and percentiles. There is no constraint on the number of samples in the second or subsequent sets as there is with incremental LHS.

Typically, this approach is used when you have an initial study with sample size N1 and you want to perform an additional N2 samples. Ideally, a Dakota restart file containing the initial N1 samples, so only N2 (instead of N1 + N2) potentially expensive function evaluations will be performed.

**Usage Tips**

The incremental approach is useful if it is uncertain how many simulations can be completed within available time.
Examples

Suppose an initial study is conducted using `sample_type random` with `samples = 50`. A follow-on study uses a new input file where `samples = 50`, and `refinement_samples = 10`, resulting in 50 reused samples (from restart) and 10 new random samples. The 10 new samples will be combined with the 50 previous samples to generate a combined sample of size 60 for the analysis.

The method block for the incremented study `input60.in` would be the following:

```plaintext
method
  sampling
  seed = 1337
  sample_type incremental_random
  samples = 50
  refinement_samples = 10
```

The syntax for running the second sample set might be:

```plaintext
dakota -i input60.in -r dakota.50.rst
```

where `dakota.50.rst` is the restart file containing the results of the previous study. A value for `seed` should be specified and must match in the initial and incremental studies to ensure that the generated samples are the same.

```plaintext
refinement_samples
```

- **Keywords Area**
- **method**
- **sampling**
- **refinement_samples**

Number of samples used to refine a probability estimate or sampling design.

**Specification**

**Alias:** none

**Argument(s):** INTEGERLIST

**Description**

Probability estimate: Specify the (scalar) number of samples used to improve a probability estimate. If using uni-modal sampling all samples are assigned to the sampling center. If using multi-modal sampling the samples are split between multiple samples according to some internally computed weights.

Sampling design: Specify one or a sequence of refinement samples to augment the initial samples in a sampling design.

```plaintext
d_optimal
```

- **Keywords Area**
- **method**
- **sampling**
- **d_optimal**

Generate a D-optimal sampling design
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none
Argument(s): none
Default: off

<table>
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<tr>
<th>Required/-Optional (Choose One)</th>
<th>Description of Group Design Strategy (Group 1)</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>candidate_designs</td>
<td>Number of candidate sampling designs from which to select the most D-optimal</td>
</tr>
</tbody>
</table>

Description

This option will generate a sampling design that is approximately determinant-optimal (D-optimal) by downselecting from a set of candidate sample points.

Default Behavior

If not specified, a standard sampling design (MC or LHS) will be generated. When d_optimal is specified, 100 candidate designs will be generated and the most D-optimal will be selected.

Usage Tips

D-optimal designs are only supported for aleatory_uncertain_variables. The default candidate-based D-optimal strategy works for all submethods except incremental LHS (lhs with refinement_samples). The Leja sampling option only works for continuous variables, and when used with LHS designs, the candidates point set will be Latin, but the final design will not be.

Examples

```plaintext
method
  sampling
    sample_type random
    samples = 20
    d_optimal

candidate_designs
```

- Keywords Area
- method
- sampling
- d_optimal
- candidate_designs

Number of candidate sampling designs from which to select the most D-optimal
6.2. METHOD

Specification

Alias: none
Argument(s): INTEGER
Default: 100

Description

Dakota will generate candidate designs using the specified sampling strategy and select the one that is more determinant-optimal (D-optimal)

Examples

```
method
  sampling
    sample_type random
    samples = 20
    d_optimal
      candidate_designs = 500
```

leja_oversample_ratio

- Keywords Area
- method
- sampling
- d_optimal
- leja_oversample_ratio

Oversampling ratio for generating candidate point set

Specification

Alias: none
Argument(s): REAL
Default: 10.0

Description

When generating a D-Optimal point set of size N, the oversample_ratio R controls the number of candidate points R x N from which the D-Optimal points are chosen.

Default Behavior

The default when not specified is to perform candidate-based sample design selection (non-Leja)

Examples

```
method
  sampling
    sample_type random
    samples = 20
    d_optimal
      oversample_ratio = 2.0
```
variance_based_decomp

- Keywords Area
- method
- sampling
- variance_based_decomp

Activates global sensitivity analysis based on decomposition of response variance into contributions from variables

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no variance-based decomposition

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>Optional Group</td>
<td>drop_tolerance</td>
<td>Description</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td></td>
<td>Suppresses output of sensitivity indices with values lower than this tolerance</td>
</tr>
</tbody>
</table>

**Description**

Dakota can calculate sensitivity indices through variance based decomposition using the keyword `variance_based_decomp`. These indicate how important the uncertainty in each input variable is in contributing to the output variance.

**Default Behavior**

Because of the computational cost, `variance_based_decomp` is turned off as a default.

If the user specified a number of samples, N, and a number of nondeterministic variables, M, variance-based decomposition requires the evaluation of N*(M+2) samples. **Note that specifying this keyword will increase the number of function evaluations above the number requested with the samples keyword since replicated sets of sample values are evaluated.**

**Expected Outputs**

When `variance_based_decomp` is specified, sensitivity indices for main effects and total effects will be reported. Main effects (roughly) represent the percent contribution of each individual variable to the variance in the model response. Total effects represent the percent contribution of each individual variable in combination with all other variables to the variance in the model response.

**Usage Tips**

To obtain sensitivity indices that are reasonably accurate, we recommend that N, the number of samples, be at least one hundred and preferably several hundred or thousands.

**Examples**

```
method,
sampling
    sample_type lhs
```
6.2. METHOD

samples = 100
variance_based_decomp

Theory
In this context, we take sensitivity analysis to be global, not local as when calculating derivatives of output variables with respect to input variables. Our definition is similar to that of[73] : “The study of how uncertainty in the output of a model can be apportioned to different sources of uncertainty in the model input.”

Variance based decomposition is a way of using sets of samples to understand how the variance of the output behaves, with respect to each input variable. A larger value of the sensitivity index, $S_i$, means that the uncertainty in the input variable $i$ has a larger effect on the variance of the output. More details on the calculations and interpretation of the sensitivity indices can be found in[73] and[87].

drop_tolerance
- Keywords Area
- method
- sampling
- variance_based_decomp
- drop_tolerance
  Suppresses output of sensitivity indices with values lower than this tolerance

Specification
Alias: none
Argument(s): REAL
Default: All VBD indices displayed

Description
The drop_tolerance keyword allows the user to specify a value below which sensitivity indices generated by variance_based_decomp are not displayed.

Default Behavior
By default, all sensitivity indices generated by variance_based_decomp are displayed.

Usage Tips
For polynomial_chaos, which outputs main, interaction, and total effects by default, the univariate_effects may be a more appropriate option. It allows suppression of the interaction effects since the output volume of these results can be prohibitive for high dimensional problems. Similar to suppression of these interactions is the covariance control, which can be selected to be diagonal_covariance or full_covariance, with the former supporting suppression of the off-diagonal covariance terms (to save compute and memory resources and reduce output volume).

Examples
method,
sampling
sample_type lhs
samples = 100
variance_based_decomp
drop_tolerance = 0.001
CHAPTER 6. KEYWORDS AREA

backfill

- Keywords Area
- method
- sampling
- backfill

Ensures that the samples of discrete variables with finite support are unique

**Specification**

Alias: none

**Argument(s):** none

**Description**

Traditional LHS can generate replicate samples when applied to discrete variables. This keyword enforces uniqueness, which is determined only over the set of discrete variables with finite support. This allows one to generate LHS for a mixed set of continuous and discrete variables whilst still enforcing that the set of discrete LHS components of all the samples are unique.

**Default Behavior**

Uniqueness of samples over discrete variables is not enforced.

**Usage Tips**

Uniqueness can be useful when applying discrete LHS to simulations without noise.

**Examples**

```plaintext
method,
  sampling
  samples = 12
  seed = 123456
  sample_type lhs backfill

variables,
  active all
  uniform_uncertain = 1
  lower_bounds = 0.
  upper_bounds = 1.
  descriptors = 'continuous-uniform'

  discrete_uncertain_set
  integer = 1
  elements_per_variable = 4
  elements 1 3 5 7
  descriptors = 'design-set-int'
  real = 1
  initial_point = 0.50
  set_values = 0.25 0.50 0.75 1.00
  descriptors = 'design-set-real'

interface,
  direct analysis_driver = 'text_book'

responses,
```

response_functions = 3
no_gradients
no_hessians

See Also

These keywords may also be of interest:

- lhs

principal_components

- Keywords Area
- method
- sampling
- principal_components

Activates principal components analysis of the response matrix of N samples * L responses.

Specification

Alias: none

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>Group</td>
<td>percent_variance_explained</td>
<td>Description</td>
</tr>
</tbody>
</table>

| Specifies the number of components to retain to explain the specified percent variance. |

Description

Dakota can calculate the principal components of the response matrix of N samples * L responses using the keyword principal_components. Principal components analysis (PCA) is a data reduction method. The Dakota implementation is under active development: the PCA capability may ultimately be specified elsewhere or used in different ways. For now, it is performed as a post-processing analysis based on a set of Latin Hypercube samples.

We now have field responses in Dakota. PCA is an initial approach in Dakota to analyze and represent the field data. Specifically, if we have a sample ensemble of field data responses, we want to identify the principal components responsible for the spread of that data. Then, we can generate a surrogate model by representing the overall response as weighted sum of M principal components, where the weights will be determined by GPs which are a function of the input uncertain variables. This reduced form then can be used for sensitivity analysis, calibration, etc.

The steps involved when one specifies principal_components in Dakota are as follows:
• Create an LHS input sample based on the uncertain variable specification and run the user-specified model at the LHS points to compute the field responses. For notation purposes, there are \( d \) input parameters, \( N \) samples, and the field length is \( L \).

• Perform PCA on the covariance matrix of the data set from the previous step. This is done by first centering the data (e.g. subtracting the mean of each column from that column) and performing a singular value decomposition on the covariance matrix of the centered data. The eigenvectors of the covariance matrix correspond to the principal components.

• Identify \( M \) principal components based on the percentage of variance explained. There is an optional keyword for principal components called percent_variance_explained, which is a threshold that determines the number of components that are retained to explain at least that amount of variance. For example, if the user specifies percent_variance_explained = 0.99, the number of components that accounts for at least 99 percent of the variance in the responses will be retained. The default for this percentage is 0.95. In many applications, only a few principal components explain the majority of the variance, resulting in significant data reduction.

• Use the principal components in a predictive sense, by constructing a prediction approximation. The basis functions for this approximation are the principal components. The coefficients of the bases are obtained by constructing GP surrogates for the factor scores of the \( M \) principal components. The GP surrogates will be functions of the uncertain inputs. The idea is that we have just performed PCA on (for example) the covariance matrix of 100 samples. Typically, those 100 samples will be generated by sampling over some \( d \) uncertain input parameters denoted by \( u \), so there should be a mapping from \( u \) to the field data, specifically to the loading coefficients and the factor scores. Currently, the final item printed from a Principal Components Analysis in Dakota is a set of prediction samples based on this prediction approximation or surrogate model that relies on the principal components.

**Default Behavior**

principal_components is turned off as a default. It may be used with either scalar responses or field responses, but it is intended to be used with large field responses as a data reduction method. For example, typically we expect the number of LHS samples, \( N \), to be less than the number of field responses, \( L \) (e.g. if there is one field, the number of responses values is the length of that field).

**Expected Outputs**

When principal_components is specified, the number of significant principal components is printed along with the predictions based on the principal components. If output debug is specified, additional information is printed, including the original response matrix, the centered data, the principal components, and the factor scores.

**Usage Tips**

This is a preliminary capability that is undergoing active development. Please contact the Dakota developers team if you have problems with using this capability or want to suggest additional features.

**Examples**

```plaintext
method,
sampling
    sample_type lhs
    samples = 100
    principal_components
    percent_variance_explained = 0.98
```
Theory

There is an extensive statistical literature available on PCA. We recommend that the interested user peruse some of this in using the PCA capability.

\texttt{percent\_variance\_explained}

- **Keywords Area**
- **method**
- **sampling**
- **principal\_components**
- **percent\_variance\_explained**

Specifies the number of components to retain to explain the specified percent variance.

**Specification**

\texttt{Alias: none}

\texttt{Argument(s): REAL}

**Description**

Dakota can calculate the principal components of the response matrix of N samples \(* L\) responses using the keyword \texttt{principal\_components}. Principal components analysis (PCA) is a data reduction method. \texttt{percent\_variance\_explained} is a threshold that determines the number of components that are retained to explain at least that amount of variance. For example, if the user specifies \texttt{percent\_variance\_explained} = 0.99, the number of components that accounts for at least 99 percent of the variance in the responses will be retained. The default for this percentage is 0.95. In many applications, only a few principal components explain the majority of the variance, resulting in significant data reduction.

**Expected Outputs**

**Usage Tips** \texttt{percent\_variance\_explained} should be a real number between 0.0 and 1.0. Typically, it will be between 0.9 and 1.0.

**Examples**

\begin{verbatim}
method, sampling
  sample_type lhs
  samples = 100
  principal\_components
  percent\_variance\_explained = 0.98
\end{verbatim}

Theory

There is an extensive statistical literature available on PCA. We recommend that the interested user peruse some of this in using the PCA capability.
wilks

- Keywords Area
- method
- sampling
- wilks

Number of samples for random sampling using Wilks statistics

**Specification**

*Alias:* none

*Argument(s):* none

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>order</td>
<td>order</td>
<td>The order of the statistics to use when determining sample sizes for random sampling using Wilks order statistics.</td>
</tr>
<tr>
<td>Optional</td>
<td>confidence_level</td>
<td>confidence_level</td>
<td>The confidence level to be used when determining sample sizes for random sampling using Wilks order statistics.</td>
</tr>
<tr>
<td>Optional</td>
<td>one-sided_lower</td>
<td>one-sided_lower</td>
<td>Specifies one-sided lower portion order statistics to be used when determining sample sizes for random sampling using Wilks order statistics.</td>
</tr>
</tbody>
</table>
## Description

The **wilks** keyword is used to compute the number of samples to execute for a random sampling study using Wilks statistics[88] and[?]. In contrast to most sampling studies where the user specifies the number of samples in advance, Wilks determines the number of samples to run to achieve a particular objective. Specifically, Wilks statistics specify a probability level, alpha, and confidence level, beta, and determines the minimum number of samples required such that there is beta% confidence that the alpha*100 percentile of the uncertain distribution on model output will fall below the actual alpha*100 percentile given by the sample when outputs are ordered from smallest to largest. Statistics can also be either one-sided or two-sided with the former reflecting a statement about uppermost sample output and the latter reflecting both the smallest and largest sample outputs. Finally, the order of the statistics can be increased to higher order such that the statement concerning probability level and confidence level applies to the uppermost M outputs (for one-sided M-order Wilks) or the lowest M and uppermost M outputs (for two-sided M-order Wilks).

### Default Behavior

By default, Wilks statistics are computed using one-sided first-order order statistics with a 95% confidence interval (beta) and 95% probability (alpha). This results in a sample size of 59.

### Usage Tips

Wilks sample sizes apply to model outputs considered one-at-a-time. Joint variation among multiple outputs requires a generalization of the Wilks approach and is not supported in Dakota at this time.

When more than one probability level is specified, the largest sample size will be performed and used to subsample for the lower probability levels.

### Examples

```plaintext
method
  sampling
    sample_type random
  wilks
    probability_levels = 0.75 0.8 0.95 0.99
    confidence_level 0.99
    two_sided
    order 2
```
order

- Keywords Area
- method
- sampling
- wilks
- order

The order of the statistics to use when determining sample sizes for random sampling using Wilks order statistics.

Specification
Alias: none
Argument(s): INTEGER

Description
Default Behavior
The default order is 1.

Examples
method
sampling
  sample_type random
  wilks
  order 2

See Also
These keywords may also be of interest:

- wilks

confidence_level

- Keywords Area
- method
- sampling
- wilks
- confidence_level

The confidence level to be used when determining sample sizes for random sampling using Wilks order statistics.
6.2. METHOD

Specification

Alias: none
  Argument(s): REAL

Description

Default Behavior
A value of 0.95 (95%) is the default for both confidence level as well as probability level resulting in 59 samples for first-order one-sided statistics.

Examples

```plaintext
method
  sampling
    sample_type random
    wilks
      confidence_level 0.99
```

See Also

These keywords may also be of interest:
- wilks method-sampling-probability_levels

one_sided_lower

- Keywords Area
- method
- sampling
- wilks
- one_sided_lower

Specifies one-sided lower portion order statistics to be used when determining sample sizes for random sampling using Wilks order statistics.

Specification

Alias: none
  Argument(s): none

Description

This option causes the sample size to be based on the lowermost N outputs for order N statistics (default N=1).

Examples

```plaintext
method
  sampling
    sample_type random
    wilks
    one_sided_lower
```
See Also
These keywords may also be of interest:

- wilks

one_sided_upper

- Keywords Area
- method
- sampling
- wilks
- one_sided_upper

Specifies one-sided upper portion order statistics to be used when determining sample sizes for random sampling using Wilks order statistics.

Specification

**Alias:** none

**Argument(s):** none

**Description**

This option causes the sample size to be based on the uppermost N outputs for order N statistics (default N=1).

**Default Behavior**  This is the default for Wilks.

**Examples**

```
method
  sampling
    sample_type random
  wilks
    one_sided_upper
```

See Also

These keywords may also be of interest:

- wilks

two_sided

- Keywords Area
- method
- sampling
- wilks
- two_sided

Specifies two-sided order statistics (an interval) to be used when determining sample sizes for random sampling using Wilks order statistics.
6.2. METHOD

Specification

Alias: none
Argument(s): none

Description

This option causes the sample size to be based on the interval defined by the lowest N and uppermost N outputs for order N statistics (default N=1).

Default Behavior  The default for Wilks is one_sided_upper.

Examples

method
sampling
  sample_type random
  wilks
two_sided

See Also

These keywords may also be of interest:

- wilks

final_moments

- Keywords Area
- method
- sampling
- final_moments

Output moments of the specified type and include them within the set of final statistics.

Specification

Alias: none
Argument(s): none
Default: standard

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group objective formulation (Group 1)</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required (Choose One)</td>
<td></td>
<td>none</td>
<td>Omit moments from the set of final statistics.</td>
</tr>
</tbody>
</table>
CHAPTER 6. KEYWORDS AREA

<table>
<thead>
<tr>
<th>standard</th>
<th>Output standardized moments and include them within the set of final statistics.</th>
</tr>
</thead>
<tbody>
<tr>
<td>central</td>
<td>Output central moments and include them within the set of final statistics.</td>
</tr>
</tbody>
</table>

**Description**

When performing a nested study that may employ moment statistics on the inner loop, it can be desirable to control the type of these moments. The `final_moments` specification supports options of `none`, `standard` (default), or `central`, corresponding to omission of moments, standardized moments (mean, standard deviation, skewness, and excess kurtosis), or central moments (mean, variance, 3rd central, and 4th central).

The presence or omission of moment results in the final statistics influences the outer level mappings in the case of a nested study. For example, `final_moments none` can allow for a more compact specification of primary and/or secondary response mappings.

**Examples**

The following method specification overrides the default to print `central` moments and include them in the set of final statistics.

```
method,
  sampling
    samples = 50 seed = 1234
    response_levels = 3.6e+11 1.2e+05 3.5e+05
    final_moments central
```

Overriding the default to `none` as follows:

```
method,
  sampling
    samples = 50 seed = 1234
    response_levels = 3.6e+11 1.2e+05 3.5e+05
    final_moments none
```

allows associated nested model mappings to be simplified from:

```
model
  nested
    sub_method_pointer = ’UQ’
    primary_response_mapping = 0. 0. 1. 0. 0. 1. 0. 0. 0.
    secondary_response_mapping = 0. 0. 0. 0. 0. 0. 0. 0. 1.
```

to a more compact version focused only on the response level mappings (two leading zeros per response function for moment mappings have been removed):

```
model
  nested
    sub_method_pointer = ’UQ’
    primary_response_mapping = 1. 1. 0.
    secondary_response_mapping = 0. 0. 1.
6.2. METHOD

none

- Keywords Area
- method
- sampling
- final_moments
- none

Omit moments from the set of final statistics.

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

The omission of moment results from the final statistics can allow for a more compact definition of primary and/or secondary response mappings within a nested model specification.

**Examples**

method,
sampling
  samples = 50 seed = 1234
  response_levels = 3.6e+11 1.2e+05 3.5e+05
  final_moments none

standard

- Keywords Area
- method
- sampling
- final_moments
- standard

Output standardized moments and include them within the set of final statistics.

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

Output standardized moments (mean, standard deviation, skewness, and excess kurtosis) and include the first two within the set of final statistics to be used at a higher level (e.g., optimization under uncertainty, mixed aleatory-epistemic UQ). This inclusion of moment results affects the primary and/or secondary response mappings in a nested model specification.
Examples
The following method specification overrides the default to print central moments and include them in the set of final statistics.

```
method,
  sampling
    samples = 50 seed = 1234
    response_levels = 3.6e+11 1.2e+05 3.5e+05
    final_moments standard
```

central
- Keywords Area
- method
- sampling
- final_moments
- central

Output central moments and include them within the set of final statistics.

Specification
Alias: none
Argument(s): none

Description
Output central moments (mean, variance, 3rd central, and 4th central) and include the first two within the set of final statistics to be used at a higher level (e.g., optimization under uncertainty, mixed aleatory-epistemic U-Q). This inclusion of moment results affects the primary and/or secondary response mappings in a nested model specification.

Examples
The following method specification overrides the default to print central moments and include them in the set of final statistics.

```
method,
  sampling
    samples = 50 seed = 1234
    response_levels = 3.6e+11 1.2e+05 3.5e+05
    final_moments central
```

reliability_levels
- Keywords Area
- method
- sampling
- reliability_levels

Specify reliability levels at which the response values will be estimated
6.2. METHOD

Specification

Alias: none

Argument(s): REALLIST

Default: No CDF/CCDF response levels to compute

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>num_reliability_levels</td>
<td>Description</td>
<td>Specify which reliability_levels correspond to which response</td>
</tr>
</tbody>
</table>

Description

Response levels are calculated for specified CDF/CCDF reliabilities by projecting out the prescribed number of sample standard deviations from the sample mean.

Theory

Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.

In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

An inverse mapping involves computing the belief and plausibility response level for either a specified probability level or a specified generalized reliability level (two results for each level mapping in the evidence-based epistemic case, instead of the one result for each level mapping in the aleatory case).

num_reliability_levels

- Keywords Area
- method
- sampling
- reliability_levels
- num_reliability_levels

Specify which reliability_levels correspond to which response

Specification

Alias: none

Argument(s): INTEGERLIST

Default: reliability_levels evenly distributed among response functions

Description

See parent page
CHAPTER 6. KEYWORDS AREA

response_levels

- Keywords Area
- method
- sampling
- response_levels

Values at which to estimate desired statistics for each response

**Specification**

**Alias:** none

**Argument(s):** REALLIST

**Default:** No CDF/CCDF probabilities/reliabilities to compute

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>num_response_levels</td>
<td>compute</td>
<td>Number of values at which to estimate desired statistics for each response</td>
</tr>
</tbody>
</table>

**Description**

The `response_levels` specification provides the target response values for which to compute probabilities, reliabilities, or generalized reliabilities (forward mapping).

**Default Behavior**

If `response_levels` are not specified, no statistics will be computed. If they are, probabilities will be computed by default.

**Expected Outputs**

If `response_levels` are specified, Dakota will create two tables in the standard output: a Probability Density function (PDF) histogram and a Cumulative Distribution Function (CDF) table. The PDF histogram has the lower and upper endpoints of each bin and the corresponding density of that bin. Note that the PDF histogram has bins defined by the `probability_levels` and/or `response_levels` in the Dakota input file. If there are not very many levels, the histogram will be coarse. Dakota does not do anything to optimize the bin size or spacing. The CDF table has the list of response levels and the corresponding probability that the response value is less than or equal to each response level threshold.

**Usage Tips**

The `num_response_levels` is used to specify which arguments of the `response_level` correspond to which response.
Examples

For example, specifying a response level of 52.3 followed with compute probabilities will result in the calculation of the probability that the response value is less than or equal to 52.3, given the uncertain distributions on the inputs.

For an example with multiple responses, the following specification

```
response_levels = 1. 2. .1 .2 .3 .4 10. 20. 30.
num_response_levels = 2 4 3
```

would assign the first two response levels (1., 2.) to response function 1, the next four response levels (.1, .2, .3, .4) to response function 2, and the final three response levels (10., 20., 30.) to response function 3. If the `num_response_levels` key were omitted from this example, then the response levels would be evenly distributed among the response functions (three levels each in this case).

The Dakota input file below specifies a sampling method with response levels of interest.

```
method,
  sampling,
  samples = 100 seed = 1
  complementary distribution
  response_levels = 3.6e+11 4.0e+11 4.4e+11
  6.0e+04 6.5e+04 7.0e+04
  3.5e+05 4.0e+05 4.5e+05
variables,
  normal_uncertain = 2
  means = 248.89, 593.33
  std_deviations = 12.4, 29.7
  descriptors = 'TF1n' 'TF2n'
  uniform_uncertain = 2
  lower_bounds = 199.3, 474.63
  upper_bounds = 298.5, 712.
  descriptors = 'TF1u' 'TF2u'
  weibull_uncertain = 2
  alphas = 12., 30.
  betas = 250., 590.
  descriptors = 'TF1w' 'TF2w'
histogram_bin_uncertain = 2
  num_pairs = 3 4
  abscissas = 5 8 10 .1 .2 .3 .4
  counts = 17 21 0 12 24 12 0
  descriptors = 'TF1h' 'TF2h'
histogram_point_uncertain
  real = 1
  num_pairs = 2
  abscissas = 3 4
  counts = 11
  descriptors = 'TF3h'
```

Given the above Dakota input file, the following excerpt from the output shows the PDF and CCDF generated. Note that the bounds on the bins of the PDF are the response values specified in the input file. The probability levels corresponding to those response values are shown in the CCDF.
Probability Density Function (PDF) histograms for each response function:

PDF for response_fn_1:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.7604749078e+11</td>
<td>3.6000000000e+11</td>
<td>5.3601733194e-12</td>
</tr>
<tr>
<td>3.6000000000e+11</td>
<td>4.0000000000e+11</td>
<td>4.2500000000e-12</td>
</tr>
<tr>
<td>4.0000000000e+11</td>
<td>4.4000000000e+11</td>
<td>3.7500000000e-12</td>
</tr>
<tr>
<td>4.4000000000e+11</td>
<td>5.4196114379e+11</td>
<td>2.2557612778e-12</td>
</tr>
</tbody>
</table>

PDF for response_fn_2:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.6431154744e+04</td>
<td>6.0000000000e+04</td>
<td>2.8742313192e-05</td>
</tr>
<tr>
<td>6.0000000000e+04</td>
<td>6.5000000000e+04</td>
<td>4.6000000000e-05</td>
</tr>
<tr>
<td>6.5000000000e+04</td>
<td>7.0000000000e+04</td>
<td>4.0000000000e-05</td>
</tr>
<tr>
<td>7.0000000000e+04</td>
<td>7.8702465755e+04</td>
<td>1.0341896485e-05</td>
</tr>
</tbody>
</table>

PDF for response_fn_3:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.3796737090e+05</td>
<td>3.5000000000e+05</td>
<td>4.2844660868e-06</td>
</tr>
<tr>
<td>3.5000000000e+05</td>
<td>4.0000000000e+05</td>
<td>8.6000000000e-06</td>
</tr>
<tr>
<td>4.0000000000e+05</td>
<td>4.5000000000e+05</td>
<td>1.8000000000e-06</td>
</tr>
</tbody>
</table>

Level mappings for each response function:

Complementary Cumulative Distribution Function (CCDF) for response_fn_1:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.6000000000e+11</td>
<td>5.5000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.0000000000e+11</td>
<td>3.8000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.4000000000e+11</td>
<td>2.3000000000e-01</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Complementary Cumulative Distribution Function (CCDF) for response_fn_2:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.0000000000e+04</td>
<td>6.1000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6.5000000000e+04</td>
<td>2.9000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7.0000000000e+04</td>
<td>9.0000000000e-02</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Complementary Cumulative Distribution Function (CCDF) for response_fn_3:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.5000000000e+05</td>
<td>5.2000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.0000000000e+05</td>
<td>9.0000000000e-02</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.5000000000e+05</td>
<td>0.0000000000e+00</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Theory**

Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.

In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

A forward mapping involves computing the belief and plausibility probability level for a specified response level.

**num_response_levels**

- Keywords Area
- method
- sampling
6.2. METHOD

- response_levels
- num_response_levels

Number of values at which to estimate desired statistics for each response

Specification

Alias: none

Argument(s): INTEGERLIST

Default: response_levels evenly distributed among response functions

Description

The num_response_levels keyword allows the user to specify the number of response values, for each response, at which estimated statistics are of interest. Statistics that can be computed are probabilities and reliabilities, both according to either a cumulative distribution function or a complementary cumulative distribution function.

Default Behavior

If num_response_levels is not specified, the response_levels will be evenly distributed among the responses.

Expected Outputs

The specific output will be determined by the type of statistics that are specified. In a general sense, the output will be a list of response level-statistic pairs that show the estimated value of the desired statistic for each response level specified.

Examples

```
method
    sampling
        samples = 100
        seed = 34785
        num_response_levels = 1 1 1
        response_levels = 0.5 0.5 0.5
compute

    Keywords Area
    method
    sampling
    response_levels
    compute

Selection of statistics to compute at each response level

Specification

Alias: none

Argument(s): none

Default: probabilities
The compute keyword is used to select which forward statistical mapping is calculated at each response level.

**Default Behavior**

If `response_levels` is not specified, no statistics are computed. If `response_levels` is specified but `compute` is not, probabilities will be computed by default. If both `response_levels` and `compute` are specified, then one of the following must be specified: `probabilities`, `reliabilities`, or `gen_reliabilities`.

**Expected Output**

The type of statistics specified by `compute` will be reported for each response level.

**Usage Tips**

CDF/CCDF probabilities are calculated for specified response levels using a simple binning approach.

CDF/CCDF reliabilities are calculated for specified response levels by computing the number of sample standard deviations separating the sample mean from the response level.

**Examples**

```
method
  sampling
    sample_type random
    samples = 100 seed = 1
    complementary distribution
    response_levels = 3.6e+11 4.0e+11 4.4e+11
                     6.0e+04 6.5e+04 7.0e+04
                     3.5e+05 4.0e+05 4.5e+05
    compute reliabilities
  probabilities
```
6.2. METHOD

- Keywords Area
- method
- sampling
- response_levels
- compute
- probabilities

Computes probabilities associated with response levels

Specification

Alias: none
Argument(s): none

Description

The `probabilities` keyword directs Dakota to compute the probability that the model response will be below (cumulative) or above (complementary cumulative) a specified response value. This is done for every response level designated for each response.

Default Behavior

If `response_levels` is specified, the probabilities are computed by default. To explicitly specify it in the Dakota input file, though, the `probabilities` keyword should be specified in conjunction with the `compute` keyword.

Expected Outputs

The Dakota output is a set of response level-probability pairs that give the probability that the model response will be below or above the corresponding response level, depending on the distribution defined.

Examples

```
method sampling
  sample_type random
  samples = 100 seed = 1
  complementary_distribution
  response_levels = 3.6e+11 4.0e+11 4.4e+11
                   6.0e+04 6.5e+04 7.0e+04
                   3.5e+05 4.0e+05 4.5e+05
  compute probabilities
```
CHAPTER 6. KEYWORDS AREA

• reliabilities

Computes reliabilities associated with response levels

Specification

Alias: none
Argument(s): none

Description

The reliabilities keyword directs Dakota to compute reliabilities according to the specified distribution for a specified response value. This is done for every response level designated for each response.

Default Behavior

If response_levels is specified, the reliabilities are not computed by default. To change this behavior, the reliabilities keyword should be specified in conjunction with the compute keyword.

Expected Outputs

The Dakota output is a set of response level-reliability pairs according to the distribution defined.

Examples

method
  sampling
    sample_type random
    samples = 100 seed = 1
    complementary distribution
    response_levels = 3.6e+11 4.0e+11 4.4e+11
                       6.0e+04 6.5e+04 7.0e+04
                       3.5e+05 4.0e+05 4.5e+05
    compute reliabilities

gen_reliabilities

• Keywords Area

• method

• sampling

• response_levels

• compute

• gen_reliabilities

Computes generalized reliabilities associated with response levels

Specification

Alias: none
Argument(s): none
6.2. METHOD

Description

The gen_reliabilities keyword directs Dakota to compute generalized reliabilities according to the specified distribution for a specified response value. This is done for every response level designated for each response.

Default Behavior

If response_levels is specified, the generalized reliabilities are not computed by default. To change this behavior, the gen_reliabilities keyword should be specified in conjunction with the compute keyword.

Expected Outputs

The Dakota output is a set of response level-generalized reliability pairs according to the distribution defined.

Examples

```
method
  sampling
    sample_type random
    samples = 100 seed = 1
  complementary distribution
    response_levels = 3.6e+11 4.0e+11 4.4e+11
    6.0e+04 6.5e+04 7.0e+04
    3.5e+05 4.0e+05 4.5e+05
  compute gen_reliabilities
```

system

- Keywords Area
- method
- sampling
- response_levels
- compute
- system

Compute system reliability (series or parallel)

Specification

Alias: none

<table>
<thead>
<tr>
<th>Required/- Optional</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Aggregate response statistics assuming a series system</td>
<td>series</td>
<td>system</td>
</tr>
</tbody>
</table>
**Description**

With the system probability/reliability option, statistics for specified response levels are calculated and reported assuming the response functions combine either in series or parallel to produce a total system response.

For a series system, the system fails when any one component (response) fails. The probability of failure is the complement of the product of the individual response success probabilities.

For a parallel system, the system fails only when all components (responses) fail. The probability of failure is the product of the individual response failure probabilities.

**series**

- Keywords Area
- method
- sampling
- response_levels
- compute
- system
- series

Aggregate response statistics assuming a series system

**Specification**

Alias: none

Argument(s): none

**Description**

See parent keyword system for description.

**parallel**

- Keywords Area
- method
- sampling
- response_levels
- compute
- system
6.2. METHOD

- parallel

Aggregate response statistics assuming a parallel system

**Specification**

Alias: none

Argument(s): none

**Description**

See parent keyword *system* for description.

**distribution**

- Keywords Area
- method
- sampling
- distribution

Selection of cumulative or complementary cumulative functions

**Specification**

Alias: none

Argument(s): none

Default: cumulative (CDF)

<table>
<thead>
<tr>
<th>Required/-Optional Required (Choose One)</th>
<th>Description of Group Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>cumulativel</td>
<td></td>
<td>complementary</td>
<td>Computes statistics according to complementary cumulative functions</td>
</tr>
</tbody>
</table>

**Description**

The *distribution* keyword allows the user to select between a cumulative distribution/belief/plausibility function and a complementary cumulative distribution/belief/plausibility function. This choice affects how probabilities and reliability indices are reported.

**Default Behavior**

If the *distribution* keyword is present, it must be accompanied by either *cumulative* or *complementary*. Otherwise, a cumulative distribution will be used by default.
CHAPTER 6. KEYWORDS AREA

Expected Outputs
Output will be a set of model response-probability pairs determined according to the choice of distribution. The choice of distribution also defines the sign of the reliability or generalized reliability indices.

Examples

method
  sampling
    sample_type lhs
    samples = 10
    distribution cumulative

Computes statistics according to cumulative functions

Specification
Alias: none
  Argument(s): none

Description
Statistics on model responses will be computed according to a cumulative distribution/belief/plausibility function.

Default Behavior
By default, a cumulative distribution/belief/plausibility function will be used. To explicitly specify it in the Dakota input file, however, the cumulative keyword must be appear in conjunction with the distribution keyword.

Expected Outputs
Output will be a set of model response-probability pairs determined according to a cumulative distribution/belief/plausibility function. The probabilities reported are the probabilities that the model response falls below given response thresholds.

Examples

method
  sampling
    sample_type lhs
    samples = 10
    distribution cumulative
6.2. METHOD

complementary
  • Keywords Area
  • method
  • sampling
  • distribution
  • complementary
  Computes statistics according to complementary cumulative functions

Specification

Alias: none
  Argument(s): none

Description

Statistics on model responses will be computed according to a complementary cumulative distribution/belief/plausibility function.
  Default Behavior
  By default, a complementary cumulative distribution/belief/plausibility function will not be used. To change that behavior, the complementary keyword must appear in conjunction with the distribution keyword.
  Expected Outputs
  Output will be a set of model response-probability pairs determined according to a complementary cumulative distribution/belief/plausibility function. The probabilities reported are the probabilities that the model response falls above given response thresholds.

Examples

method
  sampling
    sample_type lhs
    samples = 10
    distribution complementary

probability_levels
  • Keywords Area
  • method
  • sampling
  • probability_levels
  Specify probability levels at which to estimate the corresponding response value

Specification

Alias: none
  Argument(s): REALLIST
  Default: No CDF/CCDF response levels to compute
| Required/- | Description of | Dakota Keyword | Dakota Keyword |
| Optional | Group | num_probability_levels | Description |
| Optional | | | Specify which probability_levels correspond to which response |

**Description**

Response levels are calculated for specified CDF/CCDF probabilities by indexing into a sorted samples array (the response levels computed are not interpolated and will correspond to one of the sampled values).

**Expected Output**

If `probability_levels` are specified, Dakota will create two tables in the standard output: a Probability Density function (PDF) histogram and a Cumulative Distribution Function (CDF) table. The PDF histogram has the lower and upper endpoints of each bin and the corresponding density of that bin. Note that the PDF histogram has bins defined by the `probability_levels` and/or `response_levels` in the Dakota input file. If there are not very many levels, the histogram will be coarse. Dakota does not do anything to optimize the bin size or spacing. The CDF table has the list of response levels and the corresponding probability that the response value is less than or equal to each response level threshold.

**Examples**

The Dakota input file below specifies a sampling method with probability levels of interest.

```plaintext
method,
   sampling,
   samples = 100 seed = 1
   complementary distribution
   probability_levels = 1. .66 .33 0.
   1. .8 .5 0.
   1. .3 .2 0.

variables,
   normal_uncertain = 2
   means = 248.89, 593.33
   std_deviations = 12.4, 29.7
   descriptors = 'TF1n' 'TF2n'
   uniform_uncertain = 2
   lower_bounds = 199.3, 474.63
   upper_bounds = 298.5, 712.
   descriptors = 'TF1u' 'TF2u'
   weibull_uncertain = 2
   alphas = 12., 30.
   betas = 250., 590.
   descriptors = 'TF1w' 'TF2w'
   histogram_bin_uncertain = 2
   num_pairs = 3 4
   abscissas = 5 8 10 .1 .2 .3 .4
   counts = 17 21 0 12 24 12 0
   descriptors = 'TF1h' 'TF2h'
   histogram_point_uncertain
   real = 1
   num_pairs = 2
   abscissas = 3 4
   counts = 1 1
   descriptors = 'TF3h'
```


### 6.2. METHOD

Given the above Dakota input file, the following excerpt from the output shows the PDF and CCDF generated. Note that the bounds on the bins of the PDF are the response values that correspond to the probability levels specified in the input file. Those response values are also shown in the CCDF.

#### Probability Density Function (PDF) histograms for each response function:

PDF for response_fn_1:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.7604749078e+11</td>
<td>3.4221494996e+11</td>
<td>5.1384774972e-12</td>
</tr>
<tr>
<td>3.4221494996e+11</td>
<td>4.0634975300e+11</td>
<td>5.145122311e-12</td>
</tr>
<tr>
<td>4.0634975300e+11</td>
<td>5.4196114379e+11</td>
<td>2.4334239039e-12</td>
</tr>
</tbody>
</table>

PDF for response_fn_2:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.643154744e+04</td>
<td>5.6511827775e+04</td>
<td>1.9839945149e-05</td>
</tr>
<tr>
<td>5.6511827775e+04</td>
<td>6.1603813790e+04</td>
<td>5.8916108390e-05</td>
</tr>
<tr>
<td>6.1603813790e+04</td>
<td>7.8702465755e+04</td>
<td>2.9242071306e-05</td>
</tr>
</tbody>
</table>

PDF for response_fn_3:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.3796737090e+05</td>
<td>3.6997214153e+05</td>
<td>5.302386523e-06</td>
</tr>
<tr>
<td>3.6997214153e+05</td>
<td>3.8100966235e+05</td>
<td>9.0600055634e-06</td>
</tr>
<tr>
<td>3.8100966235e+05</td>
<td>4.4111498127e+05</td>
<td>3.3274923548e-06</td>
</tr>
</tbody>
</table>

Level mappings for each response function:

#### Complementary Cumulative Distribution Function (CCDF) for response_fn_1:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.7604749078e+11</td>
<td>1.0000000000e+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.4221494996e+11</td>
<td>6.6000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.0634975300e+11</td>
<td>3.3000000000e-01</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

#### Complementary Cumulative Distribution Function (CCDF) for response_fn_2:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.643154744e+04</td>
<td>1.0000000000e+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5.6511827775e+04</td>
<td>8.0000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6.1603813790e+04</td>
<td>5.0000000000e-01</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

#### Complementary Cumulative Distribution Function (CCDF) for response_fn_3:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.3796737090e+05</td>
<td>1.0000000000e+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.6997214153e+05</td>
<td>3.0000000000e-01</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Theory

Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.
In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

An inverse mapping involves computing the belief and plausibility response level for either a specified probability level or a specified generalized reliability level (two results for each level mapping in the evidence-based epistemic case, instead of the one result for each level mapping in the aleatory case).

**num_probability_levels**
- Keywords Area
- method
- sampling
- probability_levels
- num_probability_levels

Specify which `probability_levels` correspond to which response

**Specification**

Alias: none

**Argument(s):** INTEGERLIST

**Default:** probability_levels evenly distributed among response functions

**Description**
See parent page

**gen_reliability_levels**
- Keywords Area
- method
- sampling
- gen_reliability_levels

Specify generalized reliability levels at which to estimate the corresponding response value

**Specification**

Alias: none

**Argument(s):** REALLIST

**Default:** No CDF/CCDF response levels to compute

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
</table>


6.2. METHOD

| Optional | num_gen_reliability_levels | Specify which gen_reliability_levels correspond to which response |

**Description**

Response levels are calculated for specified generalized reliabilities by indexing into a sorted samples array (the response levels computed are not interpolated and will correspond to one of the sampled values).

**Theory**

Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.

In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

An inverse mapping involves computing the belief and plausibility response level for either a specified probability level or a specified generalized reliability level (two results for each level mapping in the evidence-based epistemic case, instead of the one result for each level mapping in the aleatory case).

**num_gen_reliability_levels**

- **Keywords Area**
- **method**
- **sampling**
- **gen_reliability_levels**
- **num_gen_reliability_levels**

Specify which gen_reliability_levels correspond to which response

**Specification**

**Alias:** none

**Argument(s):** INTEGERLIST

**Default:** gen_reliability_levels evenly distributed among response functions

**Description**

See parent page
**rng**

- **Keywords Area**
- **method**
- **sampling**
- **rng**

Selection of a random number generator

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** Mersenne twister (mt19937)

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required/One Group 1</td>
<td></td>
<td>mt19937</td>
<td>Generates random numbers using the Mersenne twister</td>
</tr>
<tr>
<td></td>
<td></td>
<td>rnum2</td>
<td>Generates pseudo-random numbers using the Pecos package</td>
</tr>
</tbody>
</table>

**Description**

The *rng* keyword is used to indicate a choice of random number generator.

**Default Behavior**

If specified, the *rng* keyword must be accompanied by either *rnum2* (pseudo-random numbers) or *mt19937* (random numbers generated by the Mersenne twister). Otherwise, *mt19937*, the Mersenne twister is used by default.

**Usage Tips**

The default is recommended, as the Mersenne twister is a higher quality random number generator.

**Examples**

```dakota
method
  sampling
    sample_type lhs
    samples = 10
    seed = 98765
    rng rnum2
```

**mt19937**

- **Keywords Area**
- **method**
6.2. METHOD

- sampling
- rng
- mt19937

Generates random numbers using the Mersenne twister

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

The `mt19937` keyword directs Dakota to use the Mersenne twister to generate random numbers. Additional information can be found on wikipedia: [http://en.wikipedia.org/wiki/Mersenne_twister](http://en.wikipedia.org/wiki/Mersenne_twister).

**Default Behavior**

`mt19937` is the default random number generator. To specify it explicitly in the Dakota input file, however, it must be specified in conjunction with the `rng` keyword.

**Usage Tips**

Use of the Mersenne twister random number generator (`mt19937`) is recommended.

**Examples**

```dakota
method sampling
  sample_type lhs
  samples = 10
  seed = 98765
  rng mt19937
```

**rnum2**

- **Keywords Area**
- **method**
- **sampling**
- **rng**
- **rnum2**

Generates pseudo-random numbers using the Pecos package

**Specification**

**Alias:** none

**Argument(s):** none
Description

The rnum2 keyword directs Dakota to use pseudo-random numbers generated by the Pecos package.

**Default Behavior**

rnum2 is not used by default. To change this behavior, it must be specified in conjunction with the **rng** keyword.

**Usage Tips**

Use of the Mersenne twister random number generator (mt19937) is recommended over rnum2.

Examples

```plaintext
method
  sampling
    sample_type lhs
    samples = 10
    seed = 98765
  rng rnum2
```

**model_pointer**

- **Keywords Area**
- **method**
- **sampling**
- **model_pointer**

Identifier for model block to be used by a method

Topics

This keyword is related to the topics:

- **block_pointer**

Specification

**Alias:** none

**Argument(s):** STRING

**Default:** method use of last model parsed (or use of default model if none parsed)

Description

The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

**Default Behavior**

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding **id_model** with the same name.

**Usage Tips**

When doing advanced analyses that involve using multiple methods and multiple models, defining a model-pointer for each method is imperative.

See **block_pointer** for details about pointers.
6.2. METHOD

Examples

environment
tabular_graphics_data
method_pointer = 'UQ'

method
id_method = 'UQ'
model_pointer = 'SURR'
sampling,
samples = 10
seed = 98765 rng rnum2
response_levels = 0.1 0.2 0.6
0.1 0.2 0.6
0.1 0.2 0.6
sample_type lhs
distribution cumulative

model
id_model = 'SURR'
surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
id_method = 'DACE'
model_pointer = 'DACE_M'
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = 'DACE_M'
single
interface_pointer = 'I1'

variables
uniform_uncertain = 2
lower_bounds = 0. 0.
upper_bounds = 1. 1.
descriptors = 'x1' 'x2'

interface
id_interface = 'I1'
system asynch evaluationConcurrency = 5
analysis_driver = 'text_book'

responses
response_functions = 3
no_gradients
no_hessians

6.2.51 multilevel_sampling

- Keywords Area
- method
- multilevel_sampling

Multilevel methods for sampling-based UQ
**Specification**

**Alias:** multilevel_mc  
**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>seed</td>
<td></td>
<td>Seed of the random number generator</td>
</tr>
<tr>
<td>Optional</td>
<td>fixed_seed</td>
<td></td>
<td>Reuses the same seed value for multiple random sampling sets</td>
</tr>
<tr>
<td>Optional</td>
<td>pilot_samples</td>
<td></td>
<td>Initial set of samples for multilevel sampling methods.</td>
</tr>
<tr>
<td>Optional</td>
<td>sample_type</td>
<td></td>
<td>Selection of sampling strategy</td>
</tr>
<tr>
<td>Optional</td>
<td>export_sample_sequence</td>
<td></td>
<td>Enable exporting output sample sequences on files</td>
</tr>
<tr>
<td>Optional</td>
<td>max_iterations</td>
<td></td>
<td>Stopping criterion based on number of refinement iterations within the multilevel sample allocation</td>
</tr>
<tr>
<td>Optional</td>
<td>convergence_tolerance</td>
<td></td>
<td>Stopping criterion based on relative error</td>
</tr>
<tr>
<td>Optional</td>
<td>final_moments</td>
<td></td>
<td>Output moments of the specified type and include them within the set of final statistics.</td>
</tr>
</tbody>
</table>
### Description

A nascent sampling method that utilizes both multifidelity and multilevel relationships within a hierarchical surrogate model in order to improve convergence behavior in sampling methods.

In the case of a multilevel relationship, multilevel Monte Carlo methods are used to compute an optimal sample allocation per level, and in the case of a multifidelity relationship, control variate Monte Carlo methods are used to compute an optimal sample allocation per fidelity. These two approaches can also be combined, resulting in the three approaches below.

#### Multilevel Monte Carlo

The Monte Carlo estimator for the mean is defined as

\[
\mathbb{E}[Q] \equiv \hat{Q}^{MC} = \frac{1}{N} \sum_{i=1}^{N} Q^{(i)}
\]

In a multilevel method with \( L \) levels, we replace this estimator with a telescoping sum:

\[
\mathbb{E}[Q] \equiv \hat{Q}^{ML} = \sum_{l=0}^{L} \frac{1}{N_l} \sum_{i=1}^{N_l} (Q_{l}^{(i)} - Q_{l-1}^{(i)}) = \sum_{l=0}^{L} \hat{Y}_l^{MC}
\]

This decomposition forms discrepancies for each level greater than 0, seeking reduction in the variance of the discrepancy \( Y \) relative to the variance of the original response \( Q \). The number of samples allocated for each level ( \( N_l \) ) is based on a total cost minimization procedure that incorporates the relative cost and observed variance for each of the \( Y_l \).

#### Control Variate Monte Carlo

In the case of two model fidelities (low fidelity denoted as LF and high fidelity denoted as HF), we employ a control variate approach:

\[
\hat{Q}^{CV}_{HF} = \hat{Q}^{MC}_{HF} - \beta (\hat{Q}^{MC}_{LF} - \mathbb{E}[Q_{LF}])
\]

As opposed to the traditional control variate approach, we do not know \( \mathbb{E}[Q_{LF}] \) precisely, but rather estimate it more accurately than \( \hat{Q}^{MC}_{LF} \) based on a sampling increment applied to the LF model. This sampling increment is based again on a total cost minimization procedure that incorporates the relative LF and HF costs and the

<table>
<thead>
<tr>
<th>Optional</th>
<th>distribution</th>
<th>Placeholder for future capabilities</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>probability_levels</td>
<td>Placeholder for future capabilities</td>
</tr>
<tr>
<td>Optional</td>
<td>gen_reliability_levels</td>
<td>Placeholder for future capabilities</td>
</tr>
<tr>
<td>Optional</td>
<td>mg</td>
<td>Selection of a random number generator</td>
</tr>
<tr>
<td>Optional</td>
<td>model_pointer</td>
<td>Identifier for model block to be used by a method</td>
</tr>
</tbody>
</table>
observed Pearson correlation coefficient $\rho_{LH}$ between $Q_{LF}$ and $Q_{HF}$. The coefficient $\beta$ is then determined from the observed LF-HF covariance and LF variance.

**Multilevel Control Variate Monte Carlo**

If both multifidelity and multilevel structure are included within the hierarchical model specification, then a control variate can be applied across fidelities for each level within an outer multilevel approach.

On each level a control variate is active for the discrepancy $Y_\ell$ based on

$$Y_\ell^* = Y_\ell + \alpha_\ell \left( \bar{Y}_\ell^{\text{LF}} - \mathbb{E}[Y_\ell^{\text{LF}}] \right),$$

where $Y_\ell^{\text{LF}} = \gamma_\ell Q_\ell^{\text{LF}} - Q_\ell^{\text{HF}}$.

The optimal parameter $\gamma_\ell$ is computed from the correlation properties between model forms and discretization levels (see the theory manual for further details) and the optimal allocation $N_\ell$ (per level) is finally obtained from it.

**Default Behavior**

The multilevel sampling method employs Monte Carlo sampling be default, but this default can be overridden to use Latin hypercube sampling using `sample_type lhs`.

**Expected Output**

The multilevel sampling method reports estimates of the first four moments and a summary of the evaluations performed for each model fidelity and discretization level. The method does not support any level mappings (response, probability, reliability, generalized reliability) at this time.

**Usage Tips**

The multilevel sampling method must be used in combination with a hierarchical model specification. When exploiting multiple discretization levels, it is necessary to identify the variable string identifier that controls these levels using `solution_level_control`. Associated relative costs also need to be supplied using `solution_level_cost`.

**Additional Discussion**

Also see multilevel regression in `polynomial_chaos`.

**Examples**

The following method block

```plaintext
method,
  model_pointer = 'HIERARCH'
  multilevel_sampling
    pilot_samples = 20 seed = 1237
    max_iterations = 10
    convergence_tolerance = .001

results in multilevel Monte Carlo when the HIERARCH model specification contains a single model fidelity with multiple discretization levels, in control variate Monte Carlo when the HIERARCH model specification has multiple ordered model fidelities each with a single discretization level, and multilevel control variate Monte Carlo when the HIERARCH model specification contains multiple model fidelities each with multiple discretization levels.

An example of the former (single model fidelity with multiple discretization levels) follows:

```plaintext
model,
  id_model = 'HIERARCH'
  surrogate_hierarchical
    ordered_model_fidelities = 'SIM1'
    correction additive zeroth_order

model,
  id_model = 'SIM1'
```
6.2. METHOD

```
simulation
  solution_level_control = 'N_x'
  solution_level_cost = 630. 1260. 2100. 4200.
```

Refer to dakota/test/dakota_uq_heat_eq{mlmc,cvmc,mlcvmc}.in for additional examples.

See Also

These keywords may also be of interest:

- polynomial_chaos

seed

- Keywords Area
- method
- multilevel_sampling
- seed

Seed of the random number generator

Specification

Alias: none

Argument(s): INTEGER
Default: system-generated (non-repeatable)

Description

The random seed control provides a mechanism for making a stochastic method repeatable. That is, the use of the same random seed in identical studies will generate identical results.

Default Behavior
If not specified, the seed is randomly generated.

Expected Output
If seed is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

Usage Tips
If a stochastic study was run without seed specified, and the user later wishes to repeat the study using the same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen. That value can then be added to the Dakota input file.

Examples

```
method
  sampling
    sample_type lhs
    samples = 10
    seed = 15347
```
fixed_seed

- Keywords Area
- method
- multilevel_sampling
- fixed_seed

Reuses the same seed value for multiple random sampling sets

Specification

Alias: none
Argument(s): none
Default: not fixed; pattern varies run-to-run

Description

The `fixed_seed` flag is relevant if multiple sampling sets will be generated over the course of a Dakota analysis. This occurs when using advance methods (e.g., surrogate-based optimization, optimization under uncertainty). The same seed value is reused for each of these multiple sampling sets, which can be important for reducing variability in the sampling results.

Default Behavior

The default behavior is to not use a fixed seed, as the repetition of the same sampling pattern can result in a modeling weakness that an optimizer could potentially exploit (resulting in actual reliabilities that are lower than the estimated reliabilities). For repeatable studies, the `seed` must also be specified.

Examples

```
method
  sampling
    sample_type lhs
    samples = 10
    fixed_seed
```

pilot_samples

- Keywords Area
- method
- multilevel_sampling
- pilot_samples

Initial set of samples for multilevel sampling methods.

Specification

Alias: none
Argument(s): INTEGERLIST
6.2. **METHOD**

**Description**

The pilot sample provides initial estimates of variance and/or correlation within the first iteration of a multilevel and/or control variate approach.

**Default Behavior**

100 samples per model fidelity and/or discretization level.

**Usage Tips**

The number of specified values can be none (default values used for all fidelities and levels), one (all fidelities and levels use the same specified value), the number of discretization levels for every model (each model uses the same discretization level profile), or the aggregate number of discretization levels for all models (samples for each discretization level are distinct for each model).

**sample_type**

- Keywords Area
- method
- multilevel_sampling
- sample_type

Selection of sampling strategy

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** random

<table>
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<tr>
<th>Required/Optional Required (Choose One)</th>
<th>Description of Group Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<td>lhs</td>
<td>Uses Latin Hypercube Sampling (LHS) to sample variables</td>
<td></td>
<td></td>
</tr>
<tr>
<td>random</td>
<td>Uses purely random Monte Carlo sampling to sample variables</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Description**

The `sample_type` keyword allows the user to select between two types of sampling: Monte Carlo (pure random) and Latin hypercube (stratified) sampling.

The incremental keywords are deprecated; instead use `samples` together with `refinement_samples`.

**Default Behavior**

If the `sample_type` keyword is present, it must be accompanied by `lhs` or `random`. In most contexts, `lhs` is the default (exception: `multilevel_sampling` uses Monte Carlo by default).


Examples

```
method sampling
  sample_type lhs
  samples = 20
  seed = 83921
```

lhs

- Keywords Area
- method
- multilevel_sampling
- sample_type
- lhs

Uses Latin Hypercube Sampling (LHS) to sample variables

Specification

Alias: none
Argument(s): none

Description

The `lhs` keyword invokes Latin Hypercube Sampling as the means of drawing samples of uncertain variables according to their probability distributions. This is a stratified, space-filling approach that selects variable values from a set of equi-probable bins.

**Default Behavior**

Latin Hypercube Sampling is the default sampling mode in most contexts (exception: multilevel_sampling). To explicitly specify LHS in the Dakota input file, the `lhs` keyword must appear in conjunction with the `sample_type` keyword.

**Usage Tips**

Latin Hypercube Sampling is very robust and can be applied to any problem. It is fairly effective at estimating the mean of model responses and linear correlations with a reasonably small number of samples relative to the number of variables.

Examples

```
method sampling
  sample_type lhs
  samples = 20
```

random

- Keywords Area
- method
- multilevel_sampling
6.2. METHOD

- sample_type
- random

Uses purely random Monte Carlo sampling to sample variables

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

The `random` keyword invokes Monte Carlo sampling as the means of drawing samples of uncertain variables according to their probability distributions.

**Default Behavior**

In most contexts, Monte Carlo sampling is not the default sampling mode (exception: multilevel_sampling). To change this behavior, the `random` keyword must be specified in conjunction with the `sample_type` keyword.

**Usage Tips**

Monte Carlo sampling is more computationally expensive than Latin Hypercube Sampling as it requires a larger number of samples to accurately estimate statistics.

**Examples**

```plaintext
method sampling
  sample_type random
  samples = 200
```

**export_sample_sequence**

- **Keywords Area**
- **method**
- **multilevel_sampling**
- **export_sample_sequence**

Enable exporting output sample sequences on files

**Specification**

**Alias:** none

**Argument(s):** none
## Description

If present, separate output files are written for each model form and discretization level. For the multilevel technique, separate files are written for the samples used at each iteration (pilot samples are denoted by iteration 0).

### Default Behavior

If not specified, the _annotated_ format is assumed.

### Expected Output

Separate output files are generated according to the following format: `{ml/cv}.{interface_id}.{iteration_number}.{level_number}.{number_of_samples}.dat`.

If one single model form is present the first field of the file name is _ml_, otherwise _ml_ is used for the HF model and _cv_ is used for the LF one.

## Examples

The following method block

```plaintext
method,
    model_pointer = 'HIERARCH'
    multilevel_sampling
    pilot_samples = 20 seed = 1237
    convergence_tolerance = .01
    output silent
    export_sample_sequence

results in enabling the sample output on file with the defaults _annotated_ format.
```

The following variables block

```plaintext
variables,
    id_variables = 'LF_VARS'
    uniform_uncertain = 7
    lower_bounds = 7*-1.
    upper_bounds = 7* 1.
    discrete_state_set
        integer = 2
        num_set_values = 4 1
        set_values = 5 15 30 60 # number of spatial coords
            3 # number of Fourier solution modes
        initial_state = 5 3
descriptors 'N_x' 'N_mod'
```
illustrates how to define descriptors for a model form. For instance, in this case the descriptors $N_x$ and $N_{mod}$ are reported in the sample sequences files for all the format.

**annotated**

- Keywords Area
- method
- multilevel_sampling
- export_sample_sequence
- annotated

Export sample sequences with descriptors

**Specification**

Alias: none

Argument(s): none

Default: annotated

**Description**

Sample sequences are written on file using header descriptors for the data set and a per-level progressive number, eval_id. The interface identifier, interface_id, is also reported as well as the model descriptors.

**custom_annotated**

- Keywords Area
- method
- multilevel_sampling
- export_sample_sequence
- custom_annotated

Export sample sequences enabling file format customization

**Specification**

Alias: none

Argument(s): none
### Description

Sample sequences are written on file with a user-defined format. If the keyword `header` is present the heading is used, if the keyword `eval_id` is present the sample number (per level) is included and if `interface_id` is provided then the interface identification is reported.

### Examples

The following method block

```plaintext
method,
  model_pointer = 'HIERARCH'
  multilevel_sampling
  pilot_samples = 20 seed = 1237
  convergence_tolerance = .01
  output silent
  export_sample_sequence custom_annotated eval_id
```

results in enabling the sample output on file with a customized format including only the progressive number of the sample (`eval_id`).

- **header**
  - **Keywords Area**
  - **method**
  - **multilevel_sampling**
  - **export_sample_sequence**
  - **custom_annotated**
  - **header**

Enable header row in custom-annotated tabular file

<table>
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<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<td>header</td>
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</tr>
<tr>
<td>Optional</td>
<td></td>
<td>eval_id</td>
<td>Enable evaluation ID column in custom-annotated tabular file</td>
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<tr>
<td>Optional</td>
<td></td>
<td>interface_id</td>
<td>Enable interface ID column in custom-annotated tabular file</td>
</tr>
</tbody>
</table>
6.2. METHOD

Specification

Alias: none
Argument(s): none

Description

See description of parent custom_annotated

eval_id

- Keywords Area
- method
- multilevel_sampling
- export_sample_sequence
- custom_annotated
- eval_id

Enable evaluation ID column in custom-annotated tabular file

Specification

Alias: none
Argument(s): none

Description

See description of parent custom_annotated

interface_id

- Keywords Area
- method
- multilevel_sampling
- export_sample_sequence
- custom_annotated
- interface_id

Enable interface ID column in custom-annotated tabular file

Specification

Alias: none
Argument(s): none
Description

See description of parent custom.annotated

freeform
  • Keywords Area
  • method
  • multilevel_sampling
  • export_sample_sequence
  • freeform

Export sample sequences without heading descriptors

Specification

Alias: none
Argument(s): none
Default: annotated

Description

Sample sequences are written on file without using any heading descriptors for the data set. The interface identifier, interface.id, and the model descriptors are still reported.

max_iterations
  • Keywords Area
  • method
  • multilevel_sampling
  • max_iterations

Stopping criterion based on number of refinement iterations within the multilevel sample allocation

Specification

Alias: none
Argument(s): INTEGER
Default: 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence} / efficient_global: 25*n)

Description

Multilevel sampling is an iterative procedure that estimates the optimal number of samples for each level based on cost and observed variance. On each iteration, additional samples are performed and more accurate variance estimates are computed, leading to updated sample allocations. The process terminates when either no additional samples are allocated or the max_iterations control is enforced.

Default Behavior

The default value for max_iterations varies by method. For multilevel_sampling, the default value is 25.
6.2. **METHOD**

**convergence_tolerance**
- **Keywords Area**
- **method**
- **multilevel_sampling**
- **convergence_tolerance**

Stopping criterion based on relative error

**Specification**

**Alias:** none

**Argument(s):** REAL

**Default:** 1.e-4

**Description**

Multilevel sampling seeks an error balance between the estimator variance and the remaining bias error at the highest level, the two contributors to mean squared error (MSE). Since the remaining bias error is generally unknown, the `convergence_tolerance` is used to provide an error target relative to the Monte Carlo estimator variance resulting from the pilot sample. The samples allocated at each level are proportional to \( \frac{1}{\epsilon^2} \), so each order of magnitude reduction in `convergence_tolerance` will tend to increase the sample allocation by two orders of magnitude. Therefore, this control should be used with care to avoid allocation of huge sample sets that could overrun available memory.

**Default Behavior**

The default value for `convergence_tolerance` is currently .0001, which may be too resolved for expensive simulations or high variance QoI.

**final_moments**
- **Keywords Area**
- **method**
- **multilevel_sampling**
- **final_moments**

Output moments of the specified type and include them within the set of final statistics.

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** `standard`

<table>
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<th>Dakota Keyword</th>
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CHAPTER 6. KEYWORDS AREA

<table>
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<th>Omit moments from the set of final statistics.</th>
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<tr>
<td></td>
<td></td>
<td></td>
<td>Output standardized moments and include them within the set of final statistics.</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>central</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Output central moments and include them within the set of final statistics.</td>
</tr>
</tbody>
</table>

**Description**

When performing a nested study that may employ moment statistics on the inner loop, it can be desirable to control the type of these moments. The `final_moments` specification supports options of none, standard (default), or central, corresponding to omission of moments, standardized moments (mean, standard deviation, skewness, and excess kurtosis), or central moments (mean, variance, 3rd central, and 4th central).

The presence or omission of moment results in the final statistics influences the outer level mappings in the case of a nested study. For example, `final_moments none` can allow for a more compact specification of primary and/or secondary response mappings.

**Examples**

The following method specification overrides the default to print central moments and include them in the set of final statistics.

```plaintext
method,
  sampling
    samples = 50 seed = 1234
    response_levels = 3.6e+11 1.2e+05 3.5e+05
    final_moments central

  Overriding the default to none as follows:

method,
  sampling
    samples = 50 seed = 1234
    response_levels = 3.6e+11 1.2e+05 3.5e+05
    final_moments none

allows associated nested model mappings to be simplified from:

model
  nested
    sub_method_pointer = 'UQ'
    primary_response_mapping = 0. 0. 1. 0. 0. 1. 0. 0. 0.
    secondary_response_mapping = 0. 0. 0. 0. 0. 0. 0. 0. 1.

to a more compact version focused only on the response level mappings (two leading zeros per response function for moment mappings have been removed):
6.2. METHOD

model nested
  sub_method_pointer = 'UQ'
  primary_response_mapping = 1. 1. 0.
  secondary_response_mapping = 0. 0. 1.

none
  • Keywords Area
  • method
  • multilevel_sampling
  • final_moments
  • none

Omit moments from the set of final statistics.

Specification

Alias: none
  Argument(s): none

Description

The omission of moment results from the final statistics can allow for a more compact definition of primary and/or secondary response mappings within a nested model specification.

Examples

method,
  sampling
    samples = 50 seed = 1234
    response_levels = 3.6e+11 1.2e+05 3.5e+05
    final_moments none

standard
  • Keywords Area
  • method
  • multilevel_sampling
  • final_moments
  • standard

Output standardized moments and include them within the set of final statistics.

Specification

Alias: none
  Argument(s): none
CHAPTER 6. KEYWORDS AREA

Description

Output standardized moments (mean, standard deviation, skewness, and excess kurtosis) and include the first two within the set of final statistics to be used at a higher level (e.g., optimization under uncertainty, mixed aleatory-epistemic UQ). This inclusion of moment results affects the primary and/or secondary response mappings in a nested model specification.

Examples

The following method specification overrides the default to print central moments and include them in the set of final statistics.

```
method, sampling
  samples = 50 seed = 1234
  response_levels = 3.6e+11 1.2e+05 3.5e+05
  final_moments central
```

Specification

Alias: none
Argument(s): none

Description

Output central moments (mean, variance, 3rd central, and 4th central) and include the first two within the set of final statistics to be used at a higher level (e.g., optimization under uncertainty, mixed aleatory-epistemic UQ). This inclusion of moment results affects the primary and/or secondary response mappings in a nested model specification.

Examples

The following method specification overrides the default to print central moments and include them in the set of final statistics.

```
method, sampling
  samples = 50 seed = 1234
  response_levels = 3.6e+11 1.2e+05 3.5e+05
  final_moments central
```
6.2. METHOD

distribution

- Keywords Area
- method
- multilevel_sampling
- distribution

Placeholder for future capabilities

Specification

Alias: none
Argument(s): none
Default: cumulative (CDF)

<table>
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<tr>
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<th>Dakota Keyword cumulative</th>
<th>Dakota Keyword Description Placeholder for future capabilities</th>
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<tbody>
<tr>
<td></td>
<td></td>
<td>complementary</td>
<td>Placeholder for future capabilities</td>
</tr>
</tbody>
</table>

Description

At this stage only moments are computed as output in the framework of multilevel sampling techniques. No distribution capabilities are implemented yet.

cumulative

- Keywords Area
- method
- multilevel_sampling
- distribution
- cumulative

Placeholder for future capabilities

Specification

Alias: none
Argument(s): none

Description

At this stage only moments are computed as output in the framework of multilevel sampling techniques. No distribution capabilities are implemented yet.
CHAPTER 6. KEYWORDS AREA

complementary

- Keywords Area
- method
- multilevel_sampling
- distribution
- complementary

Placeholder for future capabilities

Specification

Alias: none
Argument(s): none

Description

At this stage only moments are computed as output in the framework of multilevel sampling techniques. No distribution capabilities are implemented yet.

probability_levels

- Keywords Area
- method
- multilevel_sampling
- probability_levels

Placeholder for future capabilities

Specification

Alias: none
Argument(s): REALLIST
Default: No CDF/CCDF response levels to compute

<table>
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<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<tr>
<td>Optional</td>
<td>num_probability_-levels</td>
<td></td>
<td>Placeholder for future capabilities</td>
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</table>

Description

At this stage only moments are computed as output in the framework of multilevel sampling techniques. No distribution capabilities are implemented yet.
6.2. METHOD

num_probability_levels

- Keywords Area
- method
- multilevel_sampling
- probability_levels
- num_probability_levels

Placeholder for future capabilities

Specification

Alias: none

Argument(s): INTEGERLIST

Default: probability_levels evenly distributed among response functions

Description

At this stage only moments are computed as output in the framework of multilevel sampling techniques. No distribution capabilities are implemented yet.

gen_reliability_levels

- Keywords Area
- method
- multilevel_sampling
- gen_reliability_levels

Placeholder for future capabilities

Specification

Alias: none

Argument(s): REALLIST

Default: No CDF/CCDF response levels to compute

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword</th>
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<tr>
<td></td>
<td></td>
<td>reliability_levels</td>
<td>future capabilities</td>
</tr>
</tbody>
</table>

Description

At this stage only moments are computed as output in the framework of multilevel sampling techniques. No distribution capabilities are implemented yet.
num_gen_reliability_levels

- Keywords Area
- method
- multilevel_sampling
- gen_reliability_levels
- num_gen_reliability_levels

Placeholder for future capabilities

**Specification**

**Alias:** none

**Argument(s):** INTEGERLIST

**Default:** gen_reliability_levels evenly distributed among response functions

**Description**

At this stage only moments are computed as output in the framework of multilevel sampling techniques. No distribution capabilities are implemented yet.

**rng**

- Keywords Area
- method
- multilevel_sampling
- rng

Selection of a random number generator

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** Mersenne twister (mt19937)

<table>
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<tr>
<th>Required/Optional Required (Choose One)</th>
<th>Description of Group Group 1</th>
<th>Dakota Keyword mt19937</th>
<th>Dakota Keyword Description Generates random numbers using the Mersenne twister</th>
</tr>
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<tbody>
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</tr>
</tbody>
</table>
6.2. **METHOD**

| rnum2 | Generates pseudo-random numbers using the Pecos package |

**Description**

The **rng** keyword is used to indicate a choice of random number generator.

**Default Behavior**

If specified, the **rng** keyword must be accompanied by either **rnum2** (pseudo-random numbers) or **mt19937** (random numbers generated by the Mersenne twister). Otherwise, **mt19937**, the Mersenne twister is used by default.

**Usage Tips**

The default is recommended, as the Mersenne twister is a higher quality random number generator.

**Examples**

```plaintext
method
  sampling
    sample_type lhs
    samples = 10
    seed = 98765
    rng rnum2
```

**mt19937**

- **Keywords Area**
- **method**
- **multilevel_sampling**
- **rng**
- **mt19937**

Generates random numbers using the Mersenne twister

**Specification**

**Alias:** none  
**Argument(s):** none

**Description**

The **mt19937** keyword directs Dakota to use the Mersenne twister to generate random numbers. Additional information can be found on Wikipedia: http://en.wikipedia.org/wiki/Mersenne_twister.

**Default Behavior**

**mt19937** is the default random number generator. To specify it explicitly in the Dakota input file, however, it must be specified in conjunction with the **rng** keyword.

**Usage Tips**

Use of the Mersenne twister random number generator (**mt19937**) is recommended.
Examples

method
  sampling
    sample_type lhs
    samples = 10
    seed = 98765
    rng mt19937

rnum2
  \item Keywords Area
  \item method
  \item multilevel_sampling
  \item rng
  \item rnum2
  Generates pseudo-random numbers using the Pecos package

Specification

Alias: none
  Argument(s): none

Description

The rnum2 keyword directs Dakota to use pseudo-random numbers generated by the Pecos package.

Default Behavior
rnum2 is not used by default. To change this behavior, it must be specified in conjunction with the rng keyword.

Usage Tips
Use of the Mersenne twister random number generator (mt19937) is recommended over rnum2.

Examples

method
  sampling
    sample_type lhs
    samples = 10
    seed = 98765
    rng rnum2

model_pointer
  \item Keywords Area
  \item method
  \item multilevel_sampling
  \item model_pointer

Identifier for model block to be used by a method
6.2. METHOD

Topics

This keyword is related to the topics:

- `block_pointer`

Specification

**Alias:** none

**Argument(s):** STRING

**Default:** method use of last model parsed (or use of default model if none parsed)

Description

The `model_pointer` is used to specify which `model` block will be used to perform the function evaluations needed by the Dakota method.

**Default Behavior**

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a `model` block in the Dakota input file that has a corresponding `id_model` with the same name.

**Usage Tips**

When doing advanced analyses that involve using multiple methods and multiple models, defining a `model_pointer` for each method is imperative.

See `block_pointer` for details about pointers.

Examples

```plaintext
environment
    tabular_graphics_data
    method_pointer = 'UQ'

method
    id_method = 'UQ'
    model_pointer = 'SURR'
    sampling,
        samples = 10
        seed = 98765 rng rnum2
        response_levels = 0.1 0.2 0.6
        0.1 0.2 0.6
        0.1 0.2 0.6
    sample_type lhs
distribution cumulative

model
    id_model = 'SURR'
    surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
    id_method = 'DACE'
    model_pointer = 'DACE_M'
    sampling sample_type lhs
    samples = 121 seed = 5034 rng rnum2

model
    id_model = 'DACE_M'
single
```
interface_pointer = 'I1'

variables
  uniform_uncertain = 2
  lower_bounds = 0.0.
  upper_bounds = 1.1.
  descriptors = 'x1' 'x2'

interface
  id_interface = 'I1'
  system asynch evaluation_concurrency = 5
  analysis_driver = 'text_book'

responses
  response_functions = 3
  no_gradients
  no_hessians

6.2.52 importance_sampling

- Keywords Area
- method
- importance_sampling

Importance sampling

Topics
This keyword is related to the topics:

- uncertainty_quantification
- aleatory_uncertainty_quantification_methods
- sampling

Specification
Alias: nond_importance_sampling
Argument(s): none

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword samples</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td></td>
<td>Number of samples for sampling-based methods</td>
</tr>
<tr>
<td>Optional</td>
<td>seed</td>
<td>Seed of the random number generator</td>
<td></td>
</tr>
<tr>
<td>-------------------</td>
<td>---------------</td>
<td>--------------------------------------</td>
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<tr>
<td>Required (Choose One)</td>
<td>import</td>
<td>Sampling option</td>
<td></td>
</tr>
<tr>
<td>Group 1</td>
<td>adapt_import</td>
<td>Importance sampling option</td>
<td></td>
</tr>
<tr>
<td></td>
<td>mm_adapt_import</td>
<td>Sampling option</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>refinement_samples</td>
<td>Number of samples used to refine a probability estimate or sampling design.</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>response_levels</td>
<td>Values at which to estimate desired statistics for each response</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>max_iterations</td>
<td>Number of iterations allowed for optimizers and adaptive UQ methods</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>convergence_tolerance</td>
<td>Stopping criterion based on convergence of the objective function or statistics</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>distribution</td>
<td>Selection of cumulative or complementary cumulative functions</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>probability_levels</td>
<td>Specify probability levels at which to estimate the corresponding response value</td>
<td></td>
</tr>
</tbody>
</table>
CHAPTER 6. KEYWORDS AREA

<table>
<thead>
<tr>
<th>Optional</th>
<th>gen_reliability_levels</th>
<th>Specify generalized reliability levels at which to estimate the corresponding response value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>rng</td>
<td>Selection of a random number generator</td>
</tr>
<tr>
<td>Optional</td>
<td>model_pointer</td>
<td>Identifier for model block to be used by a method</td>
</tr>
</tbody>
</table>

### Description

The `importance_sampling` method is based on ideas in reliability modeling.

An initial Latin Hypercube sampling is performed to generate an initial set of samples. These initial samples are augmented with samples from an importance density as follows:

- The variables are transformed to standard normal space.
- In the transformed space, the importance density is a set of normal densities centered around points which are in the failure region.
- Note that this is similar in spirit to the reliability methods, in which importance sampling is centered around a Most Probable Point (MPP).
- In the case of the LHS samples, the importance sampling density will simply by a mixture of normal distributions centered around points in the failure region.

### Options

Choose one of the importance sampling options:

- import
- adapt_import
- mm_adapt_import

The options for importance sampling are as follows: `import` centers a sampling density at one of the initial LHS samples identified in the failure region. It then generates the importance samples, weights them by their probability of occurrence given the original density, and calculates the required probability (CDF or CCDF level). `adapt_import` is the same as `import` but is performed iteratively until the failure probability estimate converges. `mm_adapt_import` starts with all of the samples located in the failure region to build a multimodal sampling density. First, it uses a small number of samples around each of the initial samples in the failure region. Note that these samples are allocated to the different points based on their relative probabilities of occurrence: more probable points get more samples. This early part of the approach is done to search for "representative" points. Once these are located, the multimodal sampling density is set and then `mm_adapt_import` proceeds similarly to `adapt_import` (sample until convergence).
6.2. **METHOD**

**Theory**

Importance sampling is a method that allows one to estimate statistical quantities such as failure probabilities (e.g. the probability that a response quantity will exceed a threshold or fall below a threshold value) in a way that is more efficient than Monte Carlo sampling. The core idea in importance sampling is that one generates samples that preferentially samples important regions in the space (e.g. in or near the failure region or user-defined region of interest), and then appropriately weights the samples to obtain an unbiased estimate of the failure probability [76]. In importance sampling, the samples are generated from a density which is called the importance density: it is not the original probability density of the input distributions. The importance density should be centered near the failure region of interest. For black-box simulations such as those commonly interfaced with Dakota, it is difficult to specify the importance density a priori: the user often does not know where the failure region lies, especially in a high-dimensional space.[78]. We have developed two importance sampling approaches which do not rely on the user explicitly specifying an importance density.

**See Also**

These keywords may also be of interest:

- adaptive_sampling
- gpais
- local_reliability
- global_reliability
- sampling
- polynomial_chaos
- stoch_collocation

**samples**

- Keywords Area
- method
- importance_sampling
- samples

Number of samples for sampling-based methods

**Specification**

**Alias:** initial_samples

**Argument(s):** INTEGER

**Default:** 0
CHAPTER 6. KEYWORDS AREA

Description

The samples keyword is used to define the number of samples (i.e., randomly chosen sets of variable values) at which to execute a model.

Default Behavior
By default, Dakota will use the minimum number of samples required by the chosen method.

Usage Tips
To obtain linear sensitivities or to construct a linear response surface, at least \( \text{dim}+1 \) samples should be used, where "\( \text{dim} \)" is the number of variables. For sensitivities to quadratic terms or quadratic response surfaces, at least \( (\text{dim}+1)(\text{dim}+2)/2 \) samples are needed. For uncertainty quantification, we recommend at least \( 10^*\text{dim} \) samples.

For variance-based decomp, we recommend hundreds to thousands of samples. Note that for variance-based decomp, the number of simulations performed will be \( N*(\text{dim}+2) \).

Examples

```
method
  sampling
    sample_type lhs
    samples = 20

seed
  Keywords Area
  method
  importance_sampling
  seed

Seed of the random number generator
```

Specification

Alias: none

Argument(s): INTEGER

Default: system-generated (non-repeatable)

Description

The random seed control provides a mechanism for making a stochastic method repeatable. That is, the use of the same random seed in identical studies will generate identical results.

Default Behavior
If not specified, the seed is randomly generated.

Expected Output
If seed is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

Usage Tips
If a stochastic study was run without seed specified, and the user later wishes to repeat the study using the same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen. That value can then be added to the Dakota input file.
6.2. METHOD

Examples

```plaintext
method
  sampling
    sample_type lhs
    samples = 10
    seed = 15347
```

import

- Keywords Area
- method
- importance_sampling
- import

Sampling option

Specification

Alias: none
  Argument(s): none

Description

import centers a sampling density at one of the initial LHS samples identified in the failure region. It then generates the importance samples, weights them by their probability of occurrence given the original density, and calculates the required probability (CDF or CCDF level).

adapt_import

- Keywords Area
- method
- importance_sampling
- adapt_import

Importance sampling option

Specification

Alias: none
  Argument(s): none

Description

adapt_import centers a sampling density at one of the initial LHS samples identified in the failure region. It then generates the importance samples, weights them by their probability of occurrence given the original density, and calculates the required probability (CDF or CCDF level). This continues iteratively until the failure probability estimate converges.
**mm_adapt_import**

- Keywords Area
- method
- importance_sampling
- mm_adapt_import

Sampling option

**Specification**

**Alias:** none  
**Argument(s):** none

**Description**

*mm_adapt_import* starts with all of the samples located in the failure region to build a multimodal sampling density. First, it uses a small number of samples around each of the initial samples in the failure region. Note that these samples are allocated to the different points based on their relative probabilities of occurrence: more probable points get more samples. This early part of the approach is done to search for "representative" points. Once these are located, the multimodal sampling density is set and then *mm_adapt_import* proceeds similarly to *adapt_import* (sample until convergence).

**refinement_samples**

- Keywords Area
- method
- importance_sampling
- refinement_samples

Number of samples used to refine a probability estimate or sampling design.

**Specification**

**Alias:** none  
**Argument(s):** INTEGERLIST

**Description**

Probability estimate: Specify the (scalar) number of samples used to improve a probability estimate. If using uni-modal sampling all samples are assigned to the sampling center. If using multi-modal sampling the samples are split between multiple samples according to some internally computed weights.

Sampling design: Specify one or a sequence of refinement samples to augment the initial samples in a sampling design.
response_levels

- Keywords Area
- method
- importance_sampling
- response_levels

Values at which to estimate desired statistics for each response

**Specification**

**Alias:** none

**Argument(s):** REALLIST

**Default:** No CDF/CCDF probabilities/reliabilities to compute

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword</th>
</tr>
</thead>
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<td>Group</td>
<td>num_response-</td>
<td>Description</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>levels</td>
<td>Number of values</td>
</tr>
<tr>
<td></td>
<td></td>
<td>compute</td>
<td>at which to</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>estimate desired</td>
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<td></td>
<td></td>
<td></td>
<td>statistics for</td>
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<td>each response</td>
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<td>Selection of</td>
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<td></td>
<td>statistics to</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>compute at each</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>response level</td>
</tr>
</tbody>
</table>

**Description**

The `response_levels` specification provides the target response values for which to compute probabilities, reliabilities, or generalized reliabilities (forward mapping).

**Default Behavior**

If `response_levels` are not specified, no statistics will be computed. If they are, probabilities will be computed by default.

**Expected Outputs**

If `response_levels` are specified, Dakota will create two tables in the standard output: a Probability Density function (PDF) histogram and a Cumulative Distribution Function (CDF) table. The PDF histogram has the lower and upper endpoints of each bin and the corresponding density of that bin. Note that the PDF histogram has bins defined by the `probability_levels` and/or `response_levels` in the Dakota input file. If there are not very many levels, the histogram will be coarse. Dakota does not do anything to optimize the bin size or spacing. The CDF table has the list of response levels and the corresponding probability that the response value is less than or equal to each response level threshold.

**Usage Tips**

The `num_response_levels` is used to specify which arguments of the `response_level` correspond to which response.
Examples

For example, specifying a response level of 52.3 followed with compute probabilities will result in the calculation of the probability that the response value is less than or equal to 52.3, given the uncertain distributions on the inputs.

For an example with multiple responses, the following specification

```plaintext
response_levels = 1. 2. .1 .2 .3 .4 10. 20. 30.
num_response_levels = 2 4 3
```

would assign the first two response levels (1., 2.) to response function 1, the next four response levels (.1, .2, .3, .4) to response function 2, and the final three response levels (10., 20., 30.) to response function 3. If the num_response_levels key were omitted from this example, then the response levels would be evenly distributed among the response functions (three levels each in this case).

The Dakota input file below specifies a sampling method with response levels of interest.

```plaintext
method,
  sampling,
    samples = 100 seed = 1
  complementary distribution
    response_levels = 3.6e+11 4.0e+11 4.4e+11
    response_levels = 6.0e+04 6.5e+04 7.0e+04
    response_levels = 3.5e+05 4.0e+05 4.5e+05
variables,
  normal_uncertain = 2
    means = 248.89, 593.33
    std_deviations = 12.4, 29.7
    descriptors = 'TF1n' 'TF2n'
  uniform_uncertain = 2
    lower_bounds = 199.3, 474.63
    upper_bounds = 298.5, 712.
    descriptors = 'TF1u' 'TF2u'
  weibull_uncertain = 2
    alphas = 12., 30.
    betas = 250., 590.
    descriptors = 'TF1w' 'TF2w'
  histogram_bin_uncertain = 2
    num_pairs = 3 4
    abscissas = 5 8 10 .1 .2 .3 .4
    counts = 17 21 0 12 24 12 0
    descriptors = 'TF1h' 'TF2h'
  histogram_point_uncertain
    real = 1
      num_pairs = 2
      abscissas = 3 4
      counts = 1 1
      descriptors = 'TF3h'
interface,
  system asynch evaluation_concurrency = 5
  analysis_driver = 'text_book'
responses,
  response_functions = 3
    no_gradients
    no_hessians
```

Given the above Dakota input file, the following excerpt from the output shows the PDF and CCDF generated. Note that the bounds on the bins of the PDF are the response values specified in the input file. The probability levels corresponding to those response values are shown in the CCDF.
6.2. METHOD

Probability Density Function (PDF) histograms for each response function:

PDF for \( \text{response}_1 \):

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.7604749078e+11</td>
<td>3.6000000000e+11</td>
<td>5.3601733194e-12</td>
</tr>
<tr>
<td>3.6000000000e+11</td>
<td>4.0000000000e+11</td>
<td>4.2500000000e-12</td>
</tr>
<tr>
<td>4.0000000000e+11</td>
<td>4.4000000000e+11</td>
<td>3.7500000000e-12</td>
</tr>
<tr>
<td>4.4000000000e+11</td>
<td>5.419614379e+11</td>
<td>2.2557612778e-12</td>
</tr>
</tbody>
</table>

PDF for \( \text{response}_2 \):

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.643154744e+04</td>
<td>6.0000000000e+04</td>
<td>2.874231192e-05</td>
</tr>
<tr>
<td>6.0000000000e+04</td>
<td>6.5000000000e+04</td>
<td>6.4000000000e-05</td>
</tr>
<tr>
<td>6.5000000000e+04</td>
<td>7.0000000000e+04</td>
<td>4.0000000000e-05</td>
</tr>
<tr>
<td>7.0000000000e+04</td>
<td>7.870246575e+04</td>
<td>1.0341896485e-05</td>
</tr>
</tbody>
</table>

PDF for \( \text{response}_3 \):

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.379637790e+05</td>
<td>3.5000000000e+05</td>
<td>4.284466868e-06</td>
</tr>
<tr>
<td>3.5000000000e+05</td>
<td>4.0000000000e+05</td>
<td>8.6000000000e-06</td>
</tr>
<tr>
<td>4.0000000000e+05</td>
<td>4.5000000000e+05</td>
<td>1.9000000000e-06</td>
</tr>
</tbody>
</table>

Level mappings for each response function:

Complementary Cumulative Distribution Function (CCDF) for \( \text{response}_1 \):

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.6000000000e+11</td>
<td>5.5000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.0000000000e+11</td>
<td>3.8000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.4000000000e+11</td>
<td>2.3000000000e-01</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Complementary Cumulative Distribution Function (CCDF) for \( \text{response}_2 \):

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.0000000000e+04</td>
<td>6.1000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6.5000000000e+04</td>
<td>2.9000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7.0000000000e+04</td>
<td>9.0000000000e-02</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Complementary Cumulative Distribution Function (CCDF) for \( \text{response}_3 \):

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.5000000000e+05</td>
<td>5.2000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.0000000000e+05</td>
<td>9.0000000000e-02</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.5000000000e+05</td>
<td>0.0000000000e+00</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Theory

Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.

In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

A forward mapping involves computing the belief and plausibility probability level for a specified response level.

num_response_levels

- Keywords Area
- method
- importance_sampling
• response_levels
• num_response_levels

Number of values at which to estimate desired statistics for each response

Specification

Alias: none
Argument(s): INTEGERLIST
Default: response_levels evenly distributed among response functions

Description

The num_response_levels keyword allows the user to specify the number of response values, for each response, at which estimated statistics are of interest. Statistics that can be computed are probabilities and reliabilities, both according to either a cumulative distribution function or a complementary cumulative distribution function.

Default Behavior
If num_response_levels is not specified, the response_levels will be evenly distributed among the responses.

Expected Outputs
The specific output will be determined by the type of statistics that are specified. In a general sense, the output will be a list of response level-statistic pairs that show the estimated value of the desired statistic for each response level specified.

Examples

```
method
  sampling
    samples = 100
    seed = 34785
    num_response_levels = 1 1 1
    response_levels = 0.5 0.5 0.5

compute
```

Selection of statistics to compute at each response level

Specification

Alias: none
Argument(s): none
Default: probabilities
Description

The `compute` keyword is used to select which forward statistical mapping is calculated at each response level.

**Default Behavior**

If `response_levels` is not specified, no statistics are computed. If `response_levels` is specified but `compute` is not, probabilities will be computed by default. If both `response_levels` and `compute` are specified, then one of the following must be specified: `probabilities`, `reliabilities`, or `gen_reliabilities`.

**Expected Output**

The type of statistics specified by `compute` will be reported for each response level.

**Usage Tips**

CDF/CCDF probabilities are calculated for specified response levels using a simple binning approach. CDF/CCDF reliabilities are calculated for specified response levels by computing the number of sample standard deviations separating the sample mean from the response level.

**Examples**

```plaintext
method
  sampling
    sample_type random
    samples = 100 seed = 1
    complementary distribution
    response_levels = 3.6e+11 4.0e+11 4.4e+11
    6.0e+04 6.5e+04 7.0e+04
    3.5e+05 4.0e+05 4.5e+05
    compute reliabilities

probabilities
  
  Keywords Area
  
  method
  
  importance_sampling
```
• response_levels
• compute
• probabilities

Computes probabilities associated with response levels

**Specification**

Alias: none
Argument(s): none

**Description**

The `probabilities` keyword directs Dakota to compute the probability that the model response will be below (cumulative) or above (complementary cumulative) a specified response value. This is done for every response level designated for each response.

**Default Behavior**

If `response_levels` is specified, the probabilities are computed by default. To explicitly specify it in the Dakota input file, though, the `probabilities` keyword should be specified in conjunction with the `compute` keyword.

**Expected Outputs**

The Dakota output is a set of response level-probability pairs that give the probability that the model response will be below or above the corresponding response level, depending on the distribution defined.

**Examples**

```plaintext
method
  sampling
    sample_type random
    samples = 100 seed = 1
  complementary distribution
    response_levels = 3.6e+11 4.0e+11 4.4e+11
                     6.0e+04 6.5e+04 7.0e+04
                     3.5e+05 4.0e+05 4.5e+05
  compute probabilities

gen_reliabilities
```

Computes generalized reliabilities associated with response levels
6.2. METHOD

Specification

Alias: none
Argument(s): none

Description

The gen_reliabilities keyword directs Dakota to compute generalized reliabilities according to the specified distribution for a specified response value. This is done for every response level designated for each response.

Default Behavior

If response_levels is specified, the generalized reliabilities are not computed by default. To change this behavior, the gen_reliabilities keyword should be specified in conjunction with the compute keyword.

Expected Outputs

The Dakota output is a set of response level-generalized reliability pairs according to the distribution defined.

Examples

method
  sampling
    sample_type random
    samples = 100 seed = 1
  complementary_distribution
    response_levels = 3.6e+11 4.0e+11 4.4e+11
    6.0e+04 6.5e+04 7.0e+04
    3.5e+05 4.0e+05 4.5e+05
  compute gen_reliabilities

system

  • Keywords Area
  • method
  • importance_sampling
  • response_levels
  • compute
  • system

Compute system reliability (series or parallel)

Specification

Alias: none
Argument(s): none
<table>
<thead>
<tr>
<th>Required/- Optional Required (Choose One)</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>parallel</td>
<td>Aggregate response statistics assuming a parallel system</td>
</tr>
</tbody>
</table>

**Description**

With the system probability/reliability option, statistics for specified response levels are calculated and reported assuming the response functions combine either in series or parallel to produce a total system response.

For a series system, the system fails when any one component (response) fails. The probability of failure is the complement of the product of the individual response success probabilities.

For a parallel system, the system fails only when all components (responses) fail. The probability of failure is the product of the individual response failure probabilities.

**series**

- Keywords Area
- method
- importance_sampling
- response_levels
- compute
- system
- series

Aggregate response statistics assuming a series system

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

See parent keyword system for description.
6.2. METHOD

parallel

- Keywords Area
- method
- importance_sampling
- response_levels
- compute
- system
- parallel

Aggregate response statistics assuming a parallel system

Specification

Alias: none
Argument(s): none

Description

See parent keyword system for description.

max_iterations

- Keywords Area
- method
- importance_sampling
- max_iterations

Number of iterations allowed for optimizers and adaptive UQ methods

Topics

This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none
Argument(s): INTEGER
Default: 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence} / efficient-global: 25*n)
CHAPTER 6. KEYWORDS AREA

Description

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed \( \max_{-} \) iterations. See also \( \max_{-} \text{function_evaluations} \).

Default Behavior

Default value is 100.

convergence_tolerance

- Keywords Area
- method
- importance_sampling
- convergence_tolerance

Stopping criterion based on convergence of the objective function or statistics

Topics

This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none

Argument(s): REAL

Default: 1.e-4

Description

The \texttt{convergence_tolerance} specification provides a real value for controlling the termination of iteration. For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by convergence_tolerance, then this convergence criterion is satisfied on the current iteration.

Therefore, permissible values are between 0 and 1, non-inclusive.

Behavior Varies by Package/Library

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- DOT: must be satisfied for two consecutive iterations
• NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of convergence_tolerance approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., convergence_tolerance = 1.e-6 will result in approximately six digits of accuracy in the final objective function).

• NL2SOL: See nl2sol

distribution

• Keywords Area
• method
• importance_sampling
• distribution

Selection of cumulative or complementary cumulative functions

Specification

Alias: none
Argument(s): none
Default: cumulative (CDF)

<table>
<thead>
<tr>
<th>Required/Optional Required (Choose One)</th>
<th>Description of Group Group 1</th>
<th>Dakota Keyword cumulative</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>complementary</td>
<td>Computes statistics according to complementary cumulative functions</td>
</tr>
</tbody>
</table>

Description

The distribution keyword allows the user to select between a cumulative distribution/belief/plausibility function and a complementary cumulative distribution/belief/plausibility function. This choice affects how probabilities and reliability indices are reported.

Default Behavior

If the distribution keyword is present, it must be accompanied by either cumulative or complementary. Otherwise, a cumulative distribution will be used by default.

Expected Outputs

Output will be a set of model response-probability pairs determined according to the choice of distribution. The choice of distribution also defines the sign of the reliability or generalized reliability indices.
CHAPTER 6. KEYWORDS AREA

Examples
method
  sampling
    sample_type lhs
    samples = 10
    distribution cumulative

cumulative
  • Keywords Area
  • method
  • importance_sampling
  • distribution
  • cumulative

Computes statistics according to cumulative functions

Specification
Alias: none
  Argument(s): none

Description
Statistics on model responses will be computed according to a cumulative distribution/belief/plausibility function.

Default Behavior
By default, a cumulative distribution/belief/plausibility function will be used. To explicitly specify it in the Dakota input file, however, the cumulative keyword must be appear in conjunction with the distribution keyword.

Expected Outputs
Output will be a set of model response-probability pairs determined according to a cumulative distribution/belief/plausibility function. The probabilities reported are the probabilities that the model response falls below given response thresholds.

Examples
method
  sampling
    sample_type lhs
    samples = 10
    distribution cumulative

complementary
  • Keywords Area
  • method
  • importance_sampling
  • distribution
6.2. METHOD

- complementary

Computes statistics according to complementary cumulative functions

Specification

Alias: none
Argument(s): none

Description

Statistics on model responses will be computed according to a complementary cumulative distribution/belief/plausibility function.

Default Behavior
By default, a complementary cumulative distribution/belief/plausibility function will not be used. To change that behavior, the complementary keyword must appear in conjunction with the distribution keyword.

Expected Outputs
Output will be a set of model response-probability pairs determined according to a complementary cumulative distribution/belief/plausibility function. The probabilities reported are the probabilities that the model response falls above given response thresholds.

Examples

```dakota
method sampling
    sample_type lhs
    samples = 10
    distribution complementary
```

probability_levels

- Keywords Area
- method
- importance_sampling
- probability_levels

Specify probability levels at which to estimate the corresponding response value

Specification

Alias: none
Argument(s): REALLIST
Default: No CDF/CCDF response levels to compute
CHAPTER 6. KEYWORDS AREA

<table>
<thead>
<tr>
<th>Optional</th>
<th>num_probability_levels</th>
<th>Specify which probability_levels correspond to which response</th>
</tr>
</thead>
</table>

### Description

Response levels are calculated for specified CDF/CCDF probabilities by indexing into a sorted samples array (the response levels computed are not interpolated and will correspond to one of the sampled values).

### Expected Output

If `probability_levels` are specified, Dakota will create two tables in the standard output: a Probability Density function (PDF) histogram and a Cumulative Distribution Function (CDF) table. The PDF histogram has the lower and upper endpoints of each bin and the corresponding density of that bin. Note that the PDF histogram has bins defined by the `probability_levels` and/or `response_levels` in the Dakota input file. If there are not very many levels, the histogram will be coarse. Dakota does not do anything to optimize the bin size or spacing. The CDF table has the list of response levels and the corresponding probability that the response value is less than or equal to each response level threshold.

### Examples

The Dakota input file below specifies a sampling method with probability levels of interest.

```dakota
method, sampling,
samples = 100 seed = 1
complementary distribution
probability_levels = 1. .66 .33 0.
  .8 .5 0.
  .3 .2 0.
variables, normal_uncertain = 2
  means = 248.89, 593.33
  std_deviations = 12.4, 29.7
  descriptors = 'TF1n' 'TF2n'
uniform_uncertain = 2
  lower_bounds = 199.3, 474.63
  upper_bounds = 298.5, 712.
  descriptors = 'TF1u' 'TF2u'
weibull_uncertain = 2
  alphas = 12., 30.
  betas = 250., 590.
  descriptors = 'TF1w' 'TF2w'
histogram_bin_uncertain = 2
  num_pairs = 3 4
  abscissas = 5 8 10 .1 .2 .3 .4
  counts = 17 21 0 12 24 12 0
  descriptors = 'TF1h' 'TF2h'
histogram_point_uncertain
  real = 1
  num_pairs = 2
  abscissas = 3 4
  counts = 1 1
  descriptors = 'TF3h'
interface,
```
**6.2. METHOD**

```plaintext
system asynch evaluation_concurrency = 5
analysis_driver = 'text_book'

responses,
  response_functions = 3
  no_gradients
  no_hessians
```

Given the above Dakota input file, the following excerpt from the output shows the PDF and CCDF generated. Note that the bounds on the bins of the PDF are the response values that correspond to the probability levels specified in the input file. These response values are also shown in the CCDF.

**Probability Density Function (PDF) histograms for each response function:**

**PDF for response_fn_1:**

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Lower</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.7604749078e+11</td>
<td>3.4221499996e+11</td>
<td>5.1384774972e-12</td>
</tr>
<tr>
<td>3.4221499996e+11</td>
<td>4.0634975300e+11</td>
<td>5.145122311e-12</td>
</tr>
<tr>
<td>4.0634975300e+11</td>
<td>5.4196114379e+11</td>
<td>2.4334239039e-12</td>
</tr>
</tbody>
</table>

**PDF for response_fn_2:**

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Lower</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.6431154744e+04</td>
<td>5.6511827775e+04</td>
<td>1.9839945149e-05</td>
</tr>
<tr>
<td>5.6511827775e+04</td>
<td>6.1603813790e+04</td>
<td>5.8916108390e-05</td>
</tr>
<tr>
<td>6.1603813790e+04</td>
<td>7.8702465755e+04</td>
<td>2.9242071306e-05</td>
</tr>
</tbody>
</table>

**PDF for response_fn_3:**

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Lower</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.3796737090e+05</td>
<td>3.6997214153e+05</td>
<td>5.3028386523e-06</td>
</tr>
<tr>
<td>3.6997214153e+05</td>
<td>3.8100966235e+05</td>
<td>9.060055634e-06</td>
</tr>
<tr>
<td>3.8100966235e+05</td>
<td>4.4111498127e+05</td>
<td>3.3274925348e-06</td>
</tr>
</tbody>
</table>

**Level mappings for each response function:**

**Complementary Cumulative Distribution Function (CCDF) for response_fn_1:**

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.7604749078e+11</td>
<td>1.0000000000e+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.4221499996e+11</td>
<td>1.0000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.0634975300e+11</td>
<td>1.0000000000e-01</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Complementary Cumulative Distribution Function (CCDF) for response_fn_2:**

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.6431154744e+04</td>
<td>1.0000000000e+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5.6511827775e+04</td>
<td>1.0000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6.1603813790e+04</td>
<td>1.0000000000e-01</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Complementary Cumulative Distribution Function (CCDF) for response_fn_3:**

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.3796737090e+05</td>
<td>1.0000000000e+00</td>
<td></td>
<td></td>
</tr>
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<td>1.0000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.8100966235e+05</td>
<td>1.0000000000e-01</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Theory**

Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.
In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

An inverse mapping involves computing the belief and plausibility response level for either a specified probability level or a specified generalized reliability level (two results for each level mapping in the evidence-based epistemic case, instead of the one result for each level mapping in the aleatory case).

**num_probability_levels**

- **Keywords Area**
- **method**
- **importance_sampling**
- **probability_levels**
- **num_probability_levels**

Specify which `probability_levels` correspond to which response

**Specification**

**Alias:** none

**Argument(s):** INTEGERLIST

**Default:** probability_levels evenly distributed among response functions

**Description**

See parent page

**gen_reliability_levels**

- **Keywords Area**
- **method**
- **importance_sampling**
- **gen_reliability_levels**

Specify generalized reliability levels at which to estimate the corresponding response value

**Specification**

**Alias:** none

**Argument(s):** REALLIST

**Default:** No CDF/CCDF response levels to compute
Optional | num_gen_reliability_levels | Specify which gen_reliability_levels correspond to which response

**Description**

Response levels are calculated for specified generalized reliabilities by indexing into a sorted samples array (the response levels computed are not interpolated and will correspond to one of the sampled values).

**Theory**

Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.

In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

An inverse mapping involves computing the belief and plausibility response level for either a specified probability level or a specified generalized reliability level (two results for each level mapping in the evidence-based epistemic case, instead of the one result for each level mapping in the aleatory case).

**num_gen_reliability_levels**

- **Keywords Area**
- **method**
- **importance_sampling**
- **gen_reliability_levels**
- **num_gen_reliability_levels**

Specify which gen_reliability_levels correspond to which response

**Specification**

Alias: none

Argument(s): INTEGERLIST

Default: gen_reliability_levels evenly distributed among response functions

**Description**

See parent page
CHAPTER 6. KEYWORDS AREA

rng

- Keywords Area
- method
- importance_sampling
- rng

Selection of a random number generator

Specification

Alias: none
Argument(s): none
Default: Mersenne twister (mt19937)

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required/ - Optional Required(Choose One)</td>
<td></td>
<td>mt19937</td>
<td>Generates random numbers using the Mersenne twister</td>
</tr>
<tr>
<td></td>
<td></td>
<td>rnum2</td>
<td>Generates pseudo-random numbers using the Pecos package</td>
</tr>
</tbody>
</table>

Description

The `rng` keyword is used to indicate a choice of random number generator.

Default Behavior

If specified, the `rng` keyword must be accompanied by either `rnum2` (pseudo-random numbers) or `mt19937` (random numbers generated by the Mersenne twister). Otherwise, `mt19937`, the Mersenne twister is used by default.

Usage Tips

The default is recommended, as the Mersenne twister is a higher quality random number generator.

Examples

```plaintext
method
  sampling
    sample_type lhs
    samples = 10
    seed = 98765
    rng rnum2
```

mt19937

- Keywords Area
- method
6.2. METHOD

- importance_sampling
- rng
- mt19937

Generates random numbers using the Mersenne twister

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

The mt19937 keyword directs Dakota to use the Mersenne twister to generate random numbers. Additional information can be found on wikipedia: [http://en.wikipedia.org/wiki/Mersenne_twister](http://en.wikipedia.org/wiki/Mersenne_twister).

**Default Behavior**

mt19937 is the default random number generator. To specify it explicitly in the Dakota input file, however, it must be specified in conjunction with the rng keyword.

**Usage Tips**

Use of the Mersenne twister random number generator (mt19937) is recommended.

**Examples**

```plaintext
method sampling
    sample_type lhs
    samples = 10
    seed = 98765
    rng mt19937
```

rnum2

- Keywords Area
- method
- importance_sampling
- rng
- rnum2

Generates pseudo-random numbers using the Pecos package

**Specification**

**Alias:** none

**Argument(s):** none
CHAPTER 6. KEYWORDS AREA

Description

The `rnum2` keyword directs Dakota to use pseudo-random numbers generated by the Pecos package.

Default Behavior

`rnum2` is not used by default. To change this behavior, it must be specified in conjunction with the `rng` keyword.

Usage Tips

Use of the Mersenne twister random number generator (`mt19937`) is recommended over `rnum2`.

Examples

```
method
  sampling
    sample_type lhs
    samples = 10
    seed = 98765
    rng rnum2
```

`model_pointer`

- Keywords Area
- method
- importance_sampling
- model_pointer

Identifier for model block to be used by a method

Topics

This keyword is related to the topics:

- `block_pointer`

Specification

Alias: none

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)

Description

The `model_pointer` is used to specify which `model` block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a `model` block in the Dakota input file that has a corresponding `id_model` with the same name.

Usage Tips

When doing advanced analyses that involve using multiple methods and multiple models, defining a `model-pointer` for each method is imperative.

See `block_pointer` for details about pointers.
6.2. METHOD

**Examples**

```plaintext
environment
tabular_graphics_data
method_pointer = 'UQ'

method
id_method = 'UQ'
model_pointer = 'SURR'
sampling,
samples = 10
seed = 98765 rng rnum2
response_levels = 0.1 0.2 0.6
0.1 0.2 0.6
0.1 0.2 0.6
sample_type lhs
distribution cumulative

model
id_model = 'SURR'
surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
id_method = 'DACE'
model_pointer = 'DACE_M'
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = 'DACE_M'
single
interface_pointer = 'I1'

variables
uniform_uncertain = 2
lower_bound = 0. 0.
upper_bound = 1. 1.
descriptors = 'x1' 'x2'

interface
id_interface = 'I1'
system asynch evaluation_concurrency = 5
analysis_driver = 'text_book'

responses
response_functions = 3
no_gradients
no_hessians
```

6.2.53 gpais

- Keywords Area
- method
- gpais

Gaussian Process Adaptive Importance Sampling
**Topics**

This keyword is related to the topics:

- uncertainty quantification

**Specification**

**Alias:** gaussian_process_adaptive_importance_sampling  
**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>build_samples</td>
<td>Number of initial model evaluations used in build phase</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>seed</td>
<td>Seed of the random number generator</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>samples_on_emulator</td>
<td>Number of samples at which to evaluate an emulator (surrogate)</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>import_build_points_file</td>
<td>File containing points you wish to use to build a surrogate</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>export_approx_points_file</td>
<td>Output file for evaluations of a surrogate model</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>response_levels</td>
<td>Values at which to estimate desired statistics for each response</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>max_iterations</td>
<td>Number of iterations allowed for optimizers and adaptive UQ methods</td>
</tr>
</tbody>
</table>
6.2. METHOD

Description

gpais is recommended for problems that have a relatively small number of input variables (e.g. less than 10-20). This method, Gaussian Process Adaptive Importance Sampling, is outlined in the paper[?].

This method starts with an initial set of LHS samples and adds samples one at a time, with the goal of adaptively improving the estimate of the ideal importance density during the process. The approach uses a mixture of component densities. An iterative process is used to construct the sequence of improving component densities. At each iteration, a Gaussian process (GP) surrogate is used to help identify areas in the space where failure is likely to occur. The GPs are not used to directly calculate the failure probability; they are only used to approximate the importance density. Thus, the Gaussian process adaptive importance sampling algorithm overcomes limitations involving using a potentially inaccurate surrogate model directly in importance sampling calculations.

See Also

These keywords may also be of interest:

- adaptive_sampling
- local_reliability
- global_reliability
- sampling
- importance_sampling
• polynomial_chaos
• stoch_collocation

**build_samples**

- Keywords Area
- method
- gpais
- build_samples

Number of initial model evaluations used in build phase

**Specification**

**Alias:** samples

**Argument(s):** INTEGER

**Description**

The number of build points or training points used in the initial phase of an algorithm or model construction. Typically these are the initial set of data points used to construct (train) a surrogate model (emulator). If the number of **build_samples** is less than the minimum number of points required to build the surrogate, Dakota will augment the samples to obtain the minimum required.

**Examples**

Perform GP-based adaptive importance sampling, building the GP with 100 points and then performing 100 approximate evaluations to evaluate the probability.

```plaintext
method
gpais
    build_samples = 100
    samples_on_emulator = 100
    max_iterations = 5
    response_levels = -1.065
```

**seed**

- Keywords Area
- method
- gpais
- seed

Seed of the random number generator
6.2. METHOD

Specification

Alias: none

- **Argument(s):** INTEGER
- **Default:** system-generated (non-repeatable)

Description

The random seed control provides a mechanism for making a stochastic method repeatable. That is, the use of the same random seed in identical studies will generate identical results.

- **Default Behavior**
  - If not specified, the seed is randomly generated.

- **Expected Output**
  - If `seed` is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

- **Usage Tips**
  - If a stochastic study was run without `seed` specified, and the user later wishes to repeat the study using the same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen. That value can then be added to the Dakota input file.

Examples

```
method sampling
  sample_type lhs
  samples = 10
  seed = 15347
```

```
samples_on_emulator
  - Keywords Area
  - method
  - gpais
  - samples_on_emulator

  Number of samples at which to evaluate an emulator (surrogate)
```

Specification

Alias: none

- **Argument(s):** INTEGER
- **Default:** 10000

Description

How many approximate function evaluations to perform on the emulator model, e.g., to compute statistics

- **Default Behavior**
  - The default number of samples is method-dependent.
Examples
Perform 10000 samples on the PCE approximation of the true model:

```plaintext
method
  polynomial_chaos
    quadrature_order = 2
    samples_on_emulator = 10000
```

**import_build_points_file**
- **Keywords Area**
- **method**
- **gpais**
- **import_build_points_file**

File containing points you wish to use to build a surrogate

**Specification**

**Alias:** `import_points_file`

**Argument(s):** STRING

**Default:** no point import from a file

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group Tabular Format (Group 1)</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional (Choose One)</td>
<td>annotated</td>
<td>custom_annotated</td>
<td>Selects custom-annotated tabular file format</td>
</tr>
<tr>
<td>Optional</td>
<td>freeform</td>
<td>Selects freeform file format</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>active_only</td>
<td>Import only active variables from tabular data file</td>
<td></td>
</tr>
</tbody>
</table>

**Description**

The `import_build_points_file` allows the user to specify a file that contains a list of points and truth model responses used to construct a surrogate model. These can be used by all methods that (explicitly, e.g. surrogate-based optimization, or implicitly, e.g. efficient global optimization) operate on a surrogate. In particular, these points and responses are used in place of truth model evaluations to construct the initial surrogate. When used to construct surrogate models or emulators these are often called build points or training data.

**Default Behavior**

By default, methods do not import points from a file.

**Usage Tips**
Dakota parses input files without regard to whitespace, but the `import_build_points_file` must be in one of three formats:

- annotated (default)
- custom_annotated
- freeform

**Examples**

```plaintext
method
  polynomial_chaos
  expansion_order = 4
  import_build_points_file = 'dakota_uq_rosenbrock_pce_import.annot.pts.dat'
```

annotated

- **Keywords Area**
- **method**
- **gpais**
- **import_build_points_file**
- **annotated**

Selects annotated tabular file format

**Topics**

This keyword is related to the topics:

- **file_formats**

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** annotated format

**Description**

An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

**Default Behavior**

By default, Dakota imports and exports tabular files in annotated format. The `annotated` keyword can be used to explicitly specify this.

**Usage Tips**

- To specify pre-Dakota 6.1 tabular format, which did not include `interface_id`, specify **custom_annotated header eval_id**
Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples
Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
annotated
```

Resulting tabular file:

```
%eval_id interface   x1   x2   obj_fn nln_ineq_con_1 nln_ineq_con_2
1    NO_ID          0.9   1.1   0.0002 0.26       0.76
2    NO_ID          0.90009 1.1 0.0001996404857 0.2601620081 0.759955
3    NO_ID          0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...
```

custom_annotated

- Keywords Area
- method
- gpais
- import_build_points_file
- custom_annotated

Selects custom-annotated tabular file format

Topics
This keyword is related to the topics:

- file_formats

Specification
Alias: none
Argument(s): none
Default: annotated format

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
6.2. METHOD

<table>
<thead>
<tr>
<th>Optional</th>
<th>header</th>
<th>Enable header row in custom-annotated tabular file</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>eval_id</td>
<td>Enable evaluation ID column in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td>interface_id</td>
<td>Enable interface ID column in custom-annotated tabular file</td>
</tr>
</tbody>
</table>

### Description

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

#### Default Behavior

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

#### Usage Tips

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

#### Examples

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
custom_annotated header eval_id
```

Resulting tabular file:

```plaintext
%eval_id    x1    x2    obj_fn  nln_ineq_con_1  nln_ineq_con_2
1           0.9    1.1    0.0002  0.26    0.76
2           0.90009 1.1 0.0001996404857 0.2601620081 0.759955
3           0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...```
**header**

- Keywords Area
- method
- gpais
- import_build_points_file
- custom_annotated
- header

Enable header row in custom-annotated tabular file

**Specification**

**Alias**: none

**Argument(s)**: none

**Default**: no header

**Description**

See description of parent custom_annotated

**eval_id**

- Keywords Area
- method
- gpais
- import_build_points_file
- custom_annotated
- eval_id

Enable evaluation ID column in custom-annotated tabular file

**Specification**

**Alias**: none

**Argument(s)**: none

**Default**: no eval_id column

**Description**

See description of parent custom_annotated
6.2. METHOD

interface_id

- Keywords Area
- method
- gpais
- import_build_points_file
- custom_annotated
- interface_id

Enable interface ID column in custom-annotated tabular file

**Specification**

**Alias:** none

- **Argument(s):** none
- **Default:** no interface_id column

**Description**

See description of parent `custom_annotated`

**freeform**

- Keywords Area
- method
- gpais
- import_build_points_file
- freeform

Selects freeform file format

**Topics**

This keyword is related to the topics:

- file_formats

**Specification**

**Alias:** none

- **Argument(s):** none
- **Default:** annotated format
**Description**

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

**Default Behavior**

The *annotated* format is the default for tabular export/import. To change this behavior, specify *freeform* in the relevant export/import context.

**Usage Tips**

- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to *annotated format*, though *freeform* remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- In *freeform*, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the *freeform* option.

**Examples**

Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
freeform
```

Resulting tabular file:

```
0.9 1.1 0.0002 0.26 0.76
0.90009 1.1 0.0001996404857 0.2601620081 0.759955
0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...
```

**active_only**

- Keywords Area
- method
- gpais
- import_build_points_file
- active_only

Import only active variables from tabular data file

**Topics**

This keyword is related to the topics:

- file_formats
6.2. METHOD

Specification

Alias: none
Argument(s): none

Description

By default, files for tabular data imports are expected to contain columns for all variables, active and inactive. The keyword active_only indicates that the file to import contains only the active variables.

This option should only be used in contexts where the inactive variables have no influence, for example, building a surrogate over active variables, with the state variables held at nominal. It should not be used in more complex nested contexts, where the values of inactive variables are relevant to the function evaluations used to build the surrogate.

eexport_approx_points_file

- Keywords Area
- method
- gpais
- export_approx_points_file

Output file for evaluations of a surrogate model

Specification

Alias: export_points_file
Argument(s): STRING
Default: no point export to a file

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Optional/Choose One</th>
<th>Description of Group</th>
<th>Tabular Format (Group 1)</th>
<th>Dakota Keyword annotated</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
</table>

- custom_annotated
  Selects custom-annotated tabular file format

- freeform
  Selects freeform file format

Description

The export_approx_points_file keyword allows the user to specify a file in which the points (input variable values) at which the surrogate model is evaluated and corresponding response values computed by the surrogate model will be written. The response values are the surrogate’s predicted approximation to the truth model responses at those points.

Usage Tips

Dakota exports tabular data in one of three formats:
• annotated (default)
• custom.annotated
• freeform

**annotated**

• Keywords Area
• method
• gpais
• export.approx_points_file
• annotated

Selects annotated tabular file format

**Topics**

This keyword is related to the topics:

• file.formats

**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** annotated format

**Description**

An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

**Default Behavior**

By default, Dakota imports and exports tabular files in annotated format. The `annotated` keyword can be used to explicitly specify this.

**Usage Tips**

• To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify `custom.annotated header eval_id`

• Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

• When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

• Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the `freeform` option.
6.2. METHOD

Examples

Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```python
environment
tabular_data
    tabular_data_file = 'dakota_summary.dat'
annotated

Resulting tabular file:

%eval_id interface  x1  x2  obj_fn  nln_ineq_con_1  nln_ineq_con_2
1 NO_ID  0.9  1.1  0.0002  0.26  0.76
2 NO_ID  0.90009  1.1  0.0001996404857  0.2601620081  0.759955
3 NO_ID  0.89991  1.1  0.0002003604863  0.2598380081  0.760045
...
```

custom_annotated

- Keywords Area
- method
- gpais
- export_approx_points_file
- custom_annotated

Selects custom-annotated tabular file format

Topics

This keyword is related to the topics:

- fileFormats

Specification

Alias: none

Argument(s): none

Default: annotated format

<p>| Required/- | Description of | Dakota Keyword | Dakota Keyword |</p>
<table>
<thead>
<tr>
<th>Optional</th>
<th>Group</th>
<th>header</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td></td>
<td>Enable header row in custom-annotated tabular file</td>
</tr>
</tbody>
</table>
### Description

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval id column, and interface id column appear in the tabular file, thus bridging freeform and (fully) annotated.

**Default Behavior**

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

**Usage Tips**

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

**Examples**

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval id (no interface_id), and data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
  tabular_data_file = 'dakota_summary.dat'
custom_annotated header eval_id
```

Resulting tabular file:

```
%eval_id  x1   x2   obj_fn nln_ineq_con_1 nln_ineq_con_2
1   0.9   1.1   0.0002     0.26     0.76
2  0.90009  1.1  0.0001996404857  0.2601620081  0.759955
3  0.89991  1.1  0.0002003604863  0.2598380081  0.760045
...```

- header
  - Keywords Area
  - method
  - gpais
6.2. METHOD

- export_approx_points_file
- custom_annotated
- header

Enable header row in custom-annotated tabular file

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no header

**Description**

See description of parent custom_annotated

- eval_id
  - Keywords Area
  - method
  - gpais
  - export_approx_points_file
  - custom_annotated
  - eval_id

Enable evaluation ID column in custom-annotated tabular file

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no eval_id column

**Description**

See description of parent custom_annotated

- interface_id
  - Keywords Area
  - method
  - gpais
  - export_approx_points_file
  - custom_annotated
  - interface_id

Enable interface ID column in custom-annotated tabular file
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none
Argument(s): none
Default: no interface_id column

Description

See description of parent custom_annotated

freeform

- Keywords Area
- method
- gpais
- export_approx_points_file
- freeform

Selects freeform file format

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none
Argument(s): none
Default: annotated format

Description

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior

The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips

- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
6.2. METHOD

- In **freeform**, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the **freeform** option.

**Examples**

Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
  tabular_data_file = 'dakota_summary.dat'
  freeform
```

Resulting tabular file:

```
0.9  1.1  0.0002  0.26  0.76
0.90009 1.1  0.0001996404857  0.2601620081  0.759955
0.89991 1.1  0.0002003604863  0.2598380081  0.760045
...```

**response_levels**

- **Keywords Area**
- **method**
- **gpais**
- **response_levels**

Values at which to estimate desired statistics for each response

**Specification**

**Alias**: none

**Argument(s)**: REALLIST

**Default**: No CDF/CCDF probabilities/reliabilities to compute

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>Group</td>
<td>num_response_-</td>
<td>Description</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>levels</td>
<td>Number of values at which to estimate desired statistics for each response</td>
</tr>
</tbody>
</table>
CHAPTER 6. KEYWORDS AREA

<table>
<thead>
<tr>
<th>Optional</th>
<th>compute</th>
<th>Selection of statistics to compute at each response level</th>
</tr>
</thead>
</table>

**Description**

The `response_levels` specification provides the target response values for which to compute probabilities, reliabilities, or generalized reliabilities (forward mapping).

**Default Behavior**

If `response_levels` are not specified, no statistics will be computed. If they are, probabilities will be computed by default.

**Expected Outputs**

If `response_levels` are specified, Dakota will create two tables in the standard output: a Probability Density function (PDF) histogram and a Cumulative Distribution Function (CDF) table. The PDF histogram has the lower and upper endpoints of each bin and the corresponding density of that bin. Note that the PDF histogram has bins defined by the `probability_levels` and/or `response_levels` in the Dakota input file. If there are not very many levels, the histogram will be coarse. Dakota does not do anything to optimize the bin size or spacing. The CDF table has the list of response levels and the corresponding probability that the response value is less than or equal to each response level threshold.

**Usage Tips**

The `num_response_levels` is used to specify which arguments of the `response_level` correspond to which response.

**Examples**

For example, specifying a `response_level` of 52.3 followed with `compute probabilities` will result in the calculation of the probability that the response value is less than or equal to 52.3, given the uncertain distributions on the inputs.

For an example with multiple responses, the following specification

```
response_levels = 1. 2. .1 .2 .3 .4 10. 20. 30.
num_response_levels = 2 4 3
```

would assign the first two response levels (1., 2.) to response function 1, the next four response levels (.1, .2, .3, .4) to response function 2, and the final three response levels (10., 20., 30.) to response function 3. If the `num_response_levels` key were omitted from this example, then the response levels would be evenly distributed among the response functions (three levels each in this case).

The Dakota input file below specifies a sampling method with response levels of interest.

```
method,
sampling,
samples = 100 seed = 1
complementary distribution
response_levels = 3.6e+11 4.0e+11 4.4e+11
6.0e+04 6.5e+04 7.0e+04
3.5e+05 4.0e+05 4.5e+05

variables,
    normal_uncertain = 2
    means = 248.89, 593.33
    std_deviations = 12.4, 29.7
    descriptors = 'TF1n' 'TF2n'
```
6.2. METHOD

uniform_uncertain = 2
lower_bounds = 199.3, 474.63
upper_bounds = 298.5, 712.

weibull_uncertain = 2
alphas = 12., 30.
betas = 250., 590.

descriptors = 'TF1u' 'TF2u'

histogram_bin_uncertain = 2
num_pairs = 3 4
abscissas = 5 8 10 .1 .2 .3 .4
counts = 17 21 0 12 24 12 0
descriptors = 'TF1h' 'TF2h'

histogram_point_uncertain
real = 1
num_pairs = 2
abscissas = 3 4
counts = 1 1
descriptors = 'TF3h'

interface,
system asynch evaluation_concurrency = 5
analysis_driver = 'text_book'

responses,
response_functions = 3
no_gradients
no_hessians

Given the above Dakota input file, the following excerpt from the output shows the PDF and CCDF generated. Note that the bounds on the bins of the PDF are the response values specified in the input file. The probability levels corresponding to those response values are shown in the CCDF.

Probability Density Function (PDF) histograms for each response function:

PDF for response_fn_1:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.7604749078e+11</td>
<td>3.6000000000e+11</td>
<td>5.3601733194e-12</td>
</tr>
<tr>
<td>3.6000000000e+11</td>
<td>4.0000000000e+11</td>
<td>4.2500000000e-12</td>
</tr>
<tr>
<td>4.0000000000e+11</td>
<td>4.4000000000e+11</td>
<td>3.7500000000e-12</td>
</tr>
<tr>
<td>4.4000000000e+11</td>
<td>5.4196114379e+11</td>
<td>2.2557612778e-12</td>
</tr>
</tbody>
</table>

PDF for response_fn_2:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.6431154744e+04</td>
<td>6.0000000000e+04</td>
<td>2.8742313192e-05</td>
</tr>
<tr>
<td>6.0000000000e+04</td>
<td>6.5000000000e+04</td>
<td>6.4000000000e-05</td>
</tr>
<tr>
<td>6.5000000000e+04</td>
<td>7.0000000000e+04</td>
<td>4.0000000000e-05</td>
</tr>
<tr>
<td>7.0000000000e+04</td>
<td>7.8702465755e+04</td>
<td>1.0341896485e-05</td>
</tr>
</tbody>
</table>

PDF for response_fn_3:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.3796737090e+05</td>
<td>3.5000000000e+05</td>
<td>4.2844660868e-06</td>
</tr>
<tr>
<td>3.5000000000e+05</td>
<td>4.0000000000e+05</td>
<td>8.6000000000e-06</td>
</tr>
<tr>
<td>4.0000000000e+05</td>
<td>4.5000000000e+05</td>
<td>1.8000000000e-06</td>
</tr>
</tbody>
</table>

Level mappings for each response function:

Complementary Cumulative Distribution Function (CCDF) for response_fn_1:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.6000000000e+11</td>
<td>5.5000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.0000000000e+11</td>
<td>3.8000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.4000000000e+11</td>
<td>2.3000000000e-01</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### Chapter 6. Keywords Area

Complementary Cumulative Distribution Function (CCDF) for response_fn_2:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.0000000000e+04</td>
<td>6.1000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6.5000000000e+04</td>
<td>2.9000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7.0000000000e+04</td>
<td>9.0000000000e-02</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Complementary Cumulative Distribution Function (CCDF) for response_fn_3:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.5000000000e+05</td>
<td>5.2000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.0000000000e+05</td>
<td>9.0000000000e-02</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.5000000000e+05</td>
<td>0.0000000000e+00</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Theory**

Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.

In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

A forward mapping involves computing the belief and plausibility probability level for a specified response level.

**num_response_levels**

- Keywords Area
- method
- gpais
- response_levels
- num_response_levels

Number of values at which to estimate desired statistics for each response

**Specification**

**Alias:** none

**Argument(s):** INTEGERLIST

**Default:** response_levels evenly distributed among response functions

**Description**

The `num_response_levels` keyword allows the user to specify the number of response values, for each response, at which estimated statistics are of interest. Statistics that can be computed are probabilities and reliabilities, both according to either a cumulative distribution function or a complementary cumulative distribution function.

**Default Behavior**

If `num_response_levels` is not specified, the response_levels will be evenly distributed among the responses.

**Expected Outputs**
6.2. METHOD

The specific output will be determined by the type of statistics that are specified. In a general sense, the output will be a list of response level-statistic pairs that show the estimated value of the desired statistic for each response level specified.

Examples

```
method
  sampling
    samples = 100
    seed = 34785
    num_response_levels = 1 1 1
    response_levels = 0.5 0.5 0.5

compute
  • Keywords Area
  • method
  • gpa
  • response_levels
  • compute

Selection of statistics to compute at each response level

Specification

Alias: none
Argument(s): none
Default: probabilities

<table>
<thead>
<tr>
<th>Required/-Optional Required</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>probabilities</td>
<td>Computes probabilities associated with response levels</td>
</tr>
<tr>
<td>gen_reliabilities</td>
<td></td>
<td>gen_reliabilities</td>
<td>Computes generalized reliabilities associated with response levels</td>
</tr>
</tbody>
</table>

```
CHAPTER 6. KEYWORDS AREA

<table>
<thead>
<tr>
<th>Optional</th>
<th>system</th>
<th>Compute system reliability (series or parallel)</th>
</tr>
</thead>
</table>

Description

The `compute` keyword is used to select which forward statistical mapping is calculated at each response level.

**Default Behavior**

If `response_levels` is not specified, no statistics are computed. If `response_levels` is specified but `compute` is not, probabilities will be computed by default. If both `response_levels` and `compute` are specified, then one of the following must be specified: `probabilities`, `reliabilities`, or `gen-reliabilities`.

**Expected Output**

The type of statistics specified by `compute` will be reported for each response level.

**Usage Tips**

CDF/CCDF probabilities are calculated for specified response levels using a simple binning approach. CDF/CCDF reliabilities are calculated for specified response levels by computing the number of sample standard deviations separating the sample mean from the response level.

**Examples**

```plaintext
method sampling
  sample_type random
  samples = 100 seed = 1
  complementary distribution
  response_levels = 3.6e+11 4.0e+11 4.4e+11
                 6.0e+04 6.5e+04 7.0e+04
                 3.5e+05 4.0e+05 4.5e+05
  compute reliabilities
```

**probabilities**

- Keywords Area
- method
- gpa
- response_levels
- compute
- probabilities

Computes probabilities associated with response levels

**Specification**

**Alias:** none

**Argument(s):** none
Description

The `probabilities` keyword directs Dakota to compute the probability that the model response will be below (cumulative) or above (complementary cumulative) a specified response value. This is done for every response level designated for each response.

**Default Behavior**

If `response_levels` is specified, the probabilities are computed by default. To explicitly specify it in the Dakota input file, though, the `probabilities` keyword should be specified in conjunction with the `compute` keyword.

**Expected Outputs**

The Dakota output is a set of response level-probability pairs that give the probability that the model response will be below or above the corresponding response level, depending on the distribution defined.

Examples

```
method
sampling
  sample_type random
  samples = 100 seed = 1
complementary distribution
  response_levels = 3.6e+11 4.0e+11 4.4e+11
    6.0e+04 6.5e+04 7.0e+04
    3.5e+05 4.0e+05 4.5e+05
compute probabilities
```

**gen.reliabilities**

- **Keywords Area**
- **method**
- **gpais**
- **response_levels**
- **compute**
- **gen.reliabilities**

Computes generalized reliabilities associated with response levels

**Specification**

**Alias:** none

**Argument(s):** none

Description

The `gen.reliabilities` keyword directs Dakota to compute generalized reliabilities according to the specified distribution for a specified response value. This is done for every response level designated for each response.

**Default Behavior**

If `response_levels` is specified, the generalized reliabilities are not computed by default. To change this behavior, the `gen.reliabilities` keyword should be specified in conjunction with the `compute` keyword.

**Expected Outputs**

The Dakota output is a set of response level-generalized reliability pairs according to the distribution defined.
Examples

```
method
  sampling
    sample_type random
    samples = 100 seed = 1
    complementary distribution
    response_levels = 3.6e+11 4.0e+11 4.4e+11
                     6.0e+04 6.5e+04 7.0e+04
                     3.5e+05 4.0e+05 4.5e+05
    compute gen_reliabilities
```

```
system
```

- **Keywords Area**
- **method**
- **gpais**
- **response_levels**
- **compute**
- **system**

Compute system reliability (series or parallel)

Specification

**Alias:** none

**Argument(s):** none

| Required/- | Description of | Dakota Keyword |
| Optional/ | Group | |
| Required | Group 1 | Description |
| Choose One | | |
| series | Aggregate response statistics assuming a series system |
| parallel | Aggregate response statistics assuming a parallel system |

Description

With the system probability/reliability option, statistics for specified `response_levels` are calculated and reported assuming the response functions combine either in series or parallel to produce a total system response.

For a series system, the system fails when any one component (response) fails. The probability of failure is the complement of the product of the individual response success probabilities.

For a parallel system, the system fails only when all components (responses) fail. The probability of failure is the product of the individual response failure probabilities.
6.2. METHOD

series

- Keywords Area
- method
- gpais
- response_levels
- compute
- system
- series

Aggregate response statistics assuming a series system

Specification

Alias: none

Argument(s): none

Description

See parent keyword system for description.

parallel

- Keywords Area
- method
- gpais
- response_levels
- compute
- system
- parallel

Aggregate response statistics assuming a parallel system

Specification

Alias: none

Argument(s): none

Description

See parent keyword system for description.
max_iterations

- Keywords Area
- method
- gpais
- max_iterations

Number of iterations allowed for optimizers and adaptive UQ methods

Topics

This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none

Argument(s): INTEGER

Default: 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence} / efficient_global: 25*n)

Description

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed max_iterations iterations. See also max_function_evaluations.

Default Behavior

Default value is 100.

distribution

- Keywords Area
- method
- gpais
- distribution

Selection of cumulative or complementary cumulative functions

Specification

Alias: none

Argument(s): none

Default: cumulative (CDF)
6.2. METHOD

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Group 1</td>
<td></td>
<td>cumulative</td>
<td>Computes statistics according to cumulative functions</td>
</tr>
<tr>
<td></td>
<td></td>
<td>complementary</td>
<td>Computes statistics according to complementary cumulative functions</td>
</tr>
</tbody>
</table>

Description

The `distribution` keyword allows the user to select between a cumulative distribution/belief/plausibility function and a complementary cumulative distribution/belief/plausibility function. This choice affects how probabilities and reliability indices are reported.

**Default Behavior**

If the `distribution` keyword is present, it must be accompanied by either `cumulative` or `complementary`. Otherwise, a cumulative distribution will be used by default.

**Expected Outputs**

Output will be a set of model response-probability pairs determined according to the choice of distribution. The choice of distribution also defines the sign of the reliability or generalized reliability indices.

**Examples**

```
method
  sampling
    sample_type lhs
    samples = 10
    distribution cumulative
```

cumulative

- Keywords Area
- method
- gpais
- distribution
- cumulative

Computes statistics according to cumulative functions

**Specification**

**Alias:** none

**Argument(s):** none
**Description**

Statistics on model responses will be computed according to a cumulative distribution/belief/plausibility function.

**Default Behavior**

By default, a cumulative distribution/belief/plausibility function will be used. To explicitly specify it in the Dakota input file, however, the `cumulative` keyword must be appear in conjunction with the `distribution` keyword.

**Expected Outputs**

Output will be a set of model response probability pairs determined according to a cumulative distribution/belief/plausibility function. The probabilities reported are the probabilities that the model response falls below given response thresholds.

**Examples**

```plaintext
method
  sampling
    sample_type lhs
    samples = 10
    distribution cumulative
```

**complementary**

- **Keywords Area**
- **method**
- **gpais**
- **distribution**
- **complementary**

Computes statistics according to complementary cumulative functions.

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

Statistics on model responses will be computed according to a complementary cumulative distribution/belief/plausibility function.

**Default Behavior**

By default, a complementary cumulative distribution/belief/plausibility function will not be used. To change that behavior, the `complementary` keyword must be appear in conjunction with the `distribution` keyword.

**Expected Outputs**

Output will be a set of model response-probability pairs determined according to a complementary cumulative distribution/belief/plausibility function. The probabilities reported are the probabilities that the model response falls above given response thresholds.
6.2. METHOD

Examples

```plaintext
method
  sampling
    sample_type lhs
    samples = 10
    distribution complementary
```

probability_levels

- **Keywords Area**
- **method**
- **gpais**
- **probability_levels**

Specify probability levels at which to estimate the corresponding response value

**Specification**

**Alias:** none

**Argument(s):** REALLIST

**Default:** No CDF/CCDF response levels to compute

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>num_probability_levels</td>
<td></td>
<td></td>
<td>Specify which probability_levels correspond to which response</td>
</tr>
</tbody>
</table>

**Description**

Response levels are calculated for specified CDF/CCDF probabilities by indexing into a sorted samples array (the response levels computed are not interpolated and will correspond to one of the sampled values).

**Expected Output**

If `probability_levels` are specified, Dakota will create two tables in the standard output: a Probability Density function (PDF) histogram and a Cumulative Distribution Function (CDF) table. The PDF histogram has the lower and upper endpoints of each bin and the corresponding density of that bin. Note that the PDF histogram has bins defined by the `probability_levels` and/or `response_levels` in the Dakota input file. If there are not very many levels, the histogram will be coarse. Dakota does not do anything to optimize the bin size or spacing. The CDF table has the list of response levels and the corresponding probability that the response value is less than or equal to each response level threshold.

**Examples**

The Dakota input file below specifies a sampling method with probability levels of interest.

```plaintext
method,
  sampling,
   samples = 100 seed = 1
   complementary distribution
```
CHAPTER 6. KEYWORDS AREA

probability_levels = 1. .66 .33 0.
1. .8 .5 0.
1. .3 .2 0.

variables,

normal_uncertain = 2
means = 248.89, 593.33
std_deviations = 12.4, 29.7
descriptors = 'TF1n' 'TF2n'
uniform_uncertain = 2
lower_bounds = 199.3, 474.63
upper_bounds = 298.5, 712.
descriptors = 'TF1u' 'TF2u'
weibull_uncertain = 2
alphas = 12., 30.
betas = 250., 590.
descriptors = 'TF1w' 'TF2w'
histogram_bin_uncertain = 2
num_pairs = 3 4
abscissas = 5 8 10 .1 .2 .3 .4
counts = 17 21 0 12 24 12 0
descriptors = 'TF1h' 'TF2h'
histogram_point_uncertain
real = 1
num_pairs = 2
abscissas = 3 4
counts = 1 1
descriptors = 'TF3h'

interface,

system asynch evaluation_concurrency = 5
analysis_driver = 'text_book'

responses,
response_functions = 3
no_gradients
no_hessians

Given the above Dakota input file, the following excerpt from the output shows the PDF and CCDF generated. Note that the bounds on the bins of the PDF are the response values that correspond the probability levels specified in the input file. Those response values are also shown in the CCDF.

Probability Density Function (PDF) histograms for each response function:
PDF for response_fn_1:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.7604749078e+11</td>
<td>3.4221494996e+11</td>
<td>5.1384774972e-12</td>
</tr>
<tr>
<td>3.4221494996e+11</td>
<td>4.0634975300e+11</td>
<td>5.1454122311e-12</td>
</tr>
<tr>
<td>4.0634975300e+11</td>
<td>5.4196114379e+11</td>
<td>2.4334239039e-12</td>
</tr>
</tbody>
</table>

PDF for response_fn_2:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.6431154744e+04</td>
<td>5.6511827775e+04</td>
<td>1.9839945149e-05</td>
</tr>
<tr>
<td>5.6511827775e+04</td>
<td>6.1603813790e+04</td>
<td>5.8916108390e-05</td>
</tr>
<tr>
<td>6.1603813790e+04</td>
<td>7.8702465755e+04</td>
<td>2.9242071306e-05</td>
</tr>
</tbody>
</table>

PDF for response_fn_3:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.3796737090e+05</td>
<td>3.6997214153e+05</td>
<td>5.3028386523e-06</td>
</tr>
<tr>
<td>3.6997214153e+05</td>
<td>3.8100966235e+05</td>
<td>9.0600055634e-06</td>
</tr>
<tr>
<td>3.8100966235e+05</td>
<td>4.4111498127e+05</td>
<td>3.3274925348e-06</td>
</tr>
</tbody>
</table>
6.2. METHOD

Level mappings for each response function:

Complementary Cumulative Distribution Function (CCDF) for response_fn_1:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.7604749078e+11</td>
<td>1.0000000000e+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.4221494996e+11</td>
<td>6.6000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.0634975300e+11</td>
<td>3.3000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5.4196114379e+11</td>
<td>0.0000000000e+00</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Complementary Cumulative Distribution Function (CCDF) for response_fn_2:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.643154744e+04</td>
<td>1.0000000000e+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5.6511827775e+04</td>
<td>8.0000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6.1603813790e+04</td>
<td>5.0000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7.8702645755e+04</td>
<td>0.0000000000e+00</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Complementary Cumulative Distribution Function (CCDF) for response_fn_3:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.3796737090e+11</td>
<td>1.0000000000e+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.699724153e+05</td>
<td>3.0000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.8100966235e+05</td>
<td>2.0000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.4111498127e+05</td>
<td>0.0000000000e+00</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Theory

Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.

In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

An inverse mapping involves computing the belief and plausibility response level for either a specified probability level or a specified generalized reliability level (two results for each level mapping in the evidence-based epistemic case, instead of the one result for each level mapping in the aleatory case).

define num_probability_levels

- Keywords Area
- method
- gpais
- probability_levels
- num_probability_levels

Specify which probability_levels correspond to which response

Specification

Alias: none

Argument(s): INTEGERLIST

Default: probability_levels evenly distributed among response functions

Description

See parent page
**gen_reliability_levels**
- **Keywords Area**
- **method**
- **gpais**
- **gen_reliability_levels**

Specify generalized reliability levels at which to estimate the corresponding response value

**Specification**

**Alias:** none

**Argument(s):** REALLIST

**Default:** No CDF/CCDF response levels to compute

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>num_gen_reliability_levels</td>
<td></td>
<td>Specify which gen_reliability_levels correspond to which response</td>
</tr>
</tbody>
</table>

**Description**

Response levels are calculated for specified generalized reliabilities by indexing into a sorted samples array (the response levels computed are not interpolated and will correspond to one of the sampled values).

**Theory**

Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.

In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

An inverse mapping involves computing the belief and plausibility response level for either a specified probability level or a specified generalized reliability level (two results for each level mapping in the evidence-based epistemic case, instead of the one result for each level mapping in the aleatory case).

**num_gen_reliability_levels**
- **Keywords Area**
- **method**
- **gpais**
- **gen_reliability_levels**
- **num_gen_reliability_levels**

Specify which gen_reliability_levels correspond to which response
6.2. **METHOD**

### Specification

**Alias:** none  
**Argument(s):** INTEGERLIST  
**Default:** gen_reliability_levels evenly distributed among response functions

### Description

See parent page

**rng**

- Keywords Area
- method
- gpais
- rng

Selection of a random number generator

### Specification

**Alias:** none  
**Argument(s):** none  
**Default:** Mersenne twister ( mt19937 )

<table>
<thead>
<tr>
<th>Required/-Optional Required (Choose One)</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>mt19937</td>
<td>Generates random numbers using the Mersenne twister</td>
</tr>
<tr>
<td>rnum2</td>
<td></td>
<td></td>
<td>Generates pseudo-random numbers using the Pecos package</td>
</tr>
</tbody>
</table>

### Description

The **rng** keyword is used to indicate a choice of random number generator.

**Default Behavior**

If specified, the **rng** keyword must be accompanied by either **rnum2** (pseudo-random numbers) or **mt19937** (random numbers generated by the Mersenne twister). Otherwise, **mt19937**, the Mersenne twister is used by default.

**Usage Tips**

The default is recommended, as the Mersenne twister is a higher quality random number generator.
Examples

method
sampling
  sample_type lhs
  samples = 10
  seed = 98765
  rng rnum2

mt19937
  • Keywords Area
  • method
  • gpais
  • rng
  • mt19937

Generates random numbers using the Mersenne twister

Specification

Alias: none
  Argument(s): none

Description

The mt19937 keyword directs Dakota to use the Mersenne twister to generate random numbers. Additional information can be found on wikipedia: http://en.wikipedia.org/wiki/Mersenne_twister.

Default Behavior

mt19937 is the default random number generator. To specify it explicitly in the Dakota input file, however, it must be specified in conjunction with the rng keyword.

Usage Tips

Use of the Mersenne twister random number generator (mt19937) is recommended.

Examples

method
sampling
  sample_type lhs
  samples = 10
  seed = 98765
  rng mt19937

rnum2
  • Keywords Area
  • method
  • gpais
  • rng
Generates pseudo-random numbers using the Pecos package

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

The `rnum2` keyword directs Dakota to use pseudo-random numbers generated by the Pecos package.

**Default Behavior**

`rnum2` is not used by default. To change this behavior, it must be specified in conjunction with the `rng` keyword.

**Usage Tips**

Use of the Mersenne twister random number generator (`mt19937`) is recommended over `rnum2`.

**Examples**

```
method
  sampling
    sample_type lhs
    samples = 10
    seed = 98765
    rng rnum2

model_pointer

  Keywords Area
  method
  gpais
  model_pointer

Identifier for model block to be used by a method
```

**Topics**

This keyword is related to the topics:

- `block_pointer`

**Specification**

**Alias:** none

**Argument(s):** STRING

**Default:** method use of last model parsed (or use of default model if none parsed)
Description

The `model_pointer` is used to specify which `model` block will be used to perform the function evaluations needed by the Dakota method.

**Default Behavior**

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a `model` block in the Dakota input file that has a corresponding `id_model` with the same name.

**Usage Tips**

When doing advanced analyses that involve using multiple methods and multiple models, defining a `model-pointer` for each method is imperative.

See `block_pointer` for details about pointers.

**Examples**

```plaintext
environment
  tabular_graphics_data
  method_pointer = 'UQ'

method
  id_method = 'UQ'
  model_pointer = 'SURR'
  sampling,
    samples = 10
    seed = 98765 rng rnum2
    response_levels = 0.1 0.2 0.6
    0.1 0.2 0.6
    0.1 0.2 0.6
  sample_type lhs
  distribution cumulative

model
  id_model = 'SURR'
  surrogate global,
  dace_method_pointer = 'DACE'
  polynomial quadratic

method
  id_method = 'DACE'
  model_pointer = 'DACE_M'
  sampling sample_type lhs
    samples = 121 seed = 5034 rng rnum2

model
  id_model = 'DACE_M'
  single
  interface_pointer = 'I1'

variables
  uniform_uncertain = 2
    lower_bounds = 0. 0.
    upper_bounds = 1. 1.
  descriptors = 'x1' 'x2'

interface
  id_interface = 'I1'
  system asynch evaluation_concurrency = 5
    analysis_driver = 'text_book'

responses
```
response_functions = 3
no_gradients
no_hessians

6.2.54 adaptive_sampling

- Keywords Area
- method
- adaptive_sampling

(Experimental) Adaptively refine a Gaussian process surrogate

Topics

This keyword is related to the topics:

- uncertainty_quantification

Specification

Alias: nond_adaptive_sampling

Argument(s): none

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>initial_samples</td>
<td></td>
<td>Initial number of samples for sampling-based methods</td>
</tr>
<tr>
<td></td>
<td>seed</td>
<td></td>
<td>Seed of the random number generator</td>
</tr>
<tr>
<td></td>
<td>samples_on_emulator</td>
<td></td>
<td>Number of samples at which to evaluate an emulator (surrogate)</td>
</tr>
<tr>
<td></td>
<td>fitness_metric</td>
<td></td>
<td>(Experimental) Specify the fitness_metric used to select the next point</td>
</tr>
<tr>
<td>Optional</td>
<td>batch_selection</td>
<td>(Experimental) How to select new points</td>
<td></td>
</tr>
<tr>
<td>----------</td>
<td>------------------------------</td>
<td>----------------------------------------</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>refinement_-</td>
<td>Number of samples used to refine a probability estimate or sampling design.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>samples</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>import_build_-</td>
<td>File containing points you wish to use to build a surrogate</td>
<td></td>
</tr>
<tr>
<td></td>
<td>points_file</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>export_approx_-</td>
<td>Output file for evaluations of a surrogate model</td>
<td></td>
</tr>
<tr>
<td></td>
<td>points_file</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>response_levels</td>
<td>Values at which to estimate desired statistics for each response</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>misc_options</td>
<td>(Experimental) Hook for algorithm-specific adaptive sampling options</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>max_iterations</td>
<td>Number of iterations allowed for optimizers and adaptive UQ methods</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>distribution</td>
<td>Selection of cumulative or complementary cumulative functions</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
6.2. METHOD

### Description

This is an experimental capability that is not ready for production use at this point. It was part of an investigation into computational topology-based approaches to feature identification and surrogate refinement.

The goal in performing adaptive sampling is to construct a surrogate model that can be used as an accurate predictor to some expensive simulation, thus it is to one’s advantage to build a surrogate that minimizes the error over the entire domain of interest using as little data as possible from the expensive simulation. The adaptive part alludes to the fact that the surrogate will be refined by focusing samples of the expensive simulation on particular areas of interest rather than rely on random selection or standard space-filling techniques.

At a high-level, the adaptive sampling pipeline is a four-step process:

- Evaluate the expensive simulation (referred to as the true model) at initial sample point
  1. Fit a surrogate model
  2. Create a candidate set and score based on information from surrogate
  3. Select a candidate point to evaluate the true model
  4. Loop until done

In terms of the Dakota implementation, the adaptive sampling method currently uses Latin Hypercube sampling (LHS) to generate the initial points in Step 1 above. For Step 2, we use a Gaussian process model.

The default behavior is to add one point at a time. At each iteration (e.g., each loop of Steps 2-4 above), a Latin Hypercube sample is generated (a new one, different from the initial sample) and the surrogate model is evaluated at this points. These are the candidate points that are then evaluated according to the fitness metric. The number of candidates used in practice should be high enough to fill most of the input domain: we recommend at least hundreds of points for a low-dimensional problem. All of the candidates (samples on the emulator) are given a score and then the highest-scoring candidate is selected to be evaluated on the true model.

The adaptive sampling method also can generate batches of points to add at a time using the `batch_selection` and `batch_size` keywords.
See Also
These keywords may also be of interest:

- gpais
- local_reliability
- global_reliability
- sampling
- importance_sampling
- polynomial_chaos
- stoch_collocation

initial_samples

- Keywords Area
- method
- adaptive_sampling
- initial_samples

Initial number of samples for sampling-based methods

Specification
Alias: samples
Argument(s): INTEGER
Default: 0

Description
The initial_samples keyword is used to define the number of initial samples (i.e., randomly chosen sets of variable values) at which to execute a model. The initial samples may later be augmented in an iterative process.

Default Behavior
By default, Dakota will use the minimum number of samples required by the chosen method.

Usage Tips
To obtain linear sensitivities or to construct a linear response surface, at least dim+1 samples should be used, where "dim" is the number of variables. For sensitivities to quadratic terms or quadratic response surfaces, at least (dim+1)(dim+2)/2 samples are needed. For uncertainty quantification, we recommend at least 10*dim samples. For variance_based_decomp, we recommend hundreds to thousands of samples. Note that for variance_based_decomp, the number of simulations performed will be N*(dim+2).

Examples

```
method
  sampling
    sample_type random
    initial_samples = 20
    refinement_samples = 5
```
6.2. METHOD

**seed**

- **Keywords Area**
- **method**
- **adaptive_sampling**
- **seed**

Seed of the random number generator

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** system-generated (non-repeatable)

**Description**

The random seed control provides a mechanism for making a stochastic method repeatable. That is, the use of the same random seed in identical studies will generate identical results.

**Default Behavior**

If not specified, the seed is randomly generated.

**Expected Output**

If seed is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

**Usage Tips**

If a stochastic study was run without seed specified, and the user later wishes to repeat the study using the same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen. That value can then be added to the Dakota input file.

**Examples**

```plaintext
method
  sampling
    sample_type lhs
    samples = 10
    seed = 15347
```

**samples_on_emulator**

- **Keywords Area**
- **method**
- **adaptive_sampling**
- **samples_on_emulator**

Number of samples at which to evaluate an emulator (surrogate)
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none
  Argument(s): INTEGER
  Default: 400

Description

How many approximate function evaluations to perform on the emulator model, e.g., to compute statistics

Default Behavior
The default number of samples is method-dependent.

Examples

Perform 10000 samples on the PCE approximation of the true model:

```
method
  polynomial_chaos
    quadrature_order = 2
    samples_on_emulator = 10000
```

fitness_metric

- Keywords Area
- method
- adaptive_sampling
- fitness_metric

(Experimental) Specify the fitness_metric used to select the next point

Specification

Alias: none
  Argument(s): none
  Default: predicted_variance

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>predicted_variance</td>
<td>Pick points with highest variance</td>
</tr>
<tr>
<td>Required(Choose One)</td>
<td></td>
<td>distance</td>
<td>Space filling metric</td>
</tr>
<tr>
<td></td>
<td></td>
<td>gradient</td>
<td>Fill the range space of the surrogate</td>
</tr>
</tbody>
</table>

Description

adaptive sampling is an experimental capability that is not ready for production use at this time.

The user can specify the fitness_metric used to select the next point (or points) to evaluate and add to the set. The fitness metrics used for scoring candidate points include:

- predicted_variance
6.2. METHOD

- distance
- gradient

predicted_variance

- Keywords Area
- method
- adaptive_sampling
- fitness_metric
- predicted_variance

Pick points with highest variance

Specification

Alias: none
Argument(s): none

Description

The predicted variance metric uses the predicted variance of the Gaussian process surrogate as the score of a candidate point. Thus, the adaptively chosen points will be in areas of highest uncertainty according to the Gaussian process model.

distance

- Keywords Area
- method
- adaptive_sampling
- fitness_metric
- distance

Space filling metric

Specification

Alias: none
Argument(s): none

Description

The distance metric calculates the Euclidean distance in domain space between the candidate and its nearest neighbor in the set of points already evaluated on the true model. Therefore, the most undersampled area of the domain will always be selected. Note that this is a space-filling metric.
gradient

- Keywords Area
- method
- adaptive_sampling
- fitness_metric
- gradient

Fill the range space of the surrogate

Specification

Alias: none
 Argument(s): none

Description

The gradient metric calculates the score as the absolute value of the difference in range space (the outputs) of the two points. The output values used are predicted from the surrogate model. This method attempts to evenly fill the range space of the surrogate.

batch_selection

- Keywords Area
- method
- adaptive_sampling
- batch_selection

(Experimental) How to select new points

Specification

Alias: none
 Argument(s): none
 Default: naive

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required (Choose One)</td>
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<td>naive</td>
</tr>
<tr>
<td></td>
<td></td>
<td>distance_penalty</td>
</tr>
</tbody>
</table>

Add a penalty to spread out the points in the batch
6.2. METHOD

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>topology</td>
<td>In this selection strategy, we use information about the topology of the space from the Morse-Smale complex to identify next points to select.</td>
</tr>
<tr>
<td>constant liar</td>
<td>Use information from the existing surrogate model to predict what the surrogate upgrade will be with new points.</td>
</tr>
</tbody>
</table>

**Description**

*adaptive_sampling* is an experimental capability that is not ready for production use at this time.

With batch or multi-point selection, the true model can be evaluated in parallel and thus increase throughput before refitting our surrogate model. This proposes a new challenge as the problem of choosing a single point and choosing multiple points off a surrogate are fundamentally different. Selecting the \( n \) best scoring candidates is more than likely to generate a set of points clustered in one area which will not be conducive to adapting the surrogate.

We have implemented several strategies for batch selection of points. These are described in the User’s manual and are the subject of active research.

The **batch_selection** strategies include:

1. **naive**:
2. **distance_penalty**
3. **constant liar**
4. **topology**

**naive**

- **Keywords Area**
- **method**
- **adaptive_sampling**
- **batch_selection**
- **naive**

Take the highest scoring candidates

**Specification**

**Alias**: none

**Argument(s)**: none
Description
This strategy will select the \( n \) highest scoring candidates regardless of their position. This tends to group an entire round of points in the same area.

distance\_penalty

- Keywords Area
- method
- adaptive\_sampling
- batch\_selection
- distance\_penalty

Add a penalty to spread out the points in the batch

Specification
Alias: none
Argument(s): none

Description
In this strategy, the highest scoring candidate is selected and then all remaining candidates are re-scored with a distance penalization factor added in to the score.

topology

- Keywords Area
- method
- adaptive\_sampling
- batch\_selection
- topology

In this selection strategy, we use information about the topology of the space from the Morse-Smale complex to identify next points to select.

Specification
Alias: none
Argument(s): none

Description
In this strategy we look at the topology of the scoring function and select the \( n \) highest maxima in the topology. To determine local maxima, we construct the approximate Morse-Smale complex. This strategy does require the user to have the Morse-Smale package.
constant_liar

- Keywords Area
- method
- adaptive_sampling
- batch_selection
- constant_liar

Use information from the existing surrogate model to predict what the surrogate upgrade will be with new points.

**Specification**

**Alias:** none
**Argument(s):** none

**Description**

The strategy first selects the highest scoring candidate, and then refits the surrogate using a "lie" value at the point selected. The 'lie' value is based on the surrogate predictions and not the simulation. This process repeats until \( n \) points have been selected whereupon the lie values are removed from the surrogate and the selected points are evaluated on the true model and the surrogate is refit with these values.

refinement_samples

- Keywords Area
- method
- adaptive_sampling
- refinement_samples

Number of samples used to refine a probability estimate or sampling design.

**Specification**

**Alias:** none
**Argument(s):** INTEGERLIST

**Description**

Probability estimate: Specify the (scalar) number of samples used to improve a probability estimate. If using uni-modal sampling all samples are assigned to the sampling center. If using multi-modal sampling the samples are split between multiple samples according to some internally computed weights.

Sampling design: Specify one or a sequence of refinement samples to augment the initial samples in a sampling design.
import_build_points_file

- Keywords Area
- method
- adaptive_sampling
- import_build_points_file

File containing points you wish to use to build a surrogate

**Specification**

**Alias:** import_points_file  
**Argument(s):** STRING  
**Default:** no point import from a file

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group Tabular Format (Group 1)</th>
<th>Dakota Keyword annotated</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional (Choose One)</td>
<td></td>
<td>custom_annotated</td>
<td>Selects custom-annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>freeform</td>
<td>Selects freeform file format</td>
</tr>
</tbody>
</table>

| Optional | active_only | Import only active variables from tabular data file |

**Description**

The `import_build_points_file` allows the user to specify a file that contains a list of points and truth model responses used to construct a surrogate model. These can be used by all methods that (explicitly, e.g. surrogate-based optimization, or implicitly, e.g. efficient global optimization) operate on a surrogate. In particular, these points and responses are used in place of truth model evaluations to construct the initial surrogate. When used to construct surrogate models or emulators these are often called build points or training data.

**Default Behavior**

By default, methods do not import points from a file.

**Usage Tips**

Dakota parses input files without regard to whitespace, but the `import_build_points_file` must be in one of three formats:

- annotated (default)
- custom_annotated
- freeform
6.2. METHOD

Examples

```python
method
    polynomial_chaos
    expansion_order = 4
    import_build_points_file = 'dakota_uq_rosenbrock_pce_import.annot.pts.dat'
```

annotated

- Keywords Area
- method
- adaptive_sampling
- import_build_points_file
- annotated

Selects annotated tabular file format

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none

Argument(s): none

Default: annotated format

Description

An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior

By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips

- To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify custom_annotated_header(eval_id)

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.
CHAPTER 6. KEYWORDS AREA

Examples
Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
  tabular_data_file = 'dakota_summary.dat'
annotated

Resulting tabular file:
%eval_id interface  x1  x2  obj_fn  nln_ineq_con_1  nln_ineq_con_2
1 NO_ID 0.9 1.1 0.0002 0.26 0.76
2 NO_ID 0.90009 1.1 0.0001996404857 0.2601620081 0.759955
3 NO_ID 0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...

custom_annotated
  • Keywords Area
  • method
  • adaptive_sampling
  • import_build_points_file
  • custom_annotated

Selects custom-annotated tabular file format

Topics
This keyword is related to the topics:
  • file_formats

Specification
Alias: none
Argument(s): none
Default: annotated format

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>header</td>
<td>Enable header row in custom-annotated tabular file</td>
</tr>
</tbody>
</table>
6.2. METHOD

<table>
<thead>
<tr>
<th>Optional</th>
<th>eval_id</th>
<th>Enable evaluation ID column in custom-annotated tabular file</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>interface_id</td>
<td>Enable interface ID column in custom-annotated tabular file</td>
</tr>
</tbody>
</table>

**Description**

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

**Default Behavior**

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

**Usage Tips**

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

**Examples**

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:

```plaintext
environment
  tabular_data
    tabular_data_file = 'dakota_summary.dat'
    custom_annotated header eval_id
```

Resulting tabular file:

```
%eval_id    x1    x2    obj_fn nln_ineq_con_1 nln_ineq_con_2
1    0.9    1.1    0.0002    0.26    0.76
2    0.90009    1.1    0.0001996404857    0.2601620081    0.759955
3    0.89991    1.1    0.0002003604863    0.2598380081    0.760045
...```

**header**

- Keywords Area
- method
- adaptive_sampling
• import_build_points_file
• custom_annotated
• header

Enable header row in custom-annotated tabular file

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no header

**Description**

See description of parent *custom_annotated*

**eval_id**

• Keywords Area
• method
• adaptive_sampling
• import_build_points_file
• custom_annotated
• eval_id

Enable evaluation ID column in custom-annotated tabular file

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no eval_id column

**Description**

See description of parent *custom_annotated*

**interface_id**

• Keywords Area
• method
• adaptive_sampling
• import_build_points_file
• custom_annotated
• interface_id

Enable interface ID column in custom-annotated tabular file
6.2. **METHOD**

**Specification**

Alias: none

Argument(s): none

Default: no interface_id column

**Description**

See description of parent `custom.annotated`

**freeform**

- Keywords Area
- method
- adaptive_sampling
- import_build_points_file
- freeform

Selects freeform file format

**Topics**

This keyword is related to the topics:

- fileFormats

**Specification**

Alias: none

Argument(s): none

Default: annotated format

**Description**

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior

The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips

- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
• In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).

• Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples
Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```python
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
freeform
```

Resulting tabular file:

```
0.9 1.1 0.0002 0.26 0.76
0.90009 1.1 0.0001996404857 0.2601620081 0.759955
0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...
```

active_only

• Keywords Area
• method
• adaptive_sampling
• import_build_points_file
• active_only

Import only active variables from tabular data file

Topics
This keyword is related to the topics:

• file_formats

Specification
Alias: none

Argument(s): none

Description
By default, files for tabular data imports are expected to contain columns for all variables, active and inactive. The keyword active_only indicates that the file to import contains only the active variables.

This option should only be used in contexts where the inactive variables have no influence, for example, building a surrogate over active variables, with the state variables held at nominal. It should not be used in more complex nested contexts, where the values of inactive variables are relevant to the function evaluations used to build the surrogate.
6.2. METHOD

export_approx_points_file

- Keywords Area
- method
- adaptive_sampling
- export_approx_points_file

Output file for evaluations of a surrogate model

Specification

Alias: export_points_file

Argument(s): STRING

Default: no point export to a file

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group (Choose One)</th>
<th>Dakota Keyword annotated</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>Tabular Format (Group 1)</td>
<td>custom_annotated</td>
<td>Selects custom-annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>freeform</td>
<td>Selects freeform file format</td>
</tr>
</tbody>
</table>

Description

The export_approx_points_file keyword allows the user to specify a file in which the points (input variable values) at which the surrogate model is evaluated and corresponding response values computed by the surrogate model will be written. The response values are the surrogate’s predicted approximation to the truth model responses at those points.

Usage Tips

Dakota exports tabular data in one of three formats:

- annotated (default)
- custom_annotated
- freeform

annotated

- Keywords Area
- method
- adaptive_sampling
- export_approx_points_file
• annotated

Selects annotated tabular file format

Topics
This keyword is related to the topics:

• file_formats

Specification
Alias: none
Argument(s): none
Default: annotated format

Description
An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior
By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips

• To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify custom_annotated header eval_id

• Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

• When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

• Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples
Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
annotated
```

Resulting tabular file:

```%eval_id interface x1 x2 obj_fn nln_ineq_con_1 nln_ineq_con_2
1 NO_ID 0.9 1.1 0.0002 0.26 0.76
2 NO_ID 0.90009 1.1 0.0001996404857 0.2601620081 0.759955
3 NO_ID 0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...
```
custom.annotated

- Keywords Area
- method
- adaptive.sampling
- export.approx.points.file
- custom.annotated

Selects custom-annotated tabular file format

Topics

This keyword is related to the topics:

- file.formats

Specification

Alias: none
Argument(s): none
Default: annotated format

<p>| Required/- | Description of | Dakota Keyword | Dakota Keyword |</p>
<table>
<thead>
<tr>
<th>Optional</th>
<th>Optional Group</th>
<th>Description</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>header</td>
<td></td>
<td>Enable header row in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td>eval_id</td>
<td></td>
<td>Enable evaluation ID column in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td>interface_id</td>
<td></td>
<td>Enable interface ID column in custom-annotated tabular file</td>
</tr>
</tbody>
</table>

Description

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom.annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

Default Behavior

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom.annotated, followed by options, in the relevant export/import context.

Usage Tips
• Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to 
annotated format, though freeform remains an option.

• When importing tabular data, a warning will be generated if a specific number of data are expected, but 
extra is found and an error generated when there is insufficient data.

• Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface-
id), and data for variables and responses. Input file fragment:

```
environment
  tabular_data
    tabular_data_file = 'dakota_summary.dat'
    custom_annotated header eval_id

Resulting tabular file:

%eval_id   x1    x2    obj_fn  nln_ineq_con_1  nln_ineq_con_2
1    0.9    1.1  0.0002   0.26   0.76
2    0.90009  1.1  0.0001996404857  0.2601620081  0.759955
3    0.89991  1.1  0.0002003604863  0.2598380081  0.760045
...
```

header

• Keywords Area

• method

• adaptive_sampling

• export_approx_points_file

• custom_annotated

• header

Enable header row in custom-annotated tabular file

Specification

Alias: none
Argument(s): none
Default: no header

Description

See description of parent custom_annotated
6.2. **METHOD**

**eval_id**

- Keywords Area
- method
- adaptive_sampling
- export_approx_points_file
- custom_annotated
- eval_id

Enable evaluation ID column in custom-annotated tabular file

**Specification**

Alias: none

- **Argument(s):** none
- **Default:** no eval_id column

**Description**

See description of parent custom_annotated

**interface_id**

- Keywords Area
- method
- adaptive_sampling
- export_approx_points_file
- custom_annotated
- interface_id

Enable interface ID column in custom-annotated tabular file

**Specification**

Alias: none

- **Argument(s):** none
- **Default:** no interface_id column

**Description**

See description of parent custom_annotated
freeform

- Keywords Area
- method
- adaptive_sampling
- export_approx_points_file
- freeform

Selects freeform file format

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none
Argument(s): none
Default: annotated format

Description

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior

The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips

- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.
6.2. METHOD

Examples

Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```plaintext
environment
  tabular_data
    tabular_data_file = 'dakota_summary.dat'
  freeform
```

Resulting tabular file:

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>0.9</td>
<td>1.1</td>
<td>0.0002</td>
<td>0.26</td>
<td>0.76</td>
</tr>
<tr>
<td>0.90009</td>
<td>1.1</td>
<td>0.0001996404857</td>
<td>0.2601620081</td>
<td>0.759955</td>
</tr>
<tr>
<td>0.89991</td>
<td>1.1</td>
<td>0.0002003604863</td>
<td>0.2598380081</td>
<td>0.760045</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

response_levels

- Keywords Area
- method
- adaptive_sampling
- response_levels

Values at which to estimate desired statistics for each response

Specification

Alias: none

Argument(s): REALLIST

Default: No CDF/CCDF probabilities/reliabilities to compute

<p>| Required/- | Description of | Dakota Keyword | Dakota Keyword |</p>
<table>
<thead>
<tr>
<th>Optional</th>
<th>Optional Group</th>
<th>num_response_levels</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td></td>
<td>Number of values at which to estimate desired statistics for each response</td>
</tr>
<tr>
<td></td>
<td></td>
<td>num_response_levels</td>
<td>Selection of statistics to compute at each response level</td>
</tr>
</tbody>
</table>

Description

The response_levels specification provides the target response values for which to compute probabilities, reliabilities, or generalized reliabilities (forward mapping).

Default Behavior

If response_levels are not specified, no statistics will be computed. If they are, probabilities will be computed by default.

Expected Outputs
If `response_levels` are specified, Dakota will create two tables in the standard output: a Probability Density function (PDF) histogram and a Cumulative Distribution Function (CDF) table. The PDF histogram has the lower and upper endpoints of each bin and the corresponding density of that bin. Note that the PDF histogram has bins defined by the `probability_levels` and/or `response_levels` in the Dakota input file. If there are not very many levels, the histogram will be coarse. Dakota does not do anything to optimize the bin size or spacing. The CDF table has the list of response levels and the corresponding probability that the response value is less than or equal to each response level threshold.

**Usage Tips**

The `num_response_levels` is used to specify which arguments of the `response_level` correspond to which response.

**Examples**

For example, specifying a `response_level` of 52.3 followed with `compute probabilities` will result in the calculation of the probability that the response value is less than or equal to 52.3, given the uncertain distributions on the inputs.

For an example with multiple responses, the following specification

```plaintext
response_levels = 1. 2. .1 .2 .3 .4 10. 20. 30.
num_response_levels = 2 4 3
```

would assign the first two response levels (1., 2.) to response function 1, the next four response levels (.1, .2, .3, .4) to response function 2, and the final three response levels (10., 20., 30.) to response function 3. If the `num_response_levels` key were omitted from this example, then the response levels would be evenly distributed among the response functions (three levels each in this case).

The Dakota input file below specifies a sampling method with response levels of interest.

```plaintext
method,
  sampling,
    samples = 100 seed = 1
  complementary distribution
    response_levels = 3.6e+11 4.0e+11 4.4e+11
    6.0e+04 6.5e+04 7.0e+04
    3.5e+05 4.0e+05 4.5e+05
variables,
  normal_uncertain = 2
    means = 248.89, 593.33
    std_deviations = 12.4, 29.7
    descriptors = 'TF1n' 'TF2n'
  uniform_uncertain = 2
    lower_bounds = 199.3, 474.63
    upper_bounds = 298.5, 712.
    descriptors = 'TF1u' 'TF2u'
  weibull_uncertain = 2
    alphas = 12., 30.
    betas = 250., 590.
    descriptors = 'TF1w' 'TF2w'
  histogram_bin_uncertain = 2
    num_pairs = 3 4
    abscissas = 5 8 10 .1 .2 .3 .4
    counts = 17 21 0 12 24 12 0
    descriptors = 'TF1h' 'TF2h'
  histogram_point_uncertain
    real = 1
    num_pairs = 2
    abscissas = 3 4
    counts = 1 1
```
6.2. METHOD

\[ \text{descriptors} = \text{'TF3h'} \]

interface,
\[ \text{system} \ \text{asynch} \ \text{evaluation_concurrency} = \ 5 \]
\[ \text{analysis_driver} = \text{'text_book'} \]

responses,
\[ \text{response_functions} = \ 3 \]
\[ \text{no_gradients} \]
\[ \text{no_hessians} \]

Given the above Dakota input file, the following excerpt from the output shows the PDF and CCDF generated. Note that the bounds on the bins of the PDF are the response values specified in the input file. The probability levels corresponding to those response values are shown in the CCDF.

Probability Density Function (PDF) histograms for each response function:

**PDF for response_fn_1:**

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.7604749078e+11</td>
<td>3.6000000000e+11</td>
<td>5.3601733194e-12</td>
</tr>
<tr>
<td>3.6000000000e+11</td>
<td>4.0000000000e+11</td>
<td>4.2500000000e-12</td>
</tr>
<tr>
<td>4.0000000000e+11</td>
<td>4.4000000000e+11</td>
<td>3.7500000000e-12</td>
</tr>
<tr>
<td>4.4000000000e+11</td>
<td>5.4196114379e+11</td>
<td>2.2557612778e-12</td>
</tr>
</tbody>
</table>

**PDF for response_fn_2:**

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.6431154744e+04</td>
<td>6.0000000000e+04</td>
<td>2.8742313192e-05</td>
</tr>
<tr>
<td>6.0000000000e+04</td>
<td>6.5000000000e+04</td>
<td>6.4000000000e-05</td>
</tr>
<tr>
<td>6.5000000000e+04</td>
<td>7.0000000000e+04</td>
<td>4.0000000000e-05</td>
</tr>
<tr>
<td>7.0000000000e+04</td>
<td>7.8702465755e+04</td>
<td>1.0341896485e-05</td>
</tr>
</tbody>
</table>

**PDF for response_fn_3:**

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.3796737090e+05</td>
<td>3.5000000000e+05</td>
<td>4.2844660868e-06</td>
</tr>
<tr>
<td>3.5000000000e+05</td>
<td>4.0000000000e+05</td>
<td>8.6000000000e-06</td>
</tr>
<tr>
<td>4.0000000000e+05</td>
<td>4.5000000000e+05</td>
<td>1.8000000000e-06</td>
</tr>
</tbody>
</table>

Level mappings for each response function:

**Complementary Cumulative Distribution Function (CCDF) for response_fn_1:**

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.6000000000e+11</td>
<td>5.5000000000e+01</td>
<td>5.5000000000e+01</td>
<td></td>
</tr>
<tr>
<td>4.0000000000e+11</td>
<td>3.8000000000e+01</td>
<td>3.8000000000e+01</td>
<td></td>
</tr>
<tr>
<td>4.4000000000e+11</td>
<td>2.3000000000e+01</td>
<td>2.3000000000e+01</td>
<td></td>
</tr>
</tbody>
</table>

**Complementary Cumulative Distribution Function (CCDF) for response_fn_2:**

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.0000000000e+04</td>
<td>6.1000000000e+01</td>
<td>6.1000000000e+01</td>
<td></td>
</tr>
<tr>
<td>6.5000000000e+04</td>
<td>2.9000000000e+01</td>
<td>2.9000000000e+01</td>
<td></td>
</tr>
<tr>
<td>7.0000000000e+04</td>
<td>9.0000000000e+02</td>
<td>9.0000000000e+02</td>
<td></td>
</tr>
</tbody>
</table>

**Complementary Cumulative Distribution Function (CCDF) for response_fn_3:**

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.5000000000e+05</td>
<td>5.2000000000e+01</td>
<td>5.2000000000e+01</td>
<td></td>
</tr>
<tr>
<td>4.0000000000e+05</td>
<td>9.0000000000e+02</td>
<td>9.0000000000e+02</td>
<td></td>
</tr>
<tr>
<td>4.5000000000e+05</td>
<td>0.0000000000e+00</td>
<td>0.0000000000e+00</td>
<td></td>
</tr>
</tbody>
</table>

**Theory**

Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.
In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

A forward mapping involves computing the belief and plausibility probability level for a specified response level.

**num_response_levels**

- Keywords Area
- method
- adaptive_sampling
- response_levels
- num_response_levels

Number of values at which to estimate desired statistics for each response

**Specification**

*Alias:* none

*Argument(s):* INTEGERLIST

*Default:* response_levels evenly distributed among response functions

**Description**

The *num_response_levels* keyword allows the user to specify the number of response values, for each response, at which estimated statistics are of interest. Statistics that can be computed are probabilities and reliabilities, both according to either a cumulative distribution function or a complementary cumulative distribution function.

**Default Behavior**

If *num_response_levels* is not specified, the response_levels will be evenly distributed among the responses.

**Expected Outputs**

The specific output will be determined by the type of statistics that are specified. In a general sense, the output will be a list of response level-statistic pairs that show the estimated value of the desired statistic for each response level specified.

**Examples**

```
method
  sampling
    samples = 100
    seed = 34785
    num_response_levels = 1 1 1
    response_levels = 0.5 0.5 0.5
```
compute

- **Keywords Area**
- method
- adaptive_sampling
- response_levels
- compute

Selection of statistics to compute at each response level

### Specification

**Alias:** none  
**Argument(s):** none  
**Default:** probabilities

<table>
<thead>
<tr>
<th>Required/-Optional Required (Choose One)</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>probabilities</td>
<td>Computes probabilities associated with response levels</td>
</tr>
<tr>
<td></td>
<td></td>
<td>gen_reliabilities</td>
<td>Computes generalized reliabilities associated with response levels</td>
</tr>
<tr>
<td>Optional</td>
<td>system</td>
<td></td>
<td>Compute system reliability (series or parallel)</td>
</tr>
</tbody>
</table>

### Description

The `compute` keyword is used to select which forward statistical mapping is calculated at each response level.

**Default Behavior**

If `response_levels` is not specified, no statistics are computed. If `response_levels` is specified but `compute` is not, probabilities will be computed by default. If both `response_levels` and `compute` are specified, then one of the following must be specified: `probabilities`, `reliabilities`, or `gen_reliabilities`.

**Expected Output**

The type of statistics specified by `compute` will be reported for each response level.

**Usage Tips**

CDF/CCDF probabilities are calculated for specified response levels using a simple binning approach. CDF/CCDF reliabilities are calculated for specified response levels by computing the number of sample standard deviations separating the sample mean from the response level.
Examples

```plaintext
method
  sampling
    sample_type random
    samples = 100 seed = 1
    complementary distribution
    response_levels = 3.6e+11 4.0e+11 4.4e+11
                      6.0e+04 6.5e+04 7.0e+04
                      3.5e+05 4.0e+05 4.5e+05
    compute reliabilities

probabilities
  - Keywords Area
  - method
  - adaptive_sampling
  - response_levels
  - compute
  - probabilities

Computes probabilities associated with response levels
```

Specification

**Alias:** none
**Argument(s):** none

Description

The `probabilities` keyword directs Dakota to compute the probability that the model response will be below (cumulative) or above (complementary cumulative) a specified response value. This is done for every response level designated for each response.

**Default Behavior**

If `response_levels` is specified, the probabilities are computed by default. To explicitly specify it in the Dakota input file, though, the `probabilities` keyword should be specified in conjunction with the `compute` keyword.

**Expected Outputs**

The Dakota output is a set of response level-probability pairs that give the probability that the model response will be below or above the corresponding response level, depending on the distribution defined.

Examples

```plaintext
method
  sampling
    sample_type random
    samples = 100 seed = 1
    complementary distribution
    response_levels = 3.6e+11 4.0e+11 4.4e+11
                      6.0e+04 6.5e+04 7.0e+04
                      3.5e+05 4.0e+05 4.5e+05
    compute probabilities
```
6.2. METHOD

`gen_reliabilities`

- Keywords Area
- method
- adaptive_sampling
- response_levels
- compute
- gen_reliabilities

Computes generalized reliabilities associated with response levels

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

The `gen_reliabilities` keyword directs Dakota to compute generalized reliabilities according to the specified distribution for a specified response value. This is done for every response level designated for each response.

**Default Behavior**

If `response_levels` is specified, the generalized reliabilities are not computed by default. To change this behavior, the `gen_reliabilities` keyword should be specified in conjunction with the `compute` keyword.

**Expected Outputs**

The Dakota output is a set of response level-generalized reliability pairs according to the distribution defined.

**Examples**

```
method
  sampling
    sample_type random
    samples = 100 seed = 1
    complementary distribution
    response_levels = 3.6e+11 4.0e+11 4.4e+11
                     6.0e+04 6.5e+04 7.0e+04
                     3.5e+05 4.0e+05 4.5e+05
  compute gen_reliabilities

system
```

- Keywords Area
- method
- adaptive_sampling
- response_levels
- compute
- system

Compute system reliability (series or parallel)
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional Required</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(Choose One)</td>
<td></td>
<td></td>
<td>Aggregate response statistics assuming a series system</td>
</tr>
<tr>
<td></td>
<td></td>
<td>series</td>
<td>Aggregate response statistics assuming a parallel system</td>
</tr>
<tr>
<td>parallel</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Description

With the system probability/reliability option, statistics for specified response levels are calculated and reported assuming the response functions combine either in series or parallel to produce a total system response.

For a series system, the system fails when any one component (response) fails. The probability of failure is the complement of the product of the individual response success probabilities.

For a parallel system, the system fails only when all components (responses) fail. The probability of failure is the product of the individual response failure probabilities.

- series
  - Keywords Area
  - method
  - adaptive_sampling
  - response_levels
  - compute
  - system
  - series

Aggregate response statistics assuming a series system

Specification

Alias: none
Argument(s): none

Description

See parent keyword system for description.
6.2. METHOD

parallel
  • Keywords Area
  • method
  • adaptive_sampling
  • response_levels
  • compute
  • system
  • parallel

Aggregate response statistics assuming a parallel system

Specification
Alias: none
Argument(s): none

Description
See parent keyword system for description.

misc_options
  • Keywords Area
  • method
  • adaptive_sampling
  • misc_options

(Experimental) Hook for algorithm-specific adaptive sampling options

Specification
Alias: none
Argument(s): STRINGLIST
Default: no misc options

Description
The adaptive sampling algorithm is an experimental capability and not ready for production use at this time.
max_iterations

- Keywords Area
- method
- adaptive_sampling
- max_iterations

Number of iterations allowed for optimizers and adaptive UQ methods

Topics

This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none

Argument(s): INTEGER

Default: 100 (exceptions: fsu_cvt, local_reliability: 25; global {reliability, interval_est, evidence} / efficient-global: 25∗n)

Description

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed max_iterations iterations. See also max_function_evaluations.

Default Behavior

Default value is 100.

distribution

- Keywords Area
- method
- adaptive_sampling
- distribution

Selection of cumulative or complementary cumulative functions

Specification

Alias: none

Argument(s): none

Default: cumulative (CDF)
### Description

The `distribution` keyword allows the user to select between a cumulative distribution/belief/plausibility function and a complementary cumulative distribution/belief/plausibility function. This choice affects how probabilities and reliability indices are reported.

**Default Behavior**

If the `distribution` keyword is present, it must be accompanied by either `cumulative` or `complementary`. Otherwise, a cumulative distribution will be used by default.

**Expected Outputs**

Output will be a set of model response-probability pairs determined according to the choice of distribution. The choice of distribution also defines the sign of the reliability or generalized reliability indices.

### Examples

```plaintext
method
  sampling
    sample_type lhs
    samples = 10
    distribution cumulative
```

**cumulative**

- Keywords Area
- method
- adaptive_sampling
- distribution
- cumulative

Computes statistics according to cumulative functions

### Specification

**Alias:** none

**Argument(s):** none
Description

Statistics on model responses will be computed according to a cumulative distribution/belief/plausibility function.

Default Behavior

By default, a cumulative distribution/belief/plausibility function will be used. To explicitly specify it in the Dakota input file, however, the `cumulative` keyword must be appear in conjunction with the `distribution` keyword.

Expected Outputs

Output will be a set of model response-probability pairs determined according to a cumulative distribution/belief/plausibility function. The probabilities reported are the probabilities that the model response falls below given response thresholds.

Examples

```dakota
method
  sampling
    sample_type lhs
    samples = 10
    distribution cumulative
```

complementary

- Keywords Area
- method
- adaptive_sampling
- distribution
- complementary

Computes statistics according to complementary cumulative functions

Specification

Alias: none

Argument(s): none

Description

Statistics on model responses will be computed according to a complementary cumulative distribution/belief/plausibility function.

Default Behavior

By default, a complementary cumulative distribution/belief/plausibility function will not be used. To change that behavior, the `complementary` keyword must be appear in conjunction with the `distribution` keyword.

Expected Outputs

Output will be a set of model response-probability pairs determined according to a complementary cumulative distribution/belief/plausibility function. The probabilities reported are the probabilities that the model response falls above given response thresholds.
6.2. METHOD

Examples

```
method, sampling
  sample_type lhs
  samples = 10
  distribution complementary
```

probability_levels

- Keywords Area
- method
- adaptive_sampling
- probability_levels

Specify probability levels at which to estimate the corresponding response value

Specification

**Alias:** none

**Argument(s):** REALLIST

**Default:** No CDF/CCDF response levels to compute

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>num_probability_levels</td>
<td>Specify which probability_levels correspond to which response</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Description

Response levels are calculated for specified CDF/CCDF probabilities by indexing into a sorted samples array (the response levels computed are not interpolated and will correspond to one of the sampled values).

**Expected Output**

If `probability_levels` are specified, Dakota will create two tables in the standard output: a Probability Density function (PDF) histogram and a Cumulative Distribution Function (CDF) table. The PDF histogram has the lower and upper endpoints of each bin and the corresponding density of that bin. Note that the PDF histogram has bins defined by the `probability_levels` and/or `response_levels` in the Dakota input file. If there are not very many levels, the histogram will be coarse. Dakota does not do anything to optimize the bin size or spacing. The CDF table has the list of response levels and the corresponding probability that the response value is less than or equal to each response level threshold.

Examples

The Dakota input file below specifies a sampling method with probability levels of interest.

```
method, sampling,
  samples = 100 seed = 1
  complementary distribution
```
CHAPTER 6. KEYWORDS AREA

probability_levels = 1. .66 .33 0.
1. .8 .5 0.
1. .3 .2 0.

variables,
normal_uncertain = 2
means = 248.89, 593.33
std_deviations = 12.4, 29.7
descriptors = 'TF1n' 'TF2n'
uniform_uncertain = 2
lower_bounds = 199.3, 474.63
upper_bounds = 298.5, 712.
descriptors = 'TF1u' 'TF2u'
weibull_uncertain = 2
alphas = 12., 30.
betas = 250., 590.
descriptors = 'TF1w' 'TF2w'
histogram_bin_uncertain = 2
num_pairs = 3 4
abscissas = 5 8 10 .1 .2 .3 .4
counts = 17 21 0 12 24 12 0
descriptors = 'TF1h' 'TF2h'
histogram_point_uncertain
real = 1
num_pairs = 2
abscissas = 3 4
counts = 1 1
descriptors = 'TF3h'

interface,
system asynch evaluation_concurrency = 5
analysis_driver = 'text_book'

responses,
response_functions = 3
no_gradients
no_hessians

Given the above Dakota input file, the following excerpt from the output shows the PDF and CCDF generated. Note that the bounds on the bins of the PDF are the response values that correspond the probability levels specified in the input file. Those response values are also shown in the CCDF.

Probability Density Function (PDF) histograms for each response function:

PDF for response_fn_1:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.7604749078e+11</td>
<td>3.4221494996e+11</td>
<td>5.1384774972e-12</td>
</tr>
<tr>
<td>3.4221494996e+11</td>
<td>4.0634975300e+11</td>
<td>5.1454122311e-12</td>
</tr>
<tr>
<td>4.0634975300e+11</td>
<td>5.4196114379e+11</td>
<td>2.4334239039e-12</td>
</tr>
</tbody>
</table>

PDF for response_fn_2:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.6431154744e+04</td>
<td>5.6511827775e+04</td>
<td>1.9839945149e-05</td>
</tr>
<tr>
<td>5.6511827775e+04</td>
<td>6.1603813790e+04</td>
<td>5.8916108390e-05</td>
</tr>
<tr>
<td>6.1603813790e+04</td>
<td>7.8702465755e+04</td>
<td>2.9242071306e-05</td>
</tr>
</tbody>
</table>

PDF for response_fn_3:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.3796737090e+05</td>
<td>3.6997214153e+05</td>
<td>5.3028386523e-06</td>
</tr>
<tr>
<td>3.6997214153e+05</td>
<td>3.8100966235e+05</td>
<td>9.060055634e-06</td>
</tr>
<tr>
<td>3.8100966235e+05</td>
<td>4.1114981270e+05</td>
<td>3.3274925348e-06</td>
</tr>
</tbody>
</table>
Level mappings for each response function:

### Complementary Cumulative Distribution Function (CCDF) for response_fn_1:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.7604749078e+11</td>
<td>1.0000000000e+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.4221494996e+11</td>
<td>6.6000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.0634975300e+11</td>
<td>3.3000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5.4196114379e+11</td>
<td>0.0000000000e+00</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Complementary Cumulative Distribution Function (CCDF) for response_fn_2:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.643154744e+04</td>
<td>1.0000000000e+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5.6511827775e+04</td>
<td>8.0000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6.1603813790e+04</td>
<td>5.0000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7.8702465755e+04</td>
<td>0.0000000000e+00</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Complementary Cumulative Distribution Function (CCDF) for response_fn_3:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.3796737090e+05</td>
<td>1.0000000000e+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.699721453e+05</td>
<td>3.0000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.8100966235e+05</td>
<td>2.0000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.4111498127e+05</td>
<td>0.0000000000e+00</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Theory**

Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.

In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

An inverse mapping involves computing the belief and plausibility response level for either a specified probability level or a specified generalized reliability level (two results for each level mapping in the evidence-based epistemic case, instead of the one result for each level mapping in the aleatory case).

#### num_probability Levels

- **Keywords Area**
- **method**
- **adaptive_sampling**
- **probability_levels**
- **num_probability_levels**

Specify which probability_levels correspond to which response

**Specification**

**Alias:** none

**Argument(s):** INTEGERLIST

**Default:** probability_levels evenly distributed among response functions

**Description**

See parent page
**gen_reliability_levels**

- **Keywords Area**
- **method**
- **adaptive_sampling**
- **gen_reliability_levels**

Specify generalized reliability levels at which to estimate the corresponding response value.

### Specification

**Alias:** none  
**Argument(s):** REALLIST  
**Default:** No CDF/CCDF response levels to compute

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>num_gen_reliability_levels</td>
<td></td>
<td>Specify which gen_reliability_levels correspond to which response</td>
</tr>
</tbody>
</table>

### Description

Response levels are calculated for specified generalized reliabilities by indexing into a sorted samples array (the response levels computed are not interpolated and will correspond to one of the sampled values).

### Theory

Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.

In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

An inverse mapping involves computing the belief and plausibility response level for either a specified probability level or a specified generalized reliability level (two results for each level mapping in the evidence-based epistemic case, instead of the one result for each level mapping in the aleatory case).

**num_gen_reliability_levels**

- **Keywords Area**
- **method**
- **adaptive_sampling**
- **gen_reliability_levels**
- **num_gen_reliability_levels**

Specify which gen_reliability_levels correspond to which response
6.2. \textit{METHOD}

\textbf{Specification}

\textbf{Alias:} none

\textbf{Argument(s):} INTEGERLIST

\textbf{Default:} gen\_reliability\_levels evenly distributed among response functions

\textbf{Description}

See parent page

\textbf{rng}

- Keywords Area
- method
- adaptive\_sampling
- rng

Selection of a random number generator

\textbf{Specification}

\textbf{Alias:} none

\textbf{Argument(s):} none

\textbf{Default:} Mersenne twister (mt19937)

\begin{tabular}{|c|c|c|}
\hline
\textbf{Required/-} & \textbf{Description of} & \textbf{Dakota Keyword} & \textbf{Dakota Keyword}  \\
\textbf{Optional} & \textbf{Group} & \textbf{Description}  & \textbf{Description} \\
\textbf{Required(Choose} & \textbf{Group 1} & \textbf{mt19937} & Generates random numbers using the Mersenne twister \\
\textbf{One)}} & & & \\
\hline
\multicolumn{4}{|c|}{rnum2} & Generates pseudo-random numbers using the Pecos package \\
\hline
\end{tabular}

\textbf{Description}

The \textit{rng} keyword is used to indicate a choice of random number generator.

\textbf{Default Behavior}

If specified, the \textit{rng} keyword must be accompanied by either \textit{rnum2} (pseudo-random numbers) or \textit{mt19937} (random numbers generated by the Mersenne twister). Otherwise, \textit{mt19937}, the Mersenne twister is used by default.

\textbf{Usage Tips}

The default is recommended, as the Mersenne twister is a higher quality random number generator.
Examples

```
method
  sampling
    sample_type lhs
    samples = 10
    seed = 98765
    rng mt19937
```

**mt19937**

- **Keywords Area**
- **method**
- **adaptive_sampling**
- **rng**
- **mt19937**

Generates random numbers using the Mersenne twister

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

The `mt19937` keyword directs Dakota to use the Mersenne twister to generate random numbers. Additional information can be found on wikipedia: [http://en.wikipedia.org/wiki/Mersenne_twister](http://en.wikipedia.org/wiki/Mersenne_twister).

**Default Behavior**

`mt19937` is the default random number generator. To specify it explicitly in the Dakota input file, however, it must be specified in conjunction with the `rng` keyword.

**Usage Tips**

Use of the Mersenne twister random number generator (`mt19937`) is recommended.

Examples

```
method
  sampling
    sample_type lhs
    samples = 10
    seed = 98765
    rng mt19937
```

**rnum2**

- **Keywords Area**
- **method**
- **adaptive_sampling**
- **rng**
6.2. METHOD

- **rnum2**

  Generates pseudo-random numbers using the Pecos package

**Specification**

Alias: none

Argument(s): none

**Description**

The `rnum2` keyword directs Dakota to use pseudo-random numbers generated by the Pecos package.

**Default Behavior**

`rnum2` is not used by default. To change this behavior, it must be specified in conjunction with the `rng` keyword.

**Usage Tips**

Use of the Mersenne twister random number generator (`mt19937`) is recommended over `rnum2`.

**Examples**

```plaintext
method
  sampling
    sample_type lhs
    samples = 10
    seed = 98765
    rng rnum2

model_pointer
  ```

**Topics**

This keyword is related to the topics:

- block_pointer

**Specification**

Alias: none

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)
CHAPTER 6. KEYWORDS AREA

Description

The **model_pointer** is used to specify which **model** block will be used to perform the function evaluations needed by the Dakota method.

**Default Behavior**

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a **model** block in the Dakota input file that has a corresponding **id_model** with the same name.

**Usage Tips**

When doing advanced analyses that involve using multiple methods and multiple models, defining a **model-pointer** for each method is imperative.

See **block_pointer** for details about pointers.

**Examples**

```plaintext
environment
  tabular_graphics_data
  method_pointer = 'UQ'

method
  id_method = 'UQ'
  model_pointer = 'SURR'
  sampling,
    samples = 10
    seed = 98765 rng rnum2
    response_levels = 0.1 0.2 0.6
    0.1 0.2 0.6
    0.1 0.2 0.6
    sample_type lhs
    distribution cumulative

model
  id_model = 'SURR'
    surrogate global,
    dace_method_pointer = 'DACE'
    polynomial quadratic

method
  id_method = 'DACE'
  model_pointer = 'DACE_M'
  sampling sample_type lhs
    samples = 121 seed = 5034 rng rnum2

model
  id_model = 'DACE_M'
    single
    interface_pointer = 'I1'

variables
  uniform_uncertain = 2
    lower_bounds = 0. 0.
    upper_bounds = 1. 1.
    descriptors = 'x1' 'x2'

interface
  id_interface = 'I1'
    system asynch evaluation_concurrency = 5
    analysis_driver = 'text_book'

responses
```
6.2. METHOD

response_functions = 3
no_gradients
no_hessians

6.2.55 pof_darts

- Keywords Area
- method
- pof_darts

Probability-of-Failure (POF) darts is a novel method for estimating the probability of failure based on random sphere-packing.

Topics
This keyword is related to the topics:

- uncertainty_quantification

Specification
Alias: nond_pof_darts
Argument(s): none

| Required/- | Description of Group | Dakota Keyword | Dakota Keyword Description |
| Optional Required | | build_samples | Number of initial model evaluations used in build phase |
| Optional | seed | | Seed of the random number generator |
| Optional | lipschitz | | Select the type of Lipschitz estimation (global or local) |
| Optional | samples_on_emulator | | Number of samples at which to evaluate an emulator (surrogate) |
CHAPTER 6. KEYWORDS AREA

### Description

**pof_darts** is a novel method for estimating the probability of failure based on random sphere-packing. Random spheres are sampled from the domain with the constraint that each new sphere center has to be outside prior disks. The radius of each sphere is chosen such that the entire sphere lie either in the failure or the non-failure region. This radius depends of the function evaluation at the disk center, the failure threshold and an estimate of the function gradient at the disk center.

We utilize a global surrogate for evaluating the gradient and hence only one function evaluation is required for each sphere.

After exhausting the sampling budget specified by **samples**, which is the number of spheres per failure threshold, the domain is decomposed into two regions. These regions correspond to failure and non-failure, each represented by the union of the spheres of each type. The volume of the union of failure spheres gives a lower bound on the required estimate of the probability of failure, while the volume of the union of the non-failure spheres subtracted from the volume of the domain gives an upper estimate. We currently report the average of both estimates.

**pof_darts** handles multiple response functions and allows each to have multiple failure thresholds. For each failure threshold, **pof_darts** will insert a number of spheres specified by the user-input parameter **samples**. However, estimating the probability of failure for each failure threshold would utilize the total number of disks sampled for all failure thresholds. For each failure threshold, the sphere radii changes to generate the right spatial
6.2. METHOD

decomposition.

**build_samples**

- **Keywords Area**
- method
- pof_darts
- build_samples

Number of initial model evaluations used in build phase

**Specification**

**Alias:** samples

**Argument(s):** INTEGER

**Description**

The number of build points or training points used in the initial phase of an algorithm or model construction. Typically these are the initial set of data points used to construct (train) a surrogate model (emulator). If the number of `build_samples` is less than the minimum number of points required to build the surrogate, Dakota will augment the samples to obtain the minimum required.

**Examples**

Perform GP-based adaptive importance sampling, building the GP with 100 points and then performing 100 approximate evaluations to evaluate the probability.

```plaintext
method gpais
  build_samples = 100
  samples_on_emulator = 100
  max_iterations = 5
  response_levels = -1.065
```

**seed**

- **Keywords Area**
- method
- pof_darts
- seed

Seed of the random number generator

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** system-generated (non-repeatable)
CHAPTER 6. KEYWORDS AREA

Description

The random seed control provides a mechanism for making a stochastic method repeatable. That is, the use of
the same random seed in identical studies will generate identical results.

Default Behavior

If not specified, the seed is randomly generated.

Expected Output

If seed is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

Usage Tips

If a stochastic study was run without seed specified, and the user later wishes to repeat the study using the
same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen.
That value can then be added to the Dakota input file.

Examples

```
method
  sampling
    sample_type lhs
    samples = 10
    seed = 15347
```

lipschitz

- Keywords Area
- method
- pof_darts
- lipschitz

Select the type of Lipschitz estimation (global or local)

Specification

Alias: none

Argument(s): none

<table>
<thead>
<tr>
<th>Required/Optional Required Group 1</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>local</td>
<td>Specify local estimation of the Lipschitz constant</td>
</tr>
<tr>
<td></td>
<td></td>
<td>global</td>
<td>Specify global estimation of the Lipschitz estimate</td>
</tr>
</tbody>
</table>
6.2. METHOD

**Description**

There are two types of Lipschitz estimation used in sizing the disks used in POF Darts: *global* and *local*. The global approach uses one Lipschitz estimate for the entire domain. The local approach calculates the Lipschitz estimate separately for each Voronoi region based on nearby points. The local method is more expensive but more accurate.

**local**

- **Keywords**: Area, method, pof_darts, lipschitz, local
- **Description**: Specify local estimation of the Lipschitz constant

**Specification**

- **Alias**: none
- **Argument(s)**: none

**Description**

The local approach to estimate the Lipschitz constant calculates the Lipschitz estimate separately for each Voronoi region based on nearby points. The local method is more expensive but results in higher accuracy compared to the global method.

**global**

- **Keywords**: Area, method, pof_darts, lipschitz, global
- **Description**: Specify global estimation of the Lipschitz estimate

**Specification**

- **Alias**: none
- **Argument(s)**: none

**Description**

The global approach uses one Lipschitz estimate for the entire domain. This option is currently deactivated. Please refer to the local alternative.
samples_on_emulator

- Keywords Area
- method
- pof_darts
- samples_on_emulator

Number of samples at which to evaluate an emulator (surrogate)

**Specification**

Alias: none

**Argument(s):** INTEGER

**Description**

How many approximate function evaluations to perform on the emulator model, e.g., to compute statistics

**Default Behavior**

The default number of samples is method-dependent.

**Examples**

Perform 10000 samples on the PCE approximation of the true model:

```plaintext
method
  polynomial_chaos
  quadrature_order = 2
  samples_on_emulator = 10000
```

**response_levels**

- Keywords Area
- method
- pof_darts
- response_levels

Values at which to estimate desired statistics for each response

**Specification**

Alias: none

**Argument(s):** REALLIST

**Default:** No CDF/CCDF probabilities/reliabilities to compute
6.2. METHOD

| Optional | num_response_levels | Number of values at which to estimate desired statistics for each response |
| Optional | compute | Selection of statistics to compute at each response level |

### Description

The `response_levels` specification provides the target response values for which to compute probabilities, reliabilities, or generalized reliabilities (forward mapping).

#### Default Behavior

If `response_levels` are not specified, no statistics will be computed. If they are, probabilities will be computed by default.

#### Expected Outputs

If `response_levels` are specified, Dakota will create two tables in the standard output: a Probability Density function (PDF) histogram and a Cumulative Distribution Function (CDF) table. The PDF histogram has the lower and upper endpoints of each bin and the corresponding density of that bin. Note that the PDF histogram has bins defined by the `probability_levels` and/or `response_levels` in the Dakota input file. If there are not very many levels, the histogram will be coarse. Dakota does not do anything to optimize the bin size or spacing. The CDF table has the list of response levels and the corresponding probability that the response value is less than or equal to each response level threshold.

#### Usage Tips

The `num_response_levels` key is used to specify which arguments of the `response_level` correspond to which response.

#### Examples

For example, specifying a `response_level` of 52.3 followed with `compute probabilities` will result in the calculation of the probability that the response value is less than or equal to 52.3, given the uncertain distributions on the inputs.

For an example with multiple responses, the following specification

```plaintext
response_levels = 1. 2. .1 .2 .3 .4 10. 20. 30.
num_response_levels = 2 4 3
```

would assign the first two response levels (1., 2.) to response function 1, the next four response levels (.1, .2, .3, .4) to response function 2, and the final three response levels (10., 20., 30.) to response function 3. If the `num_response_levels` key were omitted from this example, then the response levels would be evenly distributed among the response functions (three levels each in this case).

The Dakota input file below specifies a sampling method with response levels of interest.

```plaintext
method, sampling,
samples = 100 seed = 1
complementary distribution
response_levels = 3.6e+11 4.0e+11 4.4e+11 6.0e+04 6.5e+04 7.0e+04
```
variables,
    normal_uncertain = 2
    means = 248.89, 593.33
    std_deviations = 12.4, 29.7
    descriptors = 'TF1n' 'TF2n'
    uniform_uncertain = 2
    lower_bounds = 199.3, 474.63
    upper_bounds = 298.5, 712.
    descriptors = 'TF1u' 'TF2u'
weibull_uncertain = 2
    alphas = 12., 30.
    betas = 250., 590.
    descriptors = 'TF1w' 'TF2w'
histogram_bin_uncertain = 2
    num_pairs = 3 4
    abscissas = 5 8 10 .1 .2 .3 .4
    counts = 17 21 0 12 24 12 0
    descriptors = 'TF1h' 'TF2h'
histogram_point_uncertain
    real = 1
    num_pairs = 2
    abscissas = 3 4
    counts = 1 1
    descriptors = 'TF3h'

interface,
    system asynch evaluation_concurrency = 5
    analysis_driver = 'text_book'

responses,
    response_functions = 3
    no_gradients
    no_hessians

Given the above Dakota input file, the following excerpt from the output shows the PDF and CCDF generated. Note that the bounds on the bins of the PDF are the response values specified in the input file. The probability levels corresponding to those response values are shown in the CCDF.

Probability Density Function (PDF) histograms for each response function:
PDF for response_fn_1:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.76047494078e+11</td>
<td>3.6000000000e+11</td>
<td>5.3601733194e-12</td>
</tr>
<tr>
<td>3.6000000000e+11</td>
<td>4.0000000000e+11</td>
<td>4.2500000000e-12</td>
</tr>
<tr>
<td>4.0000000000e+11</td>
<td>4.4000000000e+11</td>
<td>3.7500000000e-12</td>
</tr>
<tr>
<td>4.4000000000e+11</td>
<td>5.4196114379e+11</td>
<td>2.2557612778e-12</td>
</tr>
</tbody>
</table>

PDF for response_fn_2:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.6431154744e+04</td>
<td>6.0000000000e+04</td>
<td>2.8742313192e-05</td>
</tr>
<tr>
<td>6.0000000000e+04</td>
<td>6.5000000000e+04</td>
<td>6.4000000000e-05</td>
</tr>
<tr>
<td>6.5000000000e+04</td>
<td>7.0000000000e+04</td>
<td>4.0000000000e-05</td>
</tr>
<tr>
<td>7.0000000000e+04</td>
<td>7.8702465755e+04</td>
<td>1.0341896485e-05</td>
</tr>
</tbody>
</table>

PDF for response_fn_3:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.3796737090e+05</td>
<td>3.5000000000e+05</td>
<td>4.2844660868e-06</td>
</tr>
<tr>
<td>3.5000000000e+05</td>
<td>4.0000000000e+05</td>
<td>8.6000000000e-06</td>
</tr>
<tr>
<td>4.0000000000e+05</td>
<td>4.5000000000e+05</td>
<td>1.8000000000e-06</td>
</tr>
</tbody>
</table>
6.2. METHOD

Level mappings for each response function:

---
**Complementary Cumulative Distribution Function (CCDF) for response_fn_1:**

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.6000000000e+11</td>
<td>5.5000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.0000000000e+11</td>
<td>3.8000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.4000000000e+11</td>
<td>2.3000000000e-01</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
---
**Complementary Cumulative Distribution Function (CCDF) for response_fn_2:**

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.0000000000e+04</td>
<td>6.1000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6.5000000000e+04</td>
<td>2.9000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7.0000000000e+04</td>
<td>9.0000000000e-02</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
---
**Complementary Cumulative Distribution Function (CCDF) for response_fn_3:**

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.5000000000e+05</td>
<td>5.2000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.0000000000e+05</td>
<td>9.0000000000e-02</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.5000000000e+05</td>
<td>0.0000000000e+00</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
---

**Theory**

Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.

In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

A forward mapping involves computing the belief and plausibility probability level for a specified response level.

**num_response_levels**

- **Keywords Area**
- **method**
- **pof_darts**
- **response_levels**
- **num_response_levels**

Number of values at which to estimate desired statistics for each response

**Specification**

**Alias:** none

**Argument(s):** INTEGERLIST

**Default:** response_levels evenly distributed among response functions

**Description**

The **num_response_levels** keyword allows the user to specify the number of response values, for each response, at which estimated statistics are of interest. Statistics that can be computed are probabilities and reliabilities, both according to either a cumulative distribution function or a complementary cumulative distribution function.
**Default Behavior**

If `num_response_levels` is not specified, the response levels will be evenly distributed among the responses.

**Expected Outputs**

The specific output will be determined by the type of statistics that are specified. In a general sense, the output will be a list of response level-statistic pairs that show the estimated value of the desired statistic for each response level specified.

**Examples**

```
method
  sampling
    samples = 100
    seed = 34785
    num_response_levels = 1 1 1
    response_levels = 0.5 0.5 0.5

compute
  • Keywords Area
  • method
  • pof, darts
  • response_levels
  • compute
```

Selection of statistics to compute at each response level

**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** probabilities

<table>
<thead>
<tr>
<th>Required/-Optional Required (Choose One)</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gen Reliabilities</td>
<td>gen_reliabilities</td>
<td></td>
<td>Computes generalized reliabilities associated with response levels</td>
</tr>
</tbody>
</table>
6.2. METHOD

<table>
<thead>
<tr>
<th>Optional</th>
<th>system</th>
<th>Compute system reliability (series or parallel)</th>
</tr>
</thead>
</table>

**Description**

The `compute` keyword is used to select which forward statistical mapping is calculated at each response level.

**Default Behavior**

If `response_levels` is not specified, no statistics are computed. If `response_levels` is specified but `compute` is not, probabilities will be computed by default. If both `response_levels` and `compute` are specified, then one of the following must be specified: `probabilities`, `reliabilities`, or `gen_reliabilities`.

**Expected Output**

The type of statistics specified by `compute` will be reported for each response level.

**Usage Tips**

CDF/CCDF probabilities are calculated for specified response levels using a simple binning approach. CDF/CCDF reliabilities are calculated for specified response levels by computing the number of sample standard deviations separating the sample mean from the response level.

**Examples**

```python
method sampling
    sample_type random
    samples = 100 seed = 1
    complementary distribution
    response_levels = 3.6e+11 4.0e+11 4.4e+11
                     6.0e+04 6.5e+04 7.0e+04
                     3.5e+05 4.0e+05 4.5e+05
    compute reliabilities

probabilities
- Keywords Area
- method
- pof_darts
- response_levels
- compute
- probabilities

Computes probabilities associated with response levels
```

**Specification**

Alias: none

Argument(s): none
CHAPTER 6. KEYWORDS AREA

Description

The `probabilities` keyword directs Dakota to compute the probability that the model response will be below (cumulative) or above (complementary cumulative) a specified response value. This is done for every response level designated for each response.

Default Behavior

If `response_levels` is specified, the probabilities are computed by default. To explicitly specify it in the Dakota input file, though, the `probabilities` keyword should be specified in conjunction with the `compute` keyword.

Expected Outputs

The Dakota output is a set of response level-probability pairs that give the probability that the model response will be below or above the corresponding response level, depending on the distribution defined.

Examples

```
method
  sampling
    sample_type random
    samples = 100 seed = 1
  complementary distribution
  response_levels = 3.6e+11 4.0e+11 4.4e+11
                  6.0e+04 6.5e+04 7.0e+04
                  3.5e+05 4.0e+05 4.5e+05
  compute probabilities

gen_reliabilities
```

Computes generalized reliabilities associated with response levels

Specification

Alias: none

Argument(s): none

Description

The `gen_reliabilities` keyword directs Dakota to compute generalized reliabilities according to the specified distribution for a specified response value. This is done for every response level designated for each response.

Default Behavior

If `response_levels` is specified, the generalized reliabilities are not computed by default. To change this behavior, the `gen_reliabilities` keyword should be specified in conjunction with the `compute` keyword.

Expected Outputs

The Dakota output is a set of response level-generalized reliability pairs according to the distribution defined.
6.2. METHOD

Examples

```
method
  sampling
  sample_type random
  samples = 100 seed = 1
  complementary distribution
  response_levels = 3.6e+11 4.0e+11 4.4e+11
                   6.0e+04 6.5e+04 7.0e+04
                   3.5e+05 4.0e+05 4.5e+05
  compute gen_reliabilities
```

```
system

• Keywords Area
• method
• pof_darts
• response_levels
• compute
• system

Compute system reliability (series or parallel)
```

Specification

Alias: none

<table>
<thead>
<tr>
<th>Required/Optional Required (Choose One)</th>
<th>Description of Group Group 1</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>series</td>
</tr>
<tr>
<td></td>
<td></td>
<td>parallel</td>
</tr>
</tbody>
</table>

Description

With the system probability/reliability option, statistics for specified `response_levels` are calculated and reported assuming the response functions combine either in series or parallel to produce a total system response.

For a series system, the system fails when any one component (response) fails. The probability of failure is the complement of the product of the individual response success probabilities.

For a parallel system, the system fails only when all components (responses) fail. The probability of failure is the product of the individual response failure probabilities.
series

- Keywords Area
- method
- pof_darts
- response_levels
- compute
- system
- series

Aggregate response statistics assuming a series system

**Specification**

*Alias*: none

*Argument(s):* none

**Description**

See parent keyword `system` for description.

parallel

- Keywords Area
- method
- pof_darts
- response_levels
- compute
- system
- parallel

Aggregate response statistics assuming a parallel system

**Specification**

*Alias*: none

*Argument(s):* none

**Description**

See parent keyword `system` for description.
distribution

- **Keywords Area**
- **method**
- **pof_darts**
- **distribution**

Selection of cumulative or complementary cumulative functions

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** cumulative (CDF)

<table>
<thead>
<tr>
<th>Required/-Optional Required</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Choose One</td>
<td></td>
<td>cumulative</td>
<td>Computes statistics according to cumulative functions</td>
</tr>
<tr>
<td>complementary</td>
<td></td>
<td>complementary</td>
<td>Computes statistics according to complementary cumulative functions</td>
</tr>
</tbody>
</table>

**Description**

The `distribution` keyword allows the user to select between a cumulative distribution/belief/plausibility function and a complementary cumulative distribution/belief/plausibility function. This choice affects how probabilities and reliability indices are reported.

**Default Behavior**

If the `distribution` keyword is present, it must be accompanied by either `cumulative` or `complementary`. Otherwise, a cumulative distribution will be used by default.

**Expected Outputs**

Output will be a set of model response-probability pairs determined according to the choice of distribution. The choice of distribution also defines the sign of the reliability or generalized reliability indices.

**Examples**

```
method
  sampling
    sample_type lhs
    samples = 10
    distribution cumulative
```
cumulative

- Keywords Area
- method
- pof_darts
- distribution
- cumulative

Computes statistics according to cumulative functions

**Specification**

Alias: none

Argument(s): none

**Description**

Statistics on model responses will be computed according to a cumulative distribution/belief/plausibility function.

**Default Behavior**

By default, a cumulative distribution/belief/plausibility function will be used. To explicitly specify it in the Dakota input file, however, the cumulative keyword must be appear in conjunction with the distribution keyword.

**Expected Outputs**

Output will be a set of model response-probability pairs determined according to a cumulative distribution/belief/plausibility function. The probabilities reported are the probabilities that the model response falls below given response thresholds.

**Examples**

```plaintext
method
  sampling
    sample_type lhs
    samples = 10
    distribution cumulative
```

complementary

- Keywords Area
- method
- pof_darts
- distribution
- complementary

Computes statistics according to complementary cumulative functions
6.2. **METHOD**

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

Statistics on model responses will be computed according to a complementary cumulative distribution/belief/plausibility function.

**Default Behavior**

By default, a complementary cumulative distribution/belief/plausibility function will not be used. To change that behavior, the `complementary` keyword must appear in conjunction with the `distribution` keyword.

**Expected Outputs**

Output will be a set of model response-probability pairs determined according to a complementary cumulative distribution/belief/plausibility function. The probabilities reported are the probabilities that the model response falls above given response thresholds.

**Examples**

```plaintext
method
  sampling
    sample_type lhs
    samples = 10
    distribution complementary
```

**probability_levels**

- **Keywords Area**
- **method**
- **pof_darts**
- **probability_levels**

Specify probability levels at which to estimate the corresponding response value.

**Specification**

**Alias:** none

**Argument(s):** REALLIST

**Default:** No CDF/CCDF response levels to compute

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>num_probability_levels</td>
<td>Specify which probability_levels correspond to which response</td>
<td></td>
</tr>
</tbody>
</table>
CHAPTER 6. KEYWORDS AREA

Description

Response levels are calculated for specified CDF/CCDF probabilities by indexing into a sorted samples array (the response levels computed are not interpolated and will correspond to one of the sampled values).

Expected Output

If probability levels are specified, Dakota will create two tables in the standard output: a Probability Density function (PDF) histogram and a Cumulative Distribution Function (CDF) table. The PDF histogram has the lower and upper endpoints of each bin and the corresponding density of that bin. Note that the PDF histogram has bins defined by the probability levels and/or response levels in the Dakota input file. If there are not very many levels, the histogram will be coarse. Dakota does not do anything to optimize the bin size or spacing. The CDF table has the list of response levels and the corresponding probability that the response value is less than or equal to each response level threshold.

Examples

The Dakota input file below specifies a sampling method with probability levels of interest.

```plaintext
method,
    sampling,
    samples = 100 seed = 1
    complementary distribution
    probability_levels = 1. .66 .33 0.
        1. .8 .5 0.
        1. .3 .2 0.

variables,
    normal_uncertain = 2
        means = 248.89, 593.33
        std_deviations = 12.4, 29.7
        descriptors = 'TF1n' 'TF2n'
    uniform_uncertain = 2
        lower_bounds = 199.3, 474.63
        upper_bounds = 298.5, 712.
        descriptors = 'TF1u' 'TF2u'
    weibull_uncertain = 2
        alphas = 12., 30.
        betas = 250., 590.
        descriptors = 'TF1w' 'TF2w'
    histogram_bin_uncertain = 2
        num_pairs = 3 4
        abscissas = 5 8 10 .1 .2 .3 .4
        counts = 17 21 0 12 24 12 0
        descriptors = 'TF1h' 'TF2h'
    histogram_point_uncertain
        real = 1
        num_pairs = 2
        abscissas = 3 4
        counts = 1 1
        descriptors = 'TF3h'

interface,
    system asynch evaluation_concurrency = 5
    analysis_driver = 'text_book'

responses,
    response_functions = 3
    no_gradients
    no_hessians
```
6.2. METHOD

Given the above Dakota input file, the following excerpt from the output shows the PDF and CCDF generated. Note that the bounds on the bins of the PDF are the response values that correspond the probability levels specified in the input file. Those response values are also shown in the CCDF.

Probability Density Function (PDF) histograms for each response function:

PDF for response_fn_1:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.7604749078e+11</td>
<td>3.4221494996e+11</td>
<td>5.1384774972e-12</td>
</tr>
<tr>
<td>3.4221494996e+11</td>
<td>4.0634975300e+11</td>
<td>5.145122311e-12</td>
</tr>
<tr>
<td>4.0634975300e+11</td>
<td>5.4196114379e+11</td>
<td>2.4334239039e-12</td>
</tr>
</tbody>
</table>

PDF for response_fn_2:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.6431154744e+04</td>
<td>5.6511827775e+04</td>
<td>1.9833995419e-05</td>
</tr>
<tr>
<td>5.6511827775e+04</td>
<td>6.1603813790e+04</td>
<td>5.8916108390e-05</td>
</tr>
<tr>
<td>6.1603813790e+04</td>
<td>7.8702465755e+04</td>
<td>2.9242071306e-05</td>
</tr>
</tbody>
</table>

PDF for response_fn_3:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.3796737090e+05</td>
<td>3.6997214153e+05</td>
<td>5.3028386523e-06</td>
</tr>
<tr>
<td>3.6997214153e+05</td>
<td>3.8100966235e+05</td>
<td>9.060005634e-06</td>
</tr>
<tr>
<td>3.8100966235e+05</td>
<td>4.4111498127e+05</td>
<td>3.3274925348e-06</td>
</tr>
</tbody>
</table>

Level mappings for each response function:

Complementary Cumulative Distribution Function (CCDF) for response_fn_1:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.7604749078e+11</td>
<td>1.0000000000e+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.4221494996e+11</td>
<td>6.0000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.0634975300e+11</td>
<td>3.0000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5.4196114379e+11</td>
<td>0.0000000000e+00</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Complementary Cumulative Distribution Function (CCDF) for response_fn_2:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.6431154744e+04</td>
<td>1.0000000000e+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5.6511827775e+04</td>
<td>8.0000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6.1603813790e+04</td>
<td>5.0000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7.8702465755e+04</td>
<td>0.0000000000e+00</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Complementary Cumulative Distribution Function (CCDF) for response_fn_3:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.3796737090e+05</td>
<td>1.0000000000e+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.6997214153e+05</td>
<td>3.0000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.8100966235e+05</td>
<td>2.0000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.4111498127e+05</td>
<td>0.0000000000e+00</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Theory

Sets of response-probability pairs computed with the forward/reverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.

In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

An inverse mapping involves computing the belief and plausibility response level for either a specified probability level or a specified generalized reliability level (two results for each level mapping in the evidence-based epistemic case, instead of the one result for each level mapping in the aleatory case).

num_probability_levels
CHAPTER 6. KEYWORDS AREA

• Keywords Area
• method
• pof_darts
• probability_levels
• num_probability_levels

Specify which probability_levels correspond to which response

**Specification**

**Alias**: none

**Argument(s)**: INTEGERLIST

**Default**: probability_levels evenly distributed among response functions

**Description**

See parent page

**gen_reliability_levels**

• Keywords Area
• method
• pof_darts
• gen_reliability_levels

Specify generalized reliability levels at which to estimate the corresponding response value

**Specification**

**Alias**: none

**Argument(s)**: REALLIST

**Default**: No CDF/CCDF response levels to compute

<table>
<thead>
<tr>
<th>Required-/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>num_gen_reliability_levels</td>
<td></td>
<td>Specify which gen_reliability_levels correspond to which response</td>
</tr>
</tbody>
</table>

**Description**

Response levels are calculated for specified generalized reliabilities by indexing into a sorted samples array (the response levels computed are not interpolated and will correspond to one of the sampled values).
6.2. METHOD

Theory
Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.

In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

An inverse mapping involves computing the belief and plausibility response level for either a specified probability level or a specified generalized reliability level (two results for each level mapping in the evidence-based epistemic case, instead of the one result for each level mapping in the aleatory case).

num_gen_reliability_levels

- Keywords Area
- method
- pof_darts
- gen_reliability_levels
- num_gen_reliability_levels

Specify which gen_reliability_levels correspond to which response

Specification
Alias: none

Argument(s): INTEGERLIST
Default: gen_reliability_levels evenly distributed among response functions

Description
See parent page

rng

- Keywords Area
- method
- pof_darts
- rng

Selection of a random number generator

Specification
Alias: none

Argument(s): none
Default: Mersenne twister ( mt19937 )
<table>
<thead>
<tr>
<th>Required/Optional Required (Choose One)</th>
<th>Description of Group Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>mt19937</td>
<td>Generates random numbers using the Mersenne twister</td>
</tr>
<tr>
<td></td>
<td></td>
<td>rnum2</td>
<td>Generates pseudo-random numbers using the Pecos package</td>
</tr>
</tbody>
</table>

**Description**

The `rng` keyword is used to indicate a choice of random number generator.

**Default Behavior**

If specified, the `rng` keyword must be accompanied by either `rnum2` (pseudo-random numbers) or `mt19937` (random numbers generated by the Mersenne twister). Otherwise, `mt19937`, the Mersenne twister is used by default.

**Usage Tips**

The default is recommended, as the Mersenne twister is a higher quality random number generator.

**Examples**

```plaintext
method
  sampling
    sample_type lhs
    samples = 10
    seed = 98765
    rng rnum2
```

**mt19937**

- Keywords Area
- method
- pof_darts
- rng
- mt19937

Generates random numbers using the Mersenne twister

**Specification**

**Alias:** none

**Argument(s):** none
6.2. METHOD

Description

The mt19937 keyword directs Dakota to use the Mersenne twister to generate random numbers. Additional information can be found on wikipedia: http://en.wikipedia.org/wiki/Mersenne_twister.

Default Behavior

mt19937 is the default random number generator. To specify it explicitly in the Dakota input file, however, it must be specified in conjunction with the rng keyword.

Usage Tips

Use of the Mersenne twister random number generator (mt19937) is recommended.

Examples

method
  sampling
    sample_type lhs
    samples = 10
    seed = 98765
    rng mt19937

rnum2

  • Keywords Area
  • method
  • pof_darts
  • rng
  • rnum2

  Generates pseudo-random numbers using the Pecos package

Specification

Alias: none

Argument(s): none

Description

The rnum2 keyword directs Dakota to use pseudo-random numbers generated by the Pecos package.

Default Behavior

rnum2 is not used by default. To change this behavior, it must be specified in conjunction with the rng keyword.

Usage Tips

Use of the Mersenne twister random number generator (mt19937) is recommended over rnum2.

Examples

method
  sampling
    sample_type lhs
    samples = 10
    seed = 98765
    rng rnum2


model_pointer

- Keywords Area
- method
- pof_darts
- model_pointer

Identifier for model block to be used by a method

**Topics**

This keyword is related to the topics:
- block_pointer

**Specification**

**Alias:** none

**Argument(s):** STRING

**Default:** method use of last model parsed (or use of default model if none parsed)

**Description**

The `model_pointer` is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

**Default Behavior**

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding `id_model` with the same name.

**Usage Tips**

When doing advanced analyses that involve using multiple methods and multiple models, defining a `model_pointer` for each method is imperative.

See `block_pointer` for details about pointers.

**Examples**

```plaintext
environment
  tabular_graphics_data
  method_pointer = 'UQ'

method
  id_method = 'UQ'
  model_pointer = 'SURR'
  sampling,
    samples = 10
    seed = 98765 rng rnum2
    response_levels = 0.1 0.2 0.6
    0.1 0.2 0.6
      0.1 0.2 0.6
  sample_type lhs
  distribution cumulative

model
  id_model = 'SURR'
```

6.2. METHOD

surrogate global,
dace_method_pointer = ‘DACE’
polynomial quadratic

method
id_method = ‘DACE’
model_pointer = ‘DACE_M’
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = ‘DACE_M’
single
interface_pointer = ‘I1’

variables
uniform_uncertain = 2
lower_bounds = 0. 0.
upper_bounds = 1. 1.
descriptors = ‘x1’ ‘x2’

interface
id_interface = ‘I1’
system asynch evaluation_concurrency = 5
analysis_driver = ‘text_book’

responses
response_functions = 3
no_gradients
no_hessians

6.2.56 rkd_darts

- Keywords Area
- method
- rkd_darts

Recursive k-d (RKD) Darts: Recursive Hyperplane Sampling for Numerical Integration of High-Dimensional Functions.

Topics
This keyword is related to the topics:

- uncertainty_quantification

Specification
Alias: nond_rkd_darts
Argument(s): none
<table>
<thead>
<tr>
<th>Required</th>
<th>build_samples</th>
<th>Number of initial model evaluations used in build phase</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>seed</td>
<td>Seed of the random number generator</td>
</tr>
<tr>
<td>Optional</td>
<td>lipschitz</td>
<td>Undocumented: Recursive k-d (RKD) Darts is an experimental capability.</td>
</tr>
<tr>
<td>Optional</td>
<td>samples_on_emulator</td>
<td>Number of samples at which to evaluate an emulator (surrogate)</td>
</tr>
<tr>
<td>Optional</td>
<td>response_levels</td>
<td>Undocumented: Recursive k-d (RKD) Darts is an experimental capability.</td>
</tr>
<tr>
<td>Optional</td>
<td>distribution</td>
<td>Undocumented: Recursive k-d (RKD) Darts is an experimental capability.</td>
</tr>
<tr>
<td>Optional</td>
<td>probability_levels</td>
<td>Undocumented: Recursive k-d (RKD) Darts is an experimental capability.</td>
</tr>
<tr>
<td>Optional</td>
<td>gen_reliability_levels</td>
<td>Undocumented: Recursive k-d (RKD) Darts is an experimental capability.</td>
</tr>
<tr>
<td>Optional</td>
<td>rng</td>
<td>Undocumented: Recursive k-d (RKD) Darts is an experimental capability.</td>
</tr>
</tbody>
</table>
6.2. METHOD

<table>
<thead>
<tr>
<th>Optional</th>
<th>model_pointer</th>
<th>Identifier for model block to be used by a method</th>
</tr>
</thead>
</table>

**Description**

Disclaimer: The RKD method is currently in development mode, for further experimental verification. Please contact Dakota team if you have further questions about using this method.

Recursive k-d (RKD) darts is an algorithm to evaluate the integration of a d-dimensional black box function \( f(x) \) via recursive sampling over \( d \), using a series of hyperplanes of variable dimensionality \( k = \{d, d-1, \ldots, 0\} \). Fundamentally, we decompose the d-dimensional integration problem into a series of nested one-dimensional problems. That is, we start at the root level (the whole domain) and start sampling down using hyperplanes of one lower dimension, all the way down to zero (points). A d-dimensional domain is subsampled using \( (d-1) \) hyperplanes, a \( (d-1) \)-dimensional sub-domain is subsampled using \( (d-2) \) hyperplanes, and so on. Every hyperplane, regardless of its dimension, is evaluated using sampled hyperplanes of one lower dimension, as shown in the set of figures above. Each hyperplane has direct information exchange with its parent hyperplane of one higher dimension, and its children of one lower dimension.

In each one-dimensional problem, we construct a piecewise approximation surrogate model, using 1-dimensional Lagrange interpolation. Information is exchanged between different levels, including integration values, as well as interpolation and evaluation errors, in order to a) find the integration value up to that level, b) estimate the associated integration error, and c) guide the placement of future samples.

**build_samples**

- **Keywords Area**
- **method**
- **rkd_darts**
- **build_samples**

Number of initial model evaluations used in build phase

**Specification**

**Alias:** samples

**Argument(s):** INTEGER

**Description**

The number of build points or training points used in the initial phase of an algorithm or model construction. Typically these are the initial set of data points used to construct (train) a surrogate model (emulator). If the number of **build_samples** is less than the minimum number of points required to build the surrogate, Dakota will augment the samples to obtain the minimum required.

**Examples**

Perform GP-based adaptive importance sampling, building the GP with 100 points and then performing 100 approximate evaluations to evaluate the probability.
**seed**

- **Keywords Area**
- **method**
- **rkd_darts**
- **seed**

Seed of the random number generator

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** system-generated (non-repeatable)

**Description**

The random seed control provides a mechanism for making a stochastic method repeatable. That is, the use of the same random seed in identical studies will generate identical results.

**Default Behavior**

If not specified, the seed is randomly generated.

**Expected Output**

If `seed` is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

**Usage Tips**

If a stochastic study was run without `seed` specified, and the user later wishes to repeat the study using the same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen. That value can then be added to the Dakota input file.

**Examples**

```
method
    sampling
    sample_type lhs
    samples = 10
    seed = 15347
```

**lipschitz**

- **Keywords Area**
- **method**
- **rkd_darts**
Undocumented: Recursive k-d (RKD) Darts is an experimental capability.

### Specification

**Alias:** none  
**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/-Optional Required (Choose One)</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
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<tbody>
<tr>
<td>local</td>
<td></td>
<td>local</td>
<td>Undocumented: Recursive k-d (RKD) Darts is an experimental capability.</td>
</tr>
<tr>
<td>global</td>
<td></td>
<td>global</td>
<td>Undocumented: Recursive k-d (RKD) Darts is an experimental capability.</td>
</tr>
</tbody>
</table>

**local**

- Keywords Area
- method
- rkd_darts
- lipschitz
- local

Undocumented: Recursive k-d (RKD) Darts is an experimental capability.

### Specification

**Alias:** none  
**Argument(s):** none

**global**

- Keywords Area
- method
- rkd_darts
- lipschitz
- global

Undocumented: Recursive k-d (RKD) Darts is an experimental capability.
**Specification**

**Alias:** none

**Argument(s):** none

**samples_on_emulator**

- **Keywords Area**
- **method**
- **rkd_darts**
- **samples_on_emulator**

Number of samples at which to evaluate an emulator (surrogate)

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Description**

How many approximate function evaluations to perform on the emulator model, e.g., to compute statistics

**Default Behavior**

The default number of samples is method-dependent.

**Examples**

Perform 10000 samples on the PCE approximation of the true model:

```
method
    polynomial_chaos
        quadrature_order = 2
        samples_on_emulator = 10000
```

**response_levels**

- **Keywords Area**
- **method**
- **rkd_darts**
- **response_levels**

Undocumented: Recursive k-d (RKD) Darts is an experimental capability.

**Specification**

**Alias:** none

**Argument(s):** REALLIST

**Default:** No CDF/CCDF probabilities/reliabilities to compute
<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<tr>
<td>Optional</td>
<td>response_levels</td>
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<td>Undocumented: Recursive k-d (RKD) Darts is an experimental capability.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>compute</td>
<td></td>
</tr>
</tbody>
</table>

**num_response_levels**
- Keywords Area
- method
- rkd_darts
- response_levels
- num_response_levels

Undocumented: Recursive k-d (RKD) Darts is an experimental capability.

**Specification**

**Alias:** none

**Argument(s):** INTEGERLIST

**Default:** response_levels evenly distributed among response functions

**compute**
- Keywords Area
- method
- rkd_darts
- response_levels
- compute

Undocumented: Recursive k-d (RKD) Darts is an experimental capability.

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** probabilities
### Dakota Keyword Description

**Required/Optional:** Required (Choose One)  
**Description of Group:** Group 1  
**Dakota Keyword:** probabilities  
**Dakota Keyword Description:** Undocumented: Recursive k-d (RKD) Darts is an experimental capability.

<table>
<thead>
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<th>Required/Optional</th>
<th>Description of Group</th>
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<tbody>
<tr>
<td>Optional</td>
<td>system</td>
<td>gen_reliabilities</td>
<td>Undocumented: Recursive k-d (RKD) Darts is an experimental capability.</td>
</tr>
</tbody>
</table>

probabilities

- Keywords Area
- method
- rkd_darts
- response_levels
- compute
- probabilities

Undocumented: Recursive k-d (RKD) Darts is an experimental capability.

### Specification

**Alias:** none  
**Argument(s):** none

**gen_reliabilities**

- Keywords Area
- method
- rkd_darts
- response_levels
- compute
- gen_reliabilities

Undocumented: Recursive k-d (RKD) Darts is an experimental capability.
6.2. METHOD

Specification

Alias: none

Argument(s): none

system

- Keywords Area
- method
- rkd_darts
- response_levels
- compute
- system

Undocumented: Recursive k-d (RKD) Darts is an experimental capability.

<table>
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<tr>
<th>Required/-Optional Required (Choose One)</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>series</td>
<td></td>
<td>parallel</td>
<td>Undocumented: Recursive k-d (RKD) Darts is an experimental capability.</td>
</tr>
</tbody>
</table>

series

- Keywords Area
- method
- rkd_darts
- response_levels
- compute
- system
- series

Undocumented: Recursive k-d (RKD) Darts is an experimental capability.
CHAPTER 6. KEYWORDS AREA

Specification
Alias: none

Argument(s): none

parallel

• Keywords Area
• method
• rkd_darts
• response_levels
• compute
• system
• parallel

Undocumented: Recursive k-d (RKD) Darts is an experimental capability.

Specification
Alias: none

Argument(s): none

distribution

• Keywords Area
• method
• rkd_darts
• distribution

Undocumented: Recursive k-d (RKD) Darts is an experimental capability.

Specification
Alias: none

Argument(s): none

Default: cumulative (CDF)

<table>
<thead>
<tr>
<th>Required/-Optional Required (Choose One)</th>
<th>Description of Group 1</th>
<th>Dakota Keyword cumulative</th>
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<tr>
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<td>Undocumented: Recursive k-d (RKD) Darts is an experimental capability.</td>
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<td></td>
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</tbody>
</table>
6.2. METHOD

complementary

Undocumented: Recursive k-d (RKD) Darts is an experimental capability.

Specification

Alias: none

Argument(s): none

complementary

Undocumented: Recursive k-d (RKD) Darts is an experimental capability.

Specification

Alias: none

Argument(s): none

probability_levels

Undocumented: Recursive k-d (RKD) Darts is an experimental capability.
**Specification**

Alias: none

Argument(s): REALLIST

Default: No CDF/CCDF response levels to compute

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>num_probability_levels</td>
<td></td>
<td></td>
<td>Undocumented: Recursive k-d (RKD) Darts is an experimental capability.</td>
</tr>
</tbody>
</table>

**num_probability_levels**

- Keywords Area
- method
- rkd_darts
- probability_levels
- num_probability_levels

Undocumented: Recursive k-d (RKD) Darts is an experimental capability.

**Specification**

Alias: none

Argument(s): INTEGERLIST

Default: probability_levels evenly distributed among response functions

**gen_reliability_levels**

- Keywords Area
- method
- rkd_darts
- gen_reliability_levels

Undocumented: Recursive k-d (RKD) Darts is an experimental capability.

**Specification**

Alias: none

Argument(s): REALLIST

Default: No CDF/CCDF response levels to compute


6.2. METHOD  

| Required/- | Description of Group | Dakota Keyword     | Dakota Keyword Description |
| Optional   |                      | num_gen_reliability_levels | Undocumented: Recursive k-d (RKD) Darts is an experimental capability. |

num_gen_reliability_levels

- Keywords Area
- method
- rkd_darts
- gen_reliability_levels
- num_gen_reliability_levels

Undocumented: Recursive k-d (RKD) Darts is an experimental capability.

Specification

**Alias:** none

**Argument(s):** INTEGERLIST

**Default:** gen_reliability_levels evenly distributed among response functions

rng

- Keywords Area
- method
- rkd_darts
- rng

Undocumented: Recursive k-d (RKD) Darts is an experimental capability.

Specification

**Alias:** none

**Argument(s):** none

**Default:** Mersenne twister ( mt19937 )
<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional Requirement (Choose One)</td>
<td></td>
<td>mt19937</td>
<td>Undocumented: Recursive k-d (RKD) Darts is an experimental capability.</td>
</tr>
<tr>
<td>undoc</td>
<td></td>
<td>rnum2</td>
<td>Undocumented: Recursive k-d (RKD) Darts is an experimental capability.</td>
</tr>
</tbody>
</table>

**mt19937**
- Keywords Area
- method
- rkd_darts
- rng
- mt19937

Undocumented: Recursive k-d (RKD) Darts is an experimental capability.

**Specification**
Alias: none
Argument(s): none

**rnum2**
- Keywords Area
- method
- rkd_darts
- rng
- rnum2

Undocumented: Recursive k-d (RKD) Darts is an experimental capability.

**Specification**
Alias: none
Argument(s): none
6.2. METHOD

**model_pointer**

- **Keywords Area**
- **method**
- **rkd_darts**
- **model_pointer**

Identifier for model block to be used by a method

**Topics**

This keyword is related to the topics:

- **block_pointer**

**Specification**

**Alias:** none

**Argument(s):** STRING

**Default:** method use of last model parsed (or use of default model if none parsed)

**Description**

The `model_pointer` is used to specify which `model` block will be used to perform the function evaluations needed by the Dakota method.

**Default Behavior**

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a `model` block in the Dakota input file that has a corresponding `id_model` with the same name.

**Usage Tips**

When doing advanced analyses that involve using multiple methods and multiple models, defining a `model_pointer` for each method is imperative.

See `block_pointer` for details about pointers.

**Examples**

```plaintext
environment
tabular_graphics_data
method_pointer = 'UQ'

method
id_method = 'UQ'
model_pointer = 'SURR'
sampling,
samples = 10
seed = 98765 rng rnum2
response_levels = 0.1 0.2 0.6 0.1 0.2 0.6
sample_type lhs
distribution cumulative

model
id_model = 'SURR'
```
surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
id_method = 'DACE'
model_pointer = 'DACE_M'
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = 'DACE_M'
single
interface_pointer = 'I1'

variables
uniform_uncertain = 2
lower_bounds = 0.0
upper_bounds = 1.0
descriptors = 'x1' 'x2'

interface
id_interface = 'I1'
-system asynch evaluation_concurrency = 5
-analysis_driver = 'text_book'

responses
response_functions = 3
no_gradients
no_hessians

6.2.57 global_evidence

- Keywords Area
- method
- global_evidence

Evidence theory with evidence measures computed with global optimization methods

Topics

This keyword is related to the topics:

- epistemic_uncertainty_quantification_methods
- evidence_theory

Specification

Alias: nond_global_evidence

Argument(s): none
### 6.2. METHOD

<table>
<thead>
<tr>
<th>Optional</th>
<th>samples</th>
<th>Number of samples for sampling-based methods</th>
</tr>
</thead>
<tbody>
<tr>
<td>seed</td>
<td>seed</td>
<td>Seed of the random number generator</td>
</tr>
<tr>
<td>sbo</td>
<td>sbo</td>
<td>Use the surrogate based optimization method</td>
</tr>
<tr>
<td>ego</td>
<td>ego</td>
<td>Use the Efficient Global Optimization method</td>
</tr>
<tr>
<td>ea</td>
<td>ea</td>
<td>Use an evolutionary algorithm</td>
</tr>
<tr>
<td>lhs</td>
<td>lhs</td>
<td>Uses Latin Hypercube Sampling (LHS) to sample variables</td>
</tr>
<tr>
<td>response_levels</td>
<td>response_levels</td>
<td>Values at which to estimate desired statistics for each response</td>
</tr>
<tr>
<td>distribution</td>
<td>distribution</td>
<td>Selection of cumulative or complementary cumulative functions</td>
</tr>
<tr>
<td>probability_levels</td>
<td>probability_levels</td>
<td>Specify probability levels at which to estimate the corresponding response value</td>
</tr>
<tr>
<td>gen_reliability_levels</td>
<td>gen_reliability_levels</td>
<td>Specify generalized reliability levels at which to estimate the corresponding response value</td>
</tr>
</tbody>
</table>
CHAPTER 6. KEYWORDS AREA

| Optional | rng            | Selection of a random number generator |
| Optional | model_pointer | Identifier for model block to be used by a method |

**Description**

`global_evidence` allows the user to specify several global approaches for calculating the belief and plausibility functions:

- **lhs** - note: this takes the minimum and maximum of the samples as the bounds per "interval cell combination."
- **ego** - uses Efficient Global Optimization which is based on an adaptive Gaussian process surrogate.
- **sbo** - uses a Gaussian process surrogate (non-adaptive) within an optimization process.
- **ea** - uses an evolutionary algorithm. This can be expensive as the ea will be run for each interval cell combination.

Note that to calculate the plausibility and belief cumulative distribution functions, one has to look at all combinations of intervals for the uncertain variables. In terms of implementation, if one is using LHS sampling as outlined above, this method creates a large sample over the response surface, then examines each cell to determine the minimum and maximum sample values within each cell. To do this, one needs to set the number of samples relatively high: the default is 10,000 and we recommend at least that number. If the model you are running is a simulation that is computationally quite expensive, we recommend that you set up a surrogate model within the Dakota input file so that `global_evidence` performs its sampling and calculations on the surrogate and not on the original model. If one uses optimization methods instead to find the minimum and maximum sample values within each cell, this can also be computationally expensive.

**Additional Resources**

See the topic page `evidence_theory` for important background information and usage notes.

Refer to `variable_support` for information on supported variable types.

**Theory**

The basic idea is that one specifies an "evidence structure” on uncertain inputs and propagates that to obtain belief and plausibility functions on the response functions. The inputs are defined by sets of intervals and Basic Probability Assignments (BPAs). Evidence propagation is computationally expensive, since the minimum and maximum function value must be calculated for each "interval cell combination.” These bounds are aggregated into belief and plausibility.

**See Also**

These keywords may also be of interest:

- `global_interval_est`
- `local_evidence`
- `local_interval_est`
6.2. METHOD

samples

- Keywords Area
- method
- global_evidence
- samples

Number of samples for sampling-based methods

Specification

Alias: none

Argument(s): INTEGER

Description

The `samples` keyword is used to define the number of samples (i.e., randomly chosen sets of variable values) at which to execute a model.

Default Behavior

By default, Dakota will use the minimum number of samples required by the chosen method.

Usage Tips

To obtain linear sensitivities or to construct a linear response surface, at least \( \text{dim}+1 \) samples should be used, where "\( \text{dim} \)" is the number of variables. For sensitivities to quadratic terms or quadratic response surfaces, at least \( (\text{dim}+1)(\text{dim}+2)/2 \) samples are needed. For uncertainty quantification, we recommend at least \( 10^*\text{dim} \) samples. For \text{variance_based_decomp}, we recommend hundreds to thousands of samples. Note that for \text{variance_based_decomp}, the number of simulations performed will be \( N*(\text{dim}+2) \).

Examples

```
method sampling
  sample_type lhs
  samples = 20
```

seed

- Keywords Area
- method
- global_evidence
- seed

Seed of the random number generator

Specification

Alias: none

Argument(s): INTEGER

Default: system-generated (non-repeatable)
Description
The random seed control provides a mechanism for making a stochastic method repeatable. That is, the use of the same random seed in identical studies will generate identical results.

Default Behavior
If not specified, the seed is randomly generated.

Expected Output
If seed is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

Usage Tips
If a stochastic study was run without seed specified, and the user later wishes to repeat the study using the same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen. That value can then be added to the Dakota input file.

Examples
method
  sampling
    sample_type lhs
    samples = 10
    seed = 15347

sbo
- Keywords Area
- method
- global_evidence
- sbo

Use the surrogate based optimization method

Specification
Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>Group</td>
<td>gaussian_process</td>
<td>Description</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>use_derivatives</td>
<td>Gaussian Process</td>
</tr>
</tbody>
</table>

|                      |                      | surrogate model | surrogate models |
6.2. METHOD

Optional  

<table>
<thead>
<tr>
<th></th>
<th>import_build-points_file</th>
<th>File containing points you wish to use to build a surrogate</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>export_approx-points_file</td>
<td>Output file for evaluations of a surrogate model</td>
</tr>
</tbody>
</table>

Description

A surrogate-based optimization method will be used. The surrogate employed in sbo is a Gaussian process surrogate.

The main difference between ego and the sbo approach is the objective function being optimized. ego relies on an expected improvement function, while in sbo, the optimization proceeds using an evolutionary algorithm (coliny_ea) on the Gaussian process surrogate: it is a standard surrogate-based optimization. Also note that the sbo option can support optimization over discrete variables (the discrete variables are relaxed) while ego cannot. This is not the same as surrogate_based_global.

**gaussian_process**

- Keywords Area
- method
- global_evidence
- sbo
- gaussian_process

Gaussian Process surrogate model

Specification

**Alias:** kriging  
**Argument(s):** none  
**Default:** Surfpack Gaussian process
CHAPTER 6. KEYWORDS AREA

Select the built-in Gaussian Process surrogate

dakota

Description

Use the Gaussian process (GP) surrogate from Surfpack, which is specified using the `surfpack` keyword.

An alternate version of GP surrogates was available in prior versions of Dakota. **For now, both versions are supported but the dakota version is deprecated and intended to be removed in a future release.**

**Known Issue:** When using discrete variables, there have been sometimes significant differences in surrogate behavior observed across computing platforms in some cases. The cause has not yet been fully diagnosed and is currently under investigation. In addition, guidance on appropriate construction and use of surrogates with discrete variables is under development. In the meantime, users should therefore be aware that there is a risk of inaccurate results when using surrogates with discrete variables.

**surfpack**

- **Keywords Area**
- **method**
- **global.evidence**
- **sbo**
- **gaussian.process**
- **surfpack**

Use the Surfpack version of Gaussian Process surrogates

Specification

Alias: none

**Argument(s):** none

Description

This keyword specifies the use of the Gaussian process that is incorporated in our surface fitting library called Surfpack.

Several user options are available:

1. Optimization methods:

   Maximum Likelihood Estimation (MLE) is used to find the optimal values of the hyper-parameters governing the trend and correlation functions. By default the global optimization method DIRECT is used for MLE, but other options for the optimization method are available. See `optimization_method`.

   The total number of evaluations of the likelihood function can be controlled using the `max_trials` keyword followed by a positive integer. Note that the likelihood function does not require running the "truth" model, and is relatively inexpensive to compute.

2. Trend Function:

   The GP models incorporate a parametric trend function whose purpose is to capture large-scale variations. See `trend`. 
3. Correlation Lengths:
   Correlation lengths are usually optimized by Surfpack, however, the user can specify the lengths manually. See `correlation_lengths`.

4. Ill-conditioning
   One of the major problems in determining the governing values for a Gaussian process or Kriging model is the fact that the correlation matrix can easily become ill-conditioned when there are too many input points close together. Since the predictions from the Gaussian process model involve inverting the correlation matrix, ill-conditioning can lead to poor predictive capability and should be avoided.
   Note that a sufficiently bad sample design could require correlation lengths to be so short that any interpolatory GP model would become inept at extrapolation and interpolation.
   The `surfpack` model handles ill-conditioning internally by default, but behavior can be modified using

5. Gradient Enhanced Kriging (GEK).
   The `use_derivatives` keyword will cause the Surfpack GP to be constructed from a combination of function value and gradient information (if available).
   See notes in the Theory section.

Theory

Gradient Enhanced Kriging
   Incorporating gradient information will only be beneficial if accurate and inexpensive derivative information is available, and the derivatives are not infinite or nearly so. Here “inexpensive” means that the cost of evaluating a function value plus gradient is comparable to the cost of evaluating only the function value, for example gradients computed by analytical, automatic differentiation, or continuous adjoint techniques. It is not cost effective to use derivatives computed by finite differences. In tests, GEK models built from finite difference derivatives were also significantly less accurate than those built from analytical derivatives. Note that GEK’s correlation matrix tends to have a significantly worse condition number than Kriging for the same sample design.
   This issue was addressed by using a pivoted Cholesky factorization of Kriging’s correlation matrix (which is a small sub-matrix within GEK’s correlation matrix) to rank points by how much unique information they contain. This reordering is then applied to whole points (the function value at a point immediately followed by gradient information at the same point) in GEK’s correlation matrix. A standard non-pivoted Cholesky is then applied to the reordered GEK correlation matrix and a bisection search is used to find the last equation that meets the constraint on the (estimate of) condition number. The cost of performing pivoted Cholesky on Kriging’s correlation matrix is usually negligible compared to the cost of the non-pivoted Cholesky factorization of GEK’s correlation matrix. In tests, it also resulted in more accurate GEK models than when pivoted Cholesky or whole-point-block pivoted Cholesky was performed on GEK’s correlation matrix.

`dakota`
- Keywords Area
- method
- global_evidence
- sbo
- gaussian_process
- dakota
Select the built in Gaussian Process surrogate
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none
Argument(s): none

Description

A second version of GP surrogates was available in prior versions of Dakota. **For now, both versions are supported but the dakota version is deprecated and intended to be removed in a future release.**

Historically these models were drastically different, but in Dakota 5.1, they became quite similar. They now differ in that the Surfpack GP has a richer set of features/options and tends to be more accurate than the Dakota version. Due to how the Surfpack GP handles ill-conditioned correlation matrices (which significantly contributes to its greater accuracy), the Surfpack GP can be a factor of two or three slower than Dakota’s. As of Dakota 5.2, the Surfpack implementation is the default in all contexts except Bayesian calibration.

More details on the **gaussian_process** dakota model can be found in [58].

Dakota’s GP deals with ill-conditioning in two ways. First, when it encounters a non-invertible correlation matrix it iteratively increases the size of a “nugget,” but in such cases the resulting approximation smooths rather than interpolates the data. Second, it has a **point_selection** option (default off) that uses a greedy algorithm to select a well-spaced subset of points prior to the construction of the GP. In this case, the GP will only interpolate the selected subset. Typically, one should not need point selection in trust-region methods because a small number of points are used to develop a surrogate within each trust region. Point selection is most beneficial when constructing with a large number of points, typically more than order one hundred, though this depends on the number of variables and spacing of the sample points.

This differs from the **point_selection** option of the Dakota GP which initially chooses a well-spaced subset of points and finds the correlation parameters that are most likely for that one subset.

**use_derivatives**

- **Keywords Area**
- **method**
- **global_evidence**
- **sbo**
- **use_derivatives**

Use derivative data to construct surrogate models

Specification

Alias: none
Argument(s): none
Default: use function values only

Description

The use_derivatives flag specifies that any available derivative information should be used in global approximation builds, for those global surrogate types that support it (currently, polynomial regression and the Surfpack Gaussian process).

However, it’s use with Surfpack Gaussian process is not recommended.
import_build_points_file

- Keywords Area
- method
- global_evidence
- sbo
- import_build_points_file

File containing points you wish to use to build a surrogate

**Specification**

**Alias:** import_points_file  
**Argument(s):** STRING  
**Default:** no point import from a file

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group Tabular Format (Group 1)</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional (Choose One)</td>
<td></td>
<td>annotated</td>
<td>Selects annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>custom.annotated</td>
<td>Selects custom-annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>freeform</td>
<td>Selects freeform file format</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>active_only</td>
<td>Import only active variables from tabular data file</td>
</tr>
</tbody>
</table>

**Description**

The `import_build_points_file` allows the user to specify a file that contains a list of points and truth model responses used to construct a surrogate model. These can be used by all methods that (explicitly, e.g. surrogate-based optimization, or implicitly, e.g. efficient global optimization) operate on a surrogate. In particular, these points and responses are used in place of truth model evaluations to construct the initial surrogate. When used to construct surrogate models or emulators these are often called build points or training data.

**Default Behavior**

By default, methods do not import points from a file.

**Usage Tips**

Dakota parses input files without regard to whitespace, but the `import_build_points_file` must be in one of three formats:

- annotated (default)
- custom.annotated
- freeform
Examples

method
  polynomial_chaos
    expansion_order = 4
    import_build_points_file = 'dakota_uq_rosenbrock_pce_import.annot.pts.dat'

annotated
  - Keywords Area
  - method
  - global_evidence
  - sbo
  - import_build_points_file
  - annotated

Selects annotated tabular file format

Topics

This keyword is related to the topics:
  - file_formats

Specification

Alias: none
  Argument(s): none
  Default: annotated format

Description

An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior

By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips

- To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify custom_annotated header eval_id

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.
6.2. METHOD

Examples
Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```python
environment
tabular_data
  tabular_data_file = 'dakota_summary.dat'
annotated

Resulting tabular file:

<table>
<thead>
<tr>
<th>eval_id</th>
<th>interface</th>
<th>x1</th>
<th>x2</th>
<th>obj_fn</th>
<th>nln_ineq_con_1</th>
<th>nln_ineq_con_2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>NO_ID</td>
<td>0.9</td>
<td>1.1</td>
<td>0.0002</td>
<td>0.26</td>
<td>0.76</td>
</tr>
<tr>
<td>2</td>
<td>NO_ID</td>
<td>0.90009</td>
<td>1.1</td>
<td>0.0001996404857</td>
<td>0.2601620081</td>
<td>0.759955</td>
</tr>
<tr>
<td>3</td>
<td>NO_ID</td>
<td>0.89991</td>
<td>1.1</td>
<td>0.0002003604863</td>
<td>0.2598380081</td>
<td>0.760045</td>
</tr>
<tr>
<td>...</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

custom_annotated

- Keywords Area
- method
- global_evidence
- sbo
- import_build_points_file
- custom_annotated
  Selects custom-annotated tabular file format

Topics
This keyword is related to the topics:

- file_formats

Specification
Alias: none
Argument(s): none
Default: annotated format

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword header</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td></td>
<td>Enable header row in custom-annotated tabular file</td>
</tr>
</tbody>
</table>
Description
A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

Default Behavior
The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

Usage Tips
- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples
Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:

```
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
custom_annotated header eval_id
```

Resulting tabular file:

```
%eval_id x1 x2 obj_fn nln_ineq_con_1 nln_ineq_con_2
1 0.9 1.1 0.0002 0.26 0.76
2 0.90009 1.1 0.0001996404857 0.2601620081 0.759955
3 0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...```

header
- Keywords Area
- method
- global_evidence
6.2. METHOD

- sbo
- import_build_points_file
- custom_annotated
- header

Enable header row in custom-annotated tabular file

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no header

**Description**

See description of parent `custom_annotated`

**eval_id**

- Keywords Area
- method
- global_evidence
- sbo

- import_build_points_file
- custom_annotated

- **eval_id**

Enable evaluation ID column in custom-annotated tabular file

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no eval_id column

**Description**

See description of parent `custom_annotated`
interface_id

- Keywords Area
- method
- global_evidence
- sbo
- import_build_points_file
- custom.annotated
- interface_id

Enable interface ID column in custom-annotated tabular file

**Specification**

*Alias:* none

*Argument(s):* none

*Default:* no interface_id column

**Description**

See description of parent `custom.annotated`

**freeform**

- Keywords Area
- method
- global_evidence
- sbo
- import_build_points_file
- freeform

Selects freeform file format

**Topics**

This keyword is related to the topics:

- file.formats

**Specification**

*Alias:* none

*Argument(s):* none

*Default:* annotated format
6.2. METHOD

Description

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior

The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips

• Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.

• When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

• In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).

• Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
freeform```

Resulting tabular file:

```
0.9 1.1 0.0002 0.26 0.76
0.90009 1.1 0.0001996404857 0.2601620081 0.759955
0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...
```

active_only

• Keywords Area

• method

• global_evidence

• sbo

• import_build_points_file

• active_only

Import only active variables from tabular data file

Topics

This keyword is related to the topics:

• file_formats
**Specification**

**Alias:** none

**Argument(s):** none

**Description**

By default, files for tabular data imports are expected to contain columns for all variables, active and inactive. The keyword `active_only` indicates that the file to import contains only the active variables.

This option should only be used in contexts where the inactive variables have no influence, for example, building a surrogate over active variables, with the state variables held at nominal. It should not be used in more complex nested contexts, where the values of inactive variables are relevant to the function evaluations used to build the surrogate.

**export_approx_points_file**

- **Keywords Area**
- **method**
- **global_evidence**
- **sbo**
- **export_approx_points_file**

Output file for evaluations of a surrogate model

**Specification**

**Alias:** `export_points_file`

**Argument(s):** STRING

**Default:** no point export to a file

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Optional (Choose One)</strong></td>
<td><strong>Tabular Format (Group 1)</strong></td>
<td>annotated</td>
<td>Selects annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>custom_annotated</td>
<td>Selects custom-annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>freeform</td>
<td>Selects freeform file format</td>
</tr>
</tbody>
</table>

**Description**

The `export_approx_points_file` keyword allows the user to specify a file in which the points (input variable values) at which the surrogate model is evaluated and corresponding response values computed by the surrogate model will be written. The response values are the surrogate’s predicted approximation to the truth model responses at those points.
6.2. METHOD

Usage Tips
Dakota exports tabular data in one of three formats:
- annotated (default)
- custom.annotated
- freeform

annotated
- Keywords Area
- method
- global.evidence
- sbo
- export_approx_points_file
- annotated
  Selects annotated tabular file format

Topics
This keyword is related to the topics:
- file_formats

Specification
Alias: none
  Argument(s): none
  Default: annotated format

Description
An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

  Default Behavior
  By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

  Usage Tips
  - To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify custom.annotated header eval_id
  - Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
  - When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
  - Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.
Examples
Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```python
environment
    tabular_data
        tabular_data_file = 'dakota_summary.dat'
annotated
```

Resulting tabular file:

<table>
<thead>
<tr>
<th>%eval_id</th>
<th>interface</th>
<th>x1</th>
<th>x2</th>
<th>obj_fn</th>
<th>nln_ineq_con_1</th>
<th>nln_ineq_con_2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>NO_ID</td>
<td>0.9</td>
<td>1.1</td>
<td>0.0002</td>
<td>0.26</td>
<td>0.76</td>
</tr>
<tr>
<td>2</td>
<td>NO_ID</td>
<td>0.90009</td>
<td>1.1</td>
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<td>0.759955</td>
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<td>1.1</td>
<td>0.0002003604863</td>
<td>0.2598380081</td>
<td>0.760045</td>
</tr>
<tr>
<td>...</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

custom.annotated
• Keywords Area
• method
• global.evidence
• sbo
• export_approx_points_file
• custom.annotated

Selects custom-annotated tabular file format

Topics
This keyword is related to the topics:

• file_formats

Specification
Alias: none
Argument(s): none
Default: annotated format

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>header</td>
<td></td>
<td>Enable header row in custom-annotated tabular file</td>
</tr>
</tbody>
</table>
6.2. METHOD

<table>
<thead>
<tr>
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<th>eval_id</th>
<th>Enable evaluation ID column in custom-annotated tabular file</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>interface_id</td>
<td>Enable interface ID column in custom-annotated tabular file</td>
</tr>
</tbody>
</table>

**Description**

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

**Default Behavior**

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

**Usage Tips**

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

**Examples**

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
custom_annotated header eval_id
```

Resulting tabular file:

```plaintext
%eval_id  x1  x2  obj_fn nln_ineq_con_1 nln_ineq_con_2
1  0.9  1.1  0.0002  0.26  0.76
2  0.90009  1.1  0.0001996404857  0.2601620081  0.759955
3  0.89991  1.1  0.0002003604863  0.2598380081  0.760045
...
```

**header**

- **Keywords Area**

- **method**

- **global_evidence**
CHAPTER 6. KEYWORDS AREA

- sbo
- export_approx_points_file
- custom.annotated
- header

Enable header row in custom-annotated tabular file

**Specification**

Alias: none

Argument(s): none

Default: no header

**Description**

See description of parent custom.annotated

eval_id

- Keywords Area
- method
- global_evidence
- sbo
- export_approx_points_file
- custom.annotated
- eval_id

Enable evaluation ID column in custom-annotated tabular file

**Specification**

Alias: none

Argument(s): none

Default: no eval_id column

**Description**

See description of parent custom.annotated
6.2. METHOD

interface_id

- Keywords Area
- method
- global_evidence
- sbo
- export_approx_points_file
- custom.annotated
- interface_id

Enable interface ID column in custom-annotated tabular file

Specification

Alias: none
Argument(s): none
Default: no interface_id column

Description

See description of parent custom.annotated

freeform

- Keywords Area
- method
- global_evidence
- sbo
- export_approx_points_file
- freeform

Selects freeform file format

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none
Argument(s): none
Default: annotated format
Description

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior

The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips

- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```
environment
  tabular_data
  tabular_data_file = 'dakota_summary.dat'
  freeform
```

Resulting tabular file:

```
0.9 1.1 0.0002 0.26 0.76
0.90009 1.1 0.0001996404857 0.2601620081 0.759955
0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...```

ego

- Keywords Area
- method
- global_evidence
- ego

Use the Efficient Global Optimization method

Specification

Alias: none

Argument(s): none
### 6.2. METHOD

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>gaussian_process</td>
<td>Gaussian Process surrogate model</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>use_derivatives</td>
<td>Use derivative data to construct surrogate models</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>import_build_-points_file</td>
<td>File containing points you wish to use to build a surrogate</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>export_approx_-points_file</td>
<td>Output file for evaluations of a surrogate model</td>
</tr>
</tbody>
</table>

**Description**

In the case of `ego`, the efficient global optimization (EGO) method is used to calculate bounds. By default, the Surfpack GP (Kriging) model is used, but the Dakota implementation may be selected instead. If `use_derivatives` is specified the GP model will be built using available derivative data (Surfpack GP only). See `efficient.global` for more information.

**gaussian_process**

- **Keywords Area**
- **method**
- **global_evidence**
- **ego**
- **gaussian_process**

Gaussian Process surrogate model

**Specification**

**Alias:** kriging  
**Argument(s):** none  
**Default:** Surfpack Gaussian process

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
</table>
Description

Use the Gaussian process (GP) surrogate from Surfpack, which is specified using the surfpack keyword.

An alternate version of GP surrogates was available in prior versions of Dakota. **For now, both versions are supported but the dakota version is deprecated and intended to be removed in a future release.**

Known Issue: When using discrete variables, there have been sometimes significant differences in surrogate behavior observed across computing platforms in some cases. The cause has not yet been fully diagnosed and is currently under investigation. In addition, guidance on appropriate construction and use of surrogates with discrete variables is under development. In the meantime, users should therefore be aware that there is a risk of inaccurate results when using surrogates with discrete variables.

surfpack
- Keywords Area
- method
- global_evidence
- ego
- gaussian_process
- surfpack

Use the Surfpack version of Gaussian Process surrogates

Specification

Alias: none

Argument(s): none

Description

This keyword specifies the use of the Gaussian process that is incorporated in our surface fitting library called Surfpack.

Several user options are available:

1. Optimization methods:

   Maximum Likelihood Estimation (MLE) is used to find the optimal values of the hyper-parameters governing the trend and correlation functions. By default the global optimization method DIRECT is used for MLE, but other options for the optimization method are available. See optimization_method.

   The total number of evaluations of the likelihood function can be controlled using the max_trials keyword followed by a positive integer. Note that the likelihood function does not require running the "truth" model, and is relatively inexpensive to compute.
2. Trend Function:
The GP models incorporate a parametric trend function whose purpose is to capture large-scale variations. See trend.

3. Correlation Lengths:
Correlation lengths are usually optimized by Surfpack, however, the user can specify the lengths manually. See correlation_lengths.

4. Ill-conditioning
One of the major problems in determining the governing values for a Gaussian process or Kriging model is the fact that the correlation matrix can easily become ill-conditioned when there are too many input points close together. Since the predictions from the Gaussian process model involve inverting the correlation matrix, ill-conditioning can lead to poor predictive capability and should be avoided.

Note that a sufficiently bad sample design could require correlation lengths to be so short that any interpolatory GP model would become inept at extrapolation and interpolation.
The surfpack model handles ill-conditioning internally by default, but behavior can be modified using

5. Gradient Enhanced Kriging (GEK).
The use_derivatives keyword will cause the Surfpack GP to be constructed from a combination of function value and gradient information (if available).
See notes in the Theory section.

Theory

Gradient Enhanced Kriging
Incorporating gradient information will only be beneficial if accurate and inexpensive derivative information is available, and the derivatives are not infinite or nearly so. Here "inexpensive" means that the cost of evaluating a function value plus gradient is comparable to the cost of evaluating only the function value, for example gradients computed by analytical, automatic differentiation, or continuous adjoint techniques. It is not cost effective to use derivatives computed by finite differences. In tests, GEK models built from finite difference derivatives were also significantly less accurate than those built from analytical derivatives. Note that GEK’s correlation matrix tends to have a significantly worse condition number than Kriging for the same sample design.

This issue was addressed by using a pivoted Cholesky factorization of Kriging’s correlation matrix (which is a small sub-matrix within GEK’s correlation matrix) to rank points by how much unique information they contain. This reordering is then applied to whole points (the function value at a point immediately followed by gradient information at the same point) in GEK’s correlation matrix. A standard non-pivoted Cholesky is then applied to the reordered GEK correlation matrix and a bisection search is used to find the last equation that meets the constraint on the (estimate of) condition number. The cost of performing pivoted Cholesky on Kriging’s correlation matrix is usually negligible compared to the cost of the non-pivoted Cholesky factorization of GEK’s correlation matrix. In tests, it also resulted in more accurate GEK models than when pivoted Cholesky or whole-point-block pivoted Cholesky was performed on GEK’s correlation matrix.

dakota

- Keywords Area
- method
- global_evidence
CHAPTER 6. KEYWORDS AREA

- ego
- gaussian_process
- dakota

Select the built in Gaussian Process surrogate

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

A second version of GP surrogates was available in prior versions of Dakota. **For now, both versions are supported but the dakota version is deprecated and intended to be removed in a future release.**

Historically these models were drastically different, but in Dakota 5.1, they became quite similar. They now differ in that the Surfpack GP has a richer set of features/options and tends to be more accurate than the Dakota version. Due to how the Surfpack GP handles ill-conditioned correlation matrices (which significantly contributes to its greater accuracy), the Surfpack GP can be a factor of two or three slower than Dakota’s. As of Dakota 5.2, the Surfpack implementation is the default in all contexts except Bayesian calibration.

More details on the gaussian_process dakota model can be found in[58].

Dakota’s GP deals with ill-conditioning in two ways. First, when it encounters a non-invertible correlation matrix it iteratively increases the size of a “nugget,” but in such cases the resulting approximation smooths rather than interpolates the data. Second, it has a point_selection option (default off) that uses a greedy algorithm to select a well-spaced subset of points prior to the construction of the GP. In this case, the GP will only interpolate the selected subset. Typically, one should not need point selection in trust-region methods because a small number of points are used to develop a surrogate within each trust region. Point selection is most beneficial when constructing with a large number of points, typically more than order one hundred, though this depends on the number of variables and spacing of the sample points.

This differs from the point_selection option of the Dakota GP which initially chooses a well-spaced subset of points and finds the correlation parameters that are most likely for that one subset.

**use_derivatives**

- Keywords Area
- method
- global_evidence
- ego
- use_derivatives

Use derivative data to construct surrogate models

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** use function values only
Description

The `use_derivatives` flag specifies that any available derivative information should be used in global approximation builds, for those global surrogate types that support it (currently, polynomial regression and the Surfpack Gaussian process).

However, it’s use with Surfpack Gaussian process is not recommended.

**import_build_points_file**

- **Keywords Area**
- **method**
- **global_evidence**
- **ego**
- **import_build_points_file**

File containing points you wish to use to build a surrogate

Specification

**Alias:** import_points_file  
**Argument(s):** STRING  
**Default:** no point import from a file

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group Tabular Format (Group 1)</th>
<th>Dakota Keyword annotated</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional/Choose One</td>
<td>custom_annotated</td>
<td>Selects custom-annotated tabular file format</td>
<td></td>
</tr>
<tr>
<td>Optional/active_only</td>
<td>freeform</td>
<td>Selects freeform file format</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>active_only</td>
<td>Import only active variables from tabular data file</td>
<td></td>
</tr>
</tbody>
</table>

Description

The `import_build_points_file` allows the user to specify a file that contains a list of points and truth model responses used to construct a surrogate model. These can be used by all methods that (explicitly, e.g. surrogate-based optimization, or implicitly, e.g. efficient global optimization) operate on a surrogate. In particular, these points and responses are used in place of truth model evaluations to construct the initial surrogate. When used to construct surrogate models or emulators these are often called build points or training data.

**Default Behavior**

By default, methods do not import points from a file.
Usage Tips
Dakota parses input files without regard to whitespace, but the import_build_points_file must be in one of three formats:

- annotated (default)
- custom_annotated
- freeform

Examples

method
  polynomial_chaos
    expansion_order = 4
    import_build_points_file = 'dakota_uq_rosenbrock_pce_import.annot.pts.dat'

annotated

- Keywords Area
- method
- global_evidence
- ego
- import_build_points_file
- annotated

Selects annotated tabular file format

Topics
This keyword is related to the topics:

- file_formats

Specification
Alias: none
  Argument(s): none
  Default: annotated format

Description
An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior
By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips
6.2. METHOD

- To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify `custom_annotated` header `eval_id`.

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```environment
tabular_data
  tabular_data_file = 'dakota_summary.dat'
  annotated
```

Resulting tabular file:

```
%eval_id interface x1  x2  obj_fn nln_ineq_con_1 nln_ineq_con_2
1   NO_ID   0.9  1.1  0.0002  0.26  0.76
2   NO_ID   0.90009  1.1  0.0001996404857  0.2601620081  0.759955
3   NO_ID   0.89991  1.1  0.0002003604863  0.2598380081  0.760045
...
```

- `custom_annotated`

- **Keywords Area**
- method
- global_evidence
- ego
- import_build_points_file
- **custom_annotated**

Selects custom-annotated tabular file format

Topics

This keyword is related to the topics:

- file_formats

Specification

**Alias:** none

**Argument(s):** none

**Default:** annotated format
### Description

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

### Default Behavior

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

### Usage Tips

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

### Examples

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:

```xml
environment
  tabular_data

  tabular_data_file = 'dakota_summary.dat'

  custom_annotated header eval_id
```

Resulting tabular file:

```plaintext
%eval_id  x1     x2     obj_fn  nln_ineq_con_1  nln_ineq_con_2
1         0.9     1.1     0.0002  0.26     0.76
2         0.90009 1.1     0.0001996404857 0.2601620081 0.759955
3         0.89991 1.1     0.0002003604863 0.2598380081 0.760045
...```
6.2. METHOD

header

• Keywords Area
• method
• global_evidence
• ego
• import_build_points_file
• custom_annotated
• header

Enable header row in custom-annotated tabular file

Specification

Alias: none
Argument(s): none
Default: no header

Description

See description of parent custom_annotated

eval_id

• Keywords Area
• method
• global_evidence
• ego
• import_build_points_file
• custom_annotated
• eval_id

Enable evaluation ID column in custom-annotated tabular file

Specification

Alias: none
Argument(s): none
Default: no eval_id column

Description

See description of parent custom_annotated
interface_id

- Keywords Area
- method
- global_evidence
- ego
- import_build_points_file
- custom.annotated
- interface_id

Enable interface ID column in custom-annotated tabular file

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no interface_id column

**Description**

See description of parent custom.annotated

**freeform**

- Keywords Area
- method
- global_evidence
- ego
- import_build_points_file
- freeform

Selects freeform file format

**Topics**

This keyword is related to the topics:

- file_formats

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** annotated format
6.2. **METHOD**

**Description**

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

**Default Behavior**

The annotated format is the default for tabular export/import. To change this behavior, specify `freeform` in the relevant export/import context.

**Usage Tips**

- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though `freeform` remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- In `freeform`, the `num_rows x num_cols` total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the `freeform` option.

**Examples**

Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
freeform
```

Resulting tabular file:

```
0.9 1.1 0.0002 0.26 0.76
0.90009 1.1 0.0001996404857 0.2601620081 0.759955
0.89991 1.1 0.0002003604863 0.2598380081 0.760045
```

**active_only**

- Keywords Area
- method
- global_evidence
- ego
- `import_build_points_file`
- `active_only`

Import only active variables from tabular data file

**Topics**

This keyword is related to the topics:

- `file_formats`
**Specification**

**Alias:** none

**Argument(s):** none

**Description**

By default, files for tabular data imports are expected to contain columns for all variables, active and inactive. The keyword `active_only` indicates that the file to import contains only the active variables.

This option should only be used in contexts where the inactive variables have no influence, for example, building a surrogate over active variables, with the state variables held at nominal. It should not be used in more complex nested contexts, where the values of inactive variables are relevant to the function evaluations used to build the surrogate.

**export_approx_points_file**

- **Keywords Area**
- **method**
- **global_evidence**
- **ego**
- **export_approx_points_file**

Output file for evaluations of a surrogate model

**Specification**

**Alias:** export_points_file

**Argument(s):** STRING

**Default:** no point export to a file

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Optional(Choose One)</strong></td>
<td>Tabular Format (Group 1)</td>
<td>annotated</td>
<td>selects annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>custom_annotated</td>
<td>selects custom-annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>freeform</td>
<td>selects freeform file format</td>
</tr>
</tbody>
</table>

**Description**

The `export_approx_points_file` keyword allows the user to specify a file in which the points (input variable values) at which the surrogate model is evaluated and corresponding response values computed by the surrogate model will be written. The response values are the surrogate’s predicted approximation to the truth model responses at those points.
6.2. METHOD

Usage Tips
Dakota exports tabular data in one of three formats:

- annotated (default)
- custom_annotated
- freeform

annotated
- Keywords Area
- method
- global_evidence
- ego
- export_approx_points_file
- annotated

Selects annotated tabular file format

Topics
This keyword is related to the topics:

- file_formats

Specification

Alias: none

Argument(s): none

Default: annotated format

Description
An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior
By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips

- To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify custom_annotated header eval_id
- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.
Examples
Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```python
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
annotated

Resulting tabular file:

```
%eval_id interface x1 x2 obj_fn nln_ineq_con_1 nln_ineq_con_2
1 NO_ID 0.9 1.1 0.0002 0.26 0.76
2 NO_ID 0.90009 1.1 0.0001996404857 0.2601620081 0.759955
3 NO_ID 0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...
```

custom_annotated

- Keywords Area
- method
- global_evidence
- ego
- export_approx_points_file
- custom_annotated

Selects custom-annotated tabular file format

Topics
This keyword is related to the topics:

- file_formats

Specification
Alias: none
Argument(s): none
Default: annotated format

<p>| Required/- | Description of | Dakota Keyword |</p>
<table>
<thead>
<tr>
<th>Optional</th>
<th>Group</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>header</td>
<td></td>
</tr>
</tbody>
</table>

Dakota Keyword Description
Enable header row in custom-annotated tabular file
6.2. METHOD

<table>
<thead>
<tr>
<th>Optional</th>
<th>eval_id</th>
<th>Enable evaluation ID column in custom-annotated tabular file</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>interface_id</td>
<td>Enable interface ID column in custom-annotated tabular file</td>
</tr>
</tbody>
</table>

### Description

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval\_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

#### Default Behavior

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom\_annotated, followed by options, in the relevant export/import context.

#### Usage Tips

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

### Examples

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval\_id (no interface\_id), and data for variables and responses. Input file fragment:

```plaintext
environment
  tabular_data
      tabular_data_file = 'dakota_summary.dat'
      custom_annotated header eval_id
```

Resulting tabular file:

```
%eval_id  x1  x2  obj_fn  nl_nleq_con_1  nl_nleq_con_2
1  0.9   1.1  0.0002  0.26  0.76
2  0.90009  1.1  0.0001996404857  0.2601620081  0.759955
3  0.89991  1.1  0.0002003604863  0.2598380081  0.760045
...
```

### header
- **Keywords Area**
- **method**
- **global\_evidence**
CHAPTER 6. KEYWORDS AREA

- ego
- export_approx_points_file
- custom.annotated
- header

Enable header row in custom-annotated tabular file

**Specification**

Alias: none

Argument(s): none

Default: no header

**Description**

See description of parent `custom.annotated`

**eval_id**

- Keywords Area
- method
- global_evidence
- ego
- export_approx_points_file
- custom.annotated
- eval_id

Enable evaluation ID column in custom-annotated tabular file

**Specification**

Alias: none

Argument(s): none

Default: no eval_id column

**Description**

See description of parent `custom.annotated`
6.2. METHOD

interface_id
- Keywords Area
- method
- global_evidence
- ego
- export_approx_points_file
- custom.annotated
- interface_id

Enable interface ID column in custom-annotated tabular file

Specification
Alias: none
Argument(s): none
Default: no interface_id column

Description
See description of parent custom.annotated

freeform
- Keywords Area
- method
- global_evidence
- ego
- export_approx_points_file
- freeform

Selects freeform file format

Topics
This keyword is related to the topics:
- file_formats

Specification
Alias: none
Argument(s): none
Default: annotated format
Description

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior

The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips

- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```environment
tabular_data
    tabular_data_file = 'dakota_summary.dat'
    freeform
```

Resulting tabular file:

```
0.9 1.1 0.0002 0.26 0.76
0.90009 1.1 0.0001996404857 0.2601620081 0.759955
0.89991 1.1 0.0002003604863 0.2598380081 0.760045
... 
```

Use an evolutionary algorithm

```
  ea

  - Keywords Area
  - method
  - global_evidence
  - ea
```

Specification

Alias: none

Argument(s): none
6.2. **METHOD**

**Description**

In this approach, the evolutionary algorithm from Coliny, `coliny_ea`, is used to perform the interval optimization with no surrogate model involved. Again, this option of `ea` can support interval optimization over discrete variables.

**lhs**

- **Keywords Area**
- **method**
- **global_evidence**
- **lhs**

Uses Latin Hypercube Sampling (LHS) to sample variables

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

The `lhs` keyword invokes Latin Hypercube Sampling as the means of drawing samples of uncertain variables according to their probability distributions. This is a stratified, space-filling approach that selects variable values from a set of equi-probable bins.

**Default Behavior**

Latin Hypercube Sampling is the default sampling mode in most contexts (exception: multilevel_sampling). To explicitly specify LHS in the Dakota input file, the `lhs` keyword must appear in conjunction with the `sample_type` keyword.

**Usage Tips**

Latin Hypercube Sampling is very robust and can be applied to any problem. It is fairly effective at estimating the mean of model responses and linear correlations with a reasonably small number of samples relative to the number of variables.

**Examples**

```
method sampling
   sample_type lhs
   samples = 20
```

**response_levels**

- **Keywords Area**
- **method**
- **global_evidence**
- **response_levels**

Values at which to estimate desired statistics for each response
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): REALLIST

Default: No CDF/CCDF probabilities/reliabilities to compute

| Required/-| Description of|
| Optional | Dakota Keyword |
| Optional  | num_response_-|
|           | levels        |

<table>
<thead>
<tr>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of values at which to estimate desired statistics for each response</td>
</tr>
</tbody>
</table>

Optional

<table>
<thead>
<tr>
<th>Description of Group</th>
<th>Dakota Keyword</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>compute</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Selection of statistics to compute at each response level</td>
</tr>
</tbody>
</table>

Description

The `response_levels` specification provides the target response values for which to compute probabilities, reliabilities, or generalized reliabilities (forward mapping).

Default Behavior

If `response_levels` are not specified, no statistics will be computed. If they are, probabilities will be computed by default.

Expected Outputs

If `response_levels` are specified, Dakota will create two tables in the standard output: a Probability Density function (PDF) histogram and a Cumulative Distribution Function (CDF) table. The PDF histogram has the lower and upper endpoints of each bin and the corresponding density of that bin. Note that the PDF histogram has bins defined by the `probability_levels` and/or `response_levels` in the Dakota input file. If there are not very many levels, the histogram will be coarse. Dakota does not do anything to optimize the bin size or spacing. The CDF table has the list of response levels and the corresponding probability that the response value is less than or equal to each response level threshold.

Usage Tips

The `num_response_levels` is used to specify which arguments of the `response_level` correspond to which response.

Examples

For example, specifying a `response_level` of 52.3 followed with `compute` probabilities will result in the calculation of the probability that the response value is less than or equal to 52.3, given the uncertain distributions on the inputs.

For an example with multiple responses, the following specification

```plaintext
response_levels = 1. 2. .1 .2 .3 .4 10. 20. 30.
num_response_levels = 2 4 3
```

would assign the first two response levels (1., 2.) to response function 1, the next four response levels (.1, .2, .3, .4) to response function 2, and the final three response levels (10., 20., 30.) to response function 3. If the `num_response_levels` key were omitted from this example, then the response levels would be evenly distributed among the response functions (three levels each in this case).
6.2. METHOD

The Dakota input file below specifies a sampling method with response levels of interest.

```dakota
method,
  sampling,
  samples = 100 seed = 1
  complementary distribution
  response_levels = 3.6e+11 4.0e+11 4.4e+11
  6.0e+04 6.5e+04 7.0e+04
  3.5e+05 4.0e+05 4.5e+05
variables,
  normal_uncertain = 2
    means = 248.89, 593.33
    std_deviations = 12.4, 29.7
    descriptors = 'TF1n' 'TF2n'
  uniform_uncertain = 2
    lower_bounds = 199.3, 474.63
    upper_bounds = 298.5, 712.
    descriptors = 'TF1u' 'TF2u'
  weibull_uncertain = 2
    alphas = 12., 30.
    betas = 250., 590.
    descriptors = 'TF1w' 'TF2w'
  histogram_bin_uncertain = 2
    num_pairs = 3 4
    abscissas = 5 8 10 .1 .2 .3 .4
    counts = 17 21 0 12 24 12 0
    descriptors = 'TF1h' 'TF2h'
  histogram_point_uncertain
    real = 1
    num_pairs = 2
    abscissas = 3 4
    counts = 1 1
    descriptors = 'TF3h'
interface,
  system asynch evaluation_concurrency = 5
  analysis_driver = 'text_book'
responses,
  response_functions = 3
  no_gradients
  no_hessians
```

Given the above Dakota input file, the following excerpt from the output shows the PDF and CCDF generated. Note that the bounds on the bins of the PDF are the response values specified in the input file. The probability levels corresponding to those response values are shown in the CCDF.

```
Probability Density Function (PDF) histograms for each response function:
PDF for response_fn_1:
  Bin Lower     Bin Upper     Density Value
  ------------  ------------  ------------
  2.7604749078e+11  3.6000000000e+11  5.3601733194e-12
  3.6000000000e+11  4.0000000000e+11  4.2500000000e-12
  4.0000000000e+11  4.4000000000e+11  3.7500000000e-12
  4.4000000000e+11  5.419614379e+11  2.2557612778e-12
PDF for response_fn_2:
  Bin Lower     Bin Upper     Density Value
  ------------  ------------  ------------
  4.643154744e+04  6.0000000000e+04  2.8742313192e-05
  6.0000000000e+04  6.5000000000e+04  6.4000000000e-05
  6.5000000000e+04  7.0000000000e+04  4.0000000000e-05
```
PDF for response_fn_3:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.379673709e+05</td>
<td>3.5000000000e+05</td>
<td>4.2844660868e-06</td>
</tr>
<tr>
<td>3.5000000000e+05</td>
<td>4.0000000000e+05</td>
<td>8.6000000000e-06</td>
</tr>
<tr>
<td>4.0000000000e+05</td>
<td>4.5000000000e+05</td>
<td>1.8000000000e-06</td>
</tr>
</tbody>
</table>

Level mappings for each response function:

Complementary Cumulative Distribution Function (CCDF) for response_fn_1:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.6000000000e+11</td>
<td>5.5000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.0000000000e+11</td>
<td>3.8000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.4000000000e+11</td>
<td>2.3000000000e-01</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Complementary Cumulative Distribution Function (CCDF) for response_fn_2:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.0000000000e+04</td>
<td>6.1000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6.5000000000e+04</td>
<td>2.9000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7.0000000000e+04</td>
<td>9.0000000000e-02</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Complementary Cumulative Distribution Function (CCDF) for response_fn_3:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.5000000000e+05</td>
<td>5.2000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.0000000000e+05</td>
<td>9.0000000000e-02</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.5000000000e+05</td>
<td>5.0000000000e-00</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Theory

Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.

In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

A forward mapping involves computing the belief and plausibility probability level for a specified response level.

**num_response_levels**

- Keywords Area
- method
- global_evidence
- response_levels
- num_response_levels

Number of values at which to estimate desired statistics for each response

Specification

Alias: none

**Argument(s):** INTEGERLIST

**Default:** response_levels evenly distributed among response functions
6.2. METHOD

Description

The `num_response_levels` keyword allows the user to specify the number of response values, for each response, at which estimated statistics are of interest. Statistics that can be computed are probabilities and reliabilities, both according to either a cumulative distribution function or a complementary cumulative distribution function.

Default Behavior

If `num_response_levels` is not specified, the `response_levels` will be evenly distributed among the responses.

Expected Outputs

The specific output will be determined by the type of statistics that are specified. In a general sense, the output will be a list of response level-statistic pairs that show the estimated value of the desired statistic for each response level specified.

Examples

```plaintext
method	sampling
    samples = 100
    seed = 34785
    num_response_levels = 1 1 1
    response_levels = 0.5 0.5 0.5
```

compute

- **Keywords Area**
- **method**
- **global evidence**
- **response levels**
- **compute**

Selection of statistics to compute at each response level

Specification

**Alias:** none

**Argument(s):** none

**Default:** probabilities

<table>
<thead>
<tr>
<th>Required/-Optional Required (Choose One)</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>probabilities</td>
<td>Computes probabilities associated with response levels</td>
</tr>
</tbody>
</table>
CHAPTER 6. KEYWORDS AREA

<table>
<thead>
<tr>
<th>gen_reliabilities</th>
<th>Computes generalized reliabilities associated with response levels</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>system</td>
</tr>
<tr>
<td></td>
<td>Compute system reliability (series or parallel)</td>
</tr>
</tbody>
</table>

**Description**

The `compute` keyword is used to select which forward statistical mapping is calculated at each response level.

**Default Behavior**

- If `response_levels` is not specified, no statistics are computed. If `response_levels` is specified but `compute` is not, probabilities will be computed by default. If both `response_levels` and `compute` are specified, then one of the following must be specified: `probabilities`, `reliabilities`, or `gen_reliabilities`.

**Expected Output**

- The type of statistics specified by `compute` will be reported for each response level.

**Usage Tips**

- CDF/CCDF probabilities are calculated for specified response levels using a simple binning approach.
- CDF/CCDF reliabilities are calculated for specified response levels by computing the number of sample standard deviations separating the sample mean from the response level.

**Examples**

```plaintext
method sampling
  sample_type random
  samples = 100 seed = 1
  complementary_distribution
  response_levels = 3.6e+11 4.0e+11 4.4e+11
                   6.0e+04 6.5e+04 7.0e+04
                   3.5e+05 4.0e+05 4.5e+05
  compute reliabilities

probabilities
```

- **Keywords Area**
- **method**
- **global_evidence**
- **response_levels**
- **compute**
- **probabilities**

Computes probabilities associated with response levels
6.2. METHOD

Specification

Alias: none

Argument(s): none

Description

The `probabilities` keyword directs Dakota to compute the probability that the model response will be below (cumulative) or above (complementary cumulative) a specified response value. This is done for every response level designated for each response.

Default Behavior

If `response_levels` is specified, the probabilities are computed by default. To explicitly specify it in the Dakota input file, though, the `probabilities` keyword should be specified in conjunction with the `compute` keyword.

Expected Outputs

The Dakota output is a set of response level-probability pairs that give the probability that the model response will be below or above the corresponding response level, depending on the distribution defined.

Examples

```
method sampling
  sample_type random
  samples = 100 seed = 1
complementary distribution
  response_levels = 3.6e+11 4.0e+11 4.4e+11
                   6.0e+04 6.5e+04 7.0e+04
                   3.5e+05 4.0e+05 4.5e+05
  compute probabilities

gen_reliabilities
```

- Keywords Area
- method
- global_evidence
- response_levels
- compute
- gen_reliabilities

Computes generalized reliabilities associated with response levels

Specification

Alias: none

Argument(s): none
Description

The `gen_reliabilities` keyword directs Dakota to compute generalized reliabilities according to the specified distribution for a specified response value. This is done for every response level designated for each response.

Default Behavior

If `response_levels` is specified, the generalized reliabilities are not computed by default. To change this behavior, the `gen_reliabilities` keyword should be specified in conjunction with the `compute` keyword.

Expected Outputs

The Dakota output is a set of response level-generalized reliability pairs according to the distribution defined.

Examples

```
method
  sampling
    sample_type random
    samples = 100 seed = 1
    complementary distribution
    response_levels = 3.6e+11 4.0e+11 4.4e+11
                    6.0e+04 6.5e+04 7.0e+04
                    3.5e+05 4.0e+05 4.5e+05
    compute gen_reliabilities
```

system

- **Keywords Area**
- **method**
- **global_evidence**
- **response_levels**
- **compute**
- **system**

Compute system reliability (series or parallel)

Specification

Alias: none

Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional Required (Choose One)</th>
<th>Description of Group 1</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>None</td>
<td>Aggregate response statistics assuming a series system</td>
<td>series</td>
</tr>
</tbody>
</table>
6.2. METHOD

**parallel**

| Parallel response statistics assuming a parallel system |

**Description**

With the system probability/reliability option, statistics for specified response levels are calculated and reported assuming the response functions combine either in series or parallel to produce a total system response.

For a series system, the system fails when any one component (response) fails. The probability of failure is the complement of the product of the individual response success probabilities.

For a parallel system, the system fails only when all components (responses) fail. The probability of failure is the product of the individual response failure probabilities.

**series**

- Keywords Area
- method
- global_evidence
- response_levels
- compute
- system
- series

Aggregate response statistics assuming a series system

**Specification**

Alias: none

Argument(s): none

**Description**

See parent keyword system for description.

**parallel**

- Keywords Area
- method
- global_evidence
- response_levels
- compute
- system
• **parallel**

Aggregate response statistics assuming a parallel system

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

See parent keyword `system` for description.

**distribution**

- **Keywords Area**
- **method**
- **global**
- **evidence**
- **distribution**

Selection of cumulative or complementary cumulative functions

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** cumulative (CDF)

<table>
<thead>
<tr>
<th>Required/-Optional Required (Choose One)</th>
<th>Description of Group Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>cumulative</td>
<td>Computes statistics according to cumulative functions</td>
</tr>
<tr>
<td></td>
<td></td>
<td>complementary</td>
<td>Computes statistics according to complementary cumulative functions</td>
</tr>
</tbody>
</table>

**Description**

The `distribution` keyword allows the user to select between a cumulative distribution/belief/plausibility function and a complementary cumulative distribution/belief/plausibility function. This choice affects how probabilities and reliability indices are reported.

**Default Behavior**

If the `distribution` keyword is present, it must be accompanied by either `cumulative` or `complementary`. Otherwise, a cumulative distribution will be used by default.
6.2. METHOD

**Expected Outputs**
Output will be a set of model response-probability pairs determined according to the choice of distribution. The choice of distribution also defines the sign of the reliability or generalized reliability indices.

**Examples**

```plaintext
cumulative

- Keywords Area
- method
- global_evidence
- distribution
- cumulative

Computes statistics according to cumulative functions

**Specification**

**Alias:** none

**Argument(s):** none

**Description**
Statistics on model responses will be computed according to a cumulative distribution/belief/plausibility function.

**Default Behavior**
By default, a cumulative distribution/belief/plausibility function will be used. To explicitly specify it in the Dakota input file, however, the `cumulative` keyword must appear in conjunction with the `distribution` keyword.

**Expected Outputs**
Output will be a set of model response-probability pairs determined according to a cumulative distribution/belief/plausibility function. The probabilities reported are the probabilities that the model response falls below given response thresholds.
CHAPTER 6. KEYWORDS AREA

complementary
• Keywords Area
• method
• global_evidence
• distribution
• complementary
  Computes statistics according to complementary cumulative functions

Specification
Alias: none
Argument(s): none

Description
Statistics on model responses will be computed according to a complementary cumulative distribution/belief/plausibility function.
  Default Behavior
  By default, a complementary cumulative distribution/belief/plausibility function will not be used. To change that behavior, the complementary keyword must be appear in conjunction with the distribution keyword.
  Expected Outputs
  Output will be a set of model response-probability pairs determined according to a complementary cumulative distribution/belief/plausibility function. The probabilities reported are the probabilities that the model response falls above given response threshholds.

Examples
method
  sampling
    sample_type lhs
    samples = 10
    distribution complementary

probability_levels
• Keywords Area
• method
• global_evidence
• probability_levels
  Specify probability levels at which to estimate the corresponding response value

Specification
Alias: none
Argument(s): REALLIST
Default: No CDF/CCDF response levels to compute
6.2. METHOD

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>Group</td>
<td>num_probability_levels</td>
<td>Specify which probability_levels correspond to which response</td>
</tr>
</tbody>
</table>

**Description**

Response levels are calculated for specified CDF/CCDF probabilities by indexing into a sorted samples array (the response levels computed are not interpolated and will correspond to one of the sampled values).

**Expected Output**

If `probability_levels` are specified, Dakota will create two tables in the standard output: a Probability Density function (PDF) histogram and a Cumulative Distribution Function (CDF) table. The PDF histogram has the lower and upper endpoints of each bin and the corresponding density of that bin. Note that the PDF histogram has bins defined by the `probability_levels` and/or `response_levels` in the Dakota input file. If there are not very many levels, the histogram will be coarse. Dakota does not do anything to optimize the bin size or spacing. The CDF table has the list of response levels and the corresponding probability that the response value is less than or equal to each response level threshold.

**Examples**

The Dakota input file below specifies a sampling method with probability levels of interest.

```dakota
method,
sampling,
samples = 100 seed = 1
complementary_distribution
probability_levels = 1. .66 .33 0.
1. .8 .5 0.
1. .3 .2 0.
variables,
normal_uncertain = 2
means = 248.89, 593.33
std_deviations = 12.4, 29.7
descriptors = 'TF1n' 'TF2n'
uniform_uncertain = 2
lower_bounds = 199.3, 474.63
upper_bounds = 298.5, 712.
descriptors = 'TF1u' 'TF2u'
weibull_uncertain = 2
alphas = 12., 30.
betas = 250., 590.
descriptors = 'TF1w' 'TF2w'
histogram_bin_uncertain = 2
num_pairs = 3 4
abscissas = 5 8 10 .1 .2 .3 .4
counts = 17 21 0 12 24 12 0
descriptors = 'TF1h' 'TF2h'
histogram_point_uncertain
real = 1
num_pairs = 2
abscissas = 3 4
counts = 11
descriptors = 'TF3h'
```
interface,
    system async evaluation_concurrency = 5
    analysis_driver = 'text_book'

responses,
    response_functions = 3
    no_gradients
    no_hessians

Given the above Dakota input file, the following excerpt from the output shows the PDF and CCDF generated. Note that the bounds on the bins of the PDF are the response values that correspond the probability levels specified in the input file. Those response values are also shown in the CCDF.

---

**Probability Density Function (PDF) histograms for each response function:**

### PDF for response_fn_1:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.7604749078e+11</td>
<td>3.4221494996e+11</td>
<td>5.1384774972e-12</td>
</tr>
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<td>2.4334239039e-12</td>
</tr>
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</table>

### PDF for response_fn_2:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.6431154744e+04</td>
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<td>1.9839945149e-05</td>
</tr>
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<td>5.6511827775e+04</td>
<td>6.1603813790e+04</td>
<td>5.8916108390e-05</td>
</tr>
<tr>
<td>6.1603813790e+04</td>
<td>7.8702465755e+04</td>
<td>2.9242071306e-05</td>
</tr>
</tbody>
</table>

### PDF for response_fn_3:

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<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
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</tr>
</thead>
<tbody>
<tr>
<td>2.3796737090e+05</td>
<td>3.6997214153e+05</td>
<td>5.302836523e-06</td>
</tr>
<tr>
<td>3.6997214153e+05</td>
<td>3.8100966235e+05</td>
<td>9.0600055634e-06</td>
</tr>
<tr>
<td>3.8100966235e+05</td>
<td>4.4111498127e+05</td>
<td>3.3274925348e-06</td>
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---

**Level mappings for each response function:**

### Complementary Cumulative Distribution Function (CCDF) for response_fn_1:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.7604749078e+11</td>
<td>1.0000000000e+00</td>
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</tr>
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<td>3.4221494996e+11</td>
<td>6.0000000000e-01</td>
<td></td>
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</tr>
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<td>4.0634975300e+11</td>
<td>3.0000000000e-01</td>
<td></td>
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### Complementary Cumulative Distribution Function (CCDF) for response_fn_2:

<table>
<thead>
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<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.6431154744e+04</td>
<td>1.0000000000e+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5.6511827775e+04</td>
<td>8.0000000000e-01</td>
<td></td>
<td></td>
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<tr>
<td>6.1603813790e+04</td>
<td>5.0000000000e-01</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Complementary Cumulative Distribution Function (CCDF) for response_fn_3:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.3796737090e+05</td>
<td>1.0000000000e+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.6997214153e+05</td>
<td>3.0000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.8100966235e+05</td>
<td>2.0000000000e-01</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

---

**Theory**

Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.
In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

An inverse mapping involves computing the belief and plausibility response level for either a specified probability level or a specified generalized reliability level (two results for each level mapping in the evidence-based epistemic case, instead of the one result for each level mapping in the aleatory case).

**num_probability_levels**

- **Keywords Area**
- **method**
- **global_evidence**
- **probability_levels**
- **num_probability_levels**

Specify which probability_levels correspond to which response

**Specification**

**Alias:** none

**Argument(s):** INTEGERLIST

**Default:** probability_levels evenly distributed among response functions

**Description**

See parent page

**gen_reliability_levels**

- **Keywords Area**
- **method**
- **global_evidence**
- **gen_reliability_levels**

Specify generalized reliability levels at which to estimate the corresponding response value

**Specification**

**Alias:** none

**Argument(s):** REALLIST

**Default:** No CDF/CCDF response levels to compute
Optional

num_gen_reliability_levels

Specify which gen_reliability_levels correspond to which response

### Description

Response levels are calculated for specified generalized reliabilities by indexing into a sorted samples array (the response levels computed are not interpolated and will correspond to one of the sampled values).

### Theory

Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.

In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

An inverse mapping involves computing the belief and plausibility response level for either a specified probability level or a specified generalized reliability level (two results for each level mapping in the evidence-based epistemic case, instead of the one result for each level mapping in the aleatory case).

### num_gen_reliability_levels

- Keywords Area
- method
- global_evidence
- gen_reliability_levels
- num_gen_reliability_levels

Specify which gen_reliability_levels correspond to which response

### Specification

Alias: none

Argument(s): INTEGERLIST

Default: gen_reliability_levels evenly distributed among response functions

### Description

See parent page
6.2. METHOD

rng

• Keywords Area
• method
• global_evidence
• rng

Selection of a random number generator

Specification

Alias: none
Argument(s): none
Default: Mersenne twister (mt19937)

<table>
<thead>
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<th>Description of</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword</th>
</tr>
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<tbody>
<tr>
<td>Optional</td>
<td>Group 1</td>
<td>mt19937</td>
<td>Description</td>
</tr>
<tr>
<td>Required</td>
<td></td>
<td></td>
<td>Generates random numbers using the Mersenne twister</td>
</tr>
<tr>
<td>(Choose One)</td>
<td></td>
<td></td>
<td>rnum2</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Generates pseudo-random numbers using the Pecos package</td>
</tr>
</tbody>
</table>

Description

The rng keyword is used to indicate a choice of random number generator.

Default Behavior

If specified, the rng keyword must be accompanied by either rnum2 (pseudo-random numbers) or mt19937 (random numbers generated by the Mersenne twister). Otherwise, mt19937, the Mersenne twister is used by default.

Usage Tips

The default is recommended, as the Mersenne twister is a higher quality random number generator.

Examples

method
sampling
  sample_type lhs
  samples = 10
  seed = 98765
  rng rnum2

mt19937

• Keywords Area
• method
CHAPTER 6. KEYWORDS AREA

• global_evidence

• rng

• mt19937

Generates random numbers using the Mersenne twister

Specification

Alias: none

Argument(s): none

Description

The mt19937 keyword directs Dakota to use the Mersenne twister to generate random numbers. Additional information can be found on wikipedia: http://en.wikipedia.org/wiki/Mersenne_twister.

Default Behavior

mt19937 is the default random number generator. To specify it explicitly in the Dakota input file, however, it must be specified in conjuction with the rng keyword.

Usage Tips

Use of the Mersenne twister random number generator (mt19937) is recommended.

Examples

method
  sampling
    sample_type lhs
    samples = 10
    seed = 98765
    rng mt19937

rnum2

• Keywords Area

• method

• global_evidence

• rng

• rnum2

Generates pseudo-random numbers using the Pecos package

Specification

Alias: none

Argument(s): none
Description
The rnum2 keyword directs Dakota to use pseudo-random numbers generated by the Pecos package.

Default Behavior
rnum2 is not used by default. To change this behavior, it must be specified in conjunction with the rng keyword.

Usage Tips
Use of the Mersenne twister random number generator (mt19937) is recommended over rnum2.

Examples

```
method
  sampling
    sample_type lhs
    samples = 10
    seed = 98765
    rng rnum2
```

model_pointer
- Keywords Area
- method
- global,evidence
- model_pointer

Identifier for model block to be used by a method

Topics
This keyword is related to the topics:
- block_pointer

Specification
Alias: none
Argument(s): STRING
Default: method use of last model parsed (or use of default model if none parsed)

Description
The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior
If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.

Usage Tips
When doing advanced analyses that involve using multiple methods and multiple models, defining a model_pointer for each method is imperative.

See block_pointer for details about pointers.
Examples

```plaintext
environment
tabular_graphics_data
method_pointer = 'UQ'

method
id_method = 'UQ'
model_pointer = 'SURR'
sampling,
  samples = 10
  seed = 98765 rng rnum2
  response_levels = 0.1 0.2 0.6
  0.1 0.2 0.6
  0.1 0.2 0.6
sample_type lhs
distribution cumulative

model
id_model = 'SURR'
surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
id_method = 'DACE'
model_pointer = 'DACE_M'
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = 'DACE_M'
single
interface_pointer = 'I1'

variables
uniform_uncertain = 2
  lower_bounds = 0. 0.
  upper_bounds = 1. 1.
  descriptors = 'x1' 'x2'

interface
id_interface = 'I1'
system asynch evaluation_concurrency = 5
analysis_driver = 'text_book'

responses
response_functions = 3
no_gradients
no_hessians

6.2.58  global_interval_est

- Keywords Area

- method

- global_interval_est

Interval analysis using global optimization methods
6.2. METHOD

Topics
This keyword is related to the topics:

- uncertainty_quantification
- epistemic_uncertainty_quantification_methods
- interval_estimation

Specification
Alias: nond_global_interval_est
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>samples</td>
<td></td>
<td>Number of samples for sampling-based methods</td>
</tr>
<tr>
<td>Optional</td>
<td>seed</td>
<td></td>
<td>Seed of the random number generator</td>
</tr>
<tr>
<td>Optional</td>
<td>max_iterations</td>
<td></td>
<td>Number of iterations allowed for optimizers and adaptive UQ methods</td>
</tr>
<tr>
<td>Optional</td>
<td>convergence_-tolerance</td>
<td></td>
<td>Stopping criterion based on convergence of the objective function or statistics</td>
</tr>
<tr>
<td>Optional</td>
<td>max_function_-evaluations</td>
<td></td>
<td>Number of function evaluations allowed for optimizers</td>
</tr>
</tbody>
</table>
**CHAPTER 6. KEYWORDS AREA**

<table>
<thead>
<tr>
<th>Optional (Choose One)</th>
<th>Group 1</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>sbo</td>
<td>Use the surrogate based optimization method</td>
</tr>
<tr>
<td></td>
<td></td>
<td>ego</td>
<td>Use the Efficient Global Optimization method</td>
</tr>
<tr>
<td></td>
<td></td>
<td>ea</td>
<td>Use an evolutionary algorithm</td>
</tr>
<tr>
<td></td>
<td></td>
<td>lhs</td>
<td>Uses Latin Hypercube Sampling (LHS) to sample variables</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>rng</td>
<td>Selection of a random number generator</td>
</tr>
<tr>
<td></td>
<td></td>
<td>model_pointer</td>
<td>Identifier for model block to be used by a method</td>
</tr>
</tbody>
</table>

**Description**

In the global approach to interval estimation, one uses either a global optimization method or a sampling method to assess the bounds of the responses.

`global_interval_est` allows the user to specify several approaches to calculate interval bounds on the output responses.

- `lhs` - note: this takes the minimum and maximum of the samples as the bounds
- `ego`
- `sbo`
- `ea`

**Additional Resources**

Refer to `variable_support` for information on supported variable types.

**See Also**

These keywords may also be of interest:

- `global_evidence`
- `local_evidence`
- `local_interval_est`
6.2. METHOD

samples
- Keywords Area
- method
- global_interval_est
- samples

Number of samples for sampling-based methods

**Specification**

**Alias:** none
**Argument(s):** INTEGER

**Description**

The `samples` keyword is used to define the number of samples (i.e., randomly chosen sets of variable values) at which to execute a model.

**Default Behavior**

By default, Dakota will use the minimum number of samples required by the chosen method.

**Usage Tips**

To obtain linear sensitivities or to construct a linear response surface, at least dim+1 samples should be used, where "dim" is the number of variables. For sensitivities to quadratic terms or quadratic response surfaces, at least (dim+1)(dim+2)/2 samples are needed. For uncertainty quantification, we recommend at least 10*dim samples. For variance-based_decomp, we recommend hundreds to thousands of samples. Note that for variance-based_decomp, the number of simulations performed will be N*(dim+2).

**Examples**

```
method
  sampling
    sample_type lhs
    samples = 20
```

**seed**

- Keywords Area
- method
- global_interval_est
- seed

Seed of the random number generator

**Specification**

**Alias:** none
**Argument(s):** INTEGER
**Default:** system-generated (non-repeatable)
CHAPTER 6. KEYWORDS AREA

Description
The random seed control provides a mechanism for making a stochastic method repeatable. That is, the use of the same random seed in identical studies will generate identical results.

Default Behavior
If not specified, the seed is randomly generated.

Expected Output
If seed is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

Usage Tips
If a stochastic study was run without seed specified, and the user later wishes to repeat the study using the same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen. That value can then be added to the Dakota input file.

Examples
method sampling
   sample_type lhs
   samples = 10
   seed = 15347

max_iterations
   • Keywords Area
   • method
   • global_interval_est
   • max_iterations

   Number of iterations allowed for optimizers and adaptive UQ methods

Topics
This keyword is related to the topics:
   • method_independent_controls

Specification
Alias: none
Argument(s): INTEGER
   Default: 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence} / efficient_global: 25+n)

Description
The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed max_iterations iterations. See also max_function_evaluations.

Default Behavior
Default value is 100.
6.2. METHOD

**convergence_tolerance**

- **Keywords Area**
- **method**
- **global_interval_est**
- **convergence_tolerance**

Stopping criterion based on convergence of the objective function or statistics

**Topics**

This keyword is related to the topics:

- **method_independent_controls**

**Specification**

**Alias:** none

**Argument(s):** REAL

**Default:** 1.e-4

**Description**

The `convergence_tolerance` specification provides a real value for controlling the termination of iteration. For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by `convergence_tolerance`, then this convergence criterion is satisfied on the current iteration.

Therefore, permissible values are between 0 and 1, non-inclusive.

**Behavior Varies by Package/Library**

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

**Notes on each library:**

- **DOT:** must be satisfied for two consecutive iterations
- **NPSOL:** defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of `convergence_tolerance` approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., `convergence_tolerance = 1.e-6` will result in approximately six digits of accuracy in the final objective function).
- **NL2SOL:** See `nl2sol`
max_function_evaluations

- Keywords Area
- method
- global_interval_est
- max_function_evaluations

Number of function evaluations allowed for optimizers

Topics
This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none
Argument(s): INTEGER
Default: 1000

Description
The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed max_function_evaluations evaluations. See also max_iterations.

Default Behavior
Default value is 1000.

sbo

- Keywords Area
- method
- global_interval_est
- sbo

Use the surrogate based optimization method

Specification

Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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6.2. METHOD

<table>
<thead>
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<th>Optional</th>
<th>gaussian_process</th>
<th>Gaussian Process surrogate model</th>
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<tbody>
<tr>
<td>Optional</td>
<td>use_derivatives</td>
<td>Use derivative data to construct surrogate models</td>
</tr>
<tr>
<td>Optional</td>
<td>import_build-points_file</td>
<td>File containing points you wish to use to build a surrogate</td>
</tr>
<tr>
<td>Optional</td>
<td>export_approx-points_file</td>
<td>Output file for evaluations of a surrogate model</td>
</tr>
</tbody>
</table>

Description

A surrogate-based optimization method will be used. The surrogate employed in sbo is a Gaussian process surrogate.

The main difference between ego and the sbo approach is the objective function being optimized. ego relies on an expected improvement function, while in sbo, the optimization proceeds using an evolutionary algorithm (coliny_ea) on the Gaussian process surrogate: it is a standard surrogate-based optimization. Also note that the sbo option can support optimization over discrete variables (the discrete variables are relaxed) while ego cannot. This is not the same as surrogate_based_global.

gaussian_process

- Keywords Area
- method
- global_interval_est
- sbo
- gaussian_process

Gaussian Process surrogate model

Specification

Alias: kriging
Argument(s): none
Default: Surfpack Gaussian process

<table>
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<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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</table>
CHAPTER 6. KEYWORDS AREA

<table>
<thead>
<tr>
<th>Required</th>
<th>Group 1</th>
<th>surfpack</th>
<th>Use the Surfpack version of Gaussian Process surrogates</th>
</tr>
</thead>
</table>

### Description

Use the Gaussian process (GP) surrogate from Surfpack, which is specified using the `surfpack` keyword.

An alternate version of GP surrogates was available in prior versions of Dakota. **For now, both versions are supported but the `dakota` version is deprecated and intended to be removed in a future release.**

*Known Issue: When using discrete variables, there have been sometimes significant differences in surrogate behavior observed across computing platforms in some cases. The cause has not yet been fully diagnosed and is currently under investigation. In addition, guidance on appropriate construction and use of surrogates with discrete variables is under development. In the meantime, users should therefore be aware that there is a risk of inaccurate results when using surrogates with discrete variables.*

### surfpack

- **Keywords Area**
- **method**
- **global_interval_est**
- **sbo**
- **gaussian_process**
- **surfpack**

Use the Surfpack version of Gaussian Process surrogates

### Specification

**Alias:** none  
**Argument(s):** none

### Description

This keyword specifies the use of the Gaussian process that is incorporated in our surface fitting library called Surfpack.

Several user options are available:

1. **Optimization methods:**

   Maximum Likelihood Estimation (MLE) is used to find the optimal values of the hyper-parameters governing the trend and correlation functions. By default the global optimization method DIRECT is used for MLE, but other options for the optimization method are available. See `optimization_method`.

   The total number of evaluations of the likelihood function can be controlled using the `max_trials` keyword followed by a positive integer. Note that the likelihood function does not require running the "truth" model, and is relatively inexpensive to compute.
6.2. METHOD

2. Trend Function:
   The GP models incorporate a parametric trend function whose purpose is to capture large-scale variations. See trend.

3. Correlation Lengths:
   Correlation lengths are usually optimized by Surfpack, however, the user can specify the lengths manually. See correlation_lengths.

4. Ill-conditioning
   One of the major problems in determining the governing values for a Gaussian process or Kriging model is the fact that the correlation matrix can easily become ill-conditioned when there are too many input points close together. Since the predictions from the Gaussian process model involve inverting the correlation matrix, ill-conditioning can lead to poor predictive capability and should be avoided.
   
   Note that a sufficiently bad sample design could require correlation lengths to be so short that any interpolatory GP model would become inept at extrapolation and interpolation.
   
   The surfpack model handles ill-conditioning internally by default, but behavior can be modified using

5. Gradient Enhanced Kriging (GEK).
   The use_derivatives keyword will cause the Surfpack GP to be constructed from a combination of function value and gradient information (if available).
   
   See notes in the Theory section.

Theory

Gradient Enhanced Kriging

Incorporating gradient information will only be beneficial if accurate and inexpensive derivative information is available, and the derivatives are not infinite or nearly so. Here "inexpensive" means that the cost of evaluating a function value plus gradient is comparable to the cost of evaluating only the function value, for example gradients computed by analytical, automatic differentiation, or continuous adjoint techniques. It is not cost effective to use derivatives computed by finite differences. In tests, GEK models built from finite difference derivatives were also significantly less accurate than those built from analytical derivatives. Note that GEK’s correlation matrix tends to have a significantly worse condition number than Kriging for the same sample design.

This issue was addressed by using a pivoted Cholesky factorization of Kriging’s correlation matrix (which is a small sub-matrix within GEK’s correlation matrix) to rank points by how much unique information they contain. This reordering is then applied to whole points (the function value at a point immediately followed by gradient information at the same point) in GEK’s correlation matrix. A standard non-pivoted Cholesky is then applied to the reordered GEK correlation matrix and a bisection search is used to find the last equation that meets the constraint on the (estimate of) condition number. The cost of performing pivoted Cholesky on Kriging’s correlation matrix is usually negligible compared to the cost of the non-pivoted Cholesky factorization of GEK’s correlation matrix. In tests, it also resulted in more accurate GEK models than when pivoted Cholesky or whole-point-block pivoted Cholesky was performed on GEK’s correlation matrix.

dakota

- Keywords Area
- method
- global_interval_est
CHAPTER 6. KEYWORDS AREA

- sbo
- gaussian_process
- dakota

Select the built-in Gaussian Process surrogate

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

A second version of GP surrogates was available in prior versions of Dakota. **For now, both versions are supported but the dakota version is deprecated and intended to be removed in a future release.**

Historically these models were drastically different, but in Dakota 5.1, they became quite similar. They now differ in that the Surfpack GP has a richer set of features/options and tends to be more accurate than the Dakota version. Due to how the Surfpack GP handles ill-conditioned correlation matrices (which significantly contributes to its greater accuracy), the Surfpack GP can be a factor of two or three slower than Dakota’s. As of Dakota 5.2, the Surfpack implementation is the default in all contexts except Bayesian calibration.

More details on the **gaussian_process dakota** model can be found in[58].

Dakota’s GP deals with ill-conditioning in two ways. First, when it encounters a non-invertible correlation matrix it iteratively increases the size of a “nugget,” but in such cases the resulting approximation smooths rather than interpolates the data. Second, it has a **point_selection** option (default off) that uses a greedy algorithm to select a well-spaced subset of points prior to the construction of the GP. In this case, the GP will only interpolate the selected subset. Typically, one should not need point selection in trust-region methods because a small number of points are used to develop a surrogate within each trust region. Point selection is most beneficial when constructing with a large number of points, typically more than order one hundred, though this depends on the number of variables and spacing of the sample points.

This differs from the **point_selection** option of the Dakota GP which initially chooses a well-spaced subset of points and finds the correlation parameters that are most likely for that one subset.

**use_derivatives**

- **Keywords Area**
- **method**
- **global_interval_est**
- **sbo**
- **use_derivatives**

Use derivative data to construct surrogate models

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** use function values only
Description

The `use_derivatives` flag specifies that any available derivative information should be used in global approximation builds, for those global surrogate types that support it (currently, polynomial regression and the Surfpack Gaussian process).

However, its use with Surfpack Gaussian process is not recommended.

**import_build_points_file**

- **Keywords Area**
- **method**
- **global_interval_est**
- **sbo**
- **import_build_points_file**

File containing points you wish to use to build a surrogate

**Specification**

Alias: import_points_file

Argument(s): STRING

Default: no point import from a file

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group Tabular Format (Group 1)</th>
<th>Dakota Keyword annotated</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional (Choose One)</td>
<td>annotated</td>
<td>custom_annotated</td>
<td>Selects annotated tabular file format</td>
</tr>
<tr>
<td>Optional(Choose One)</td>
<td>annotated</td>
<td>custom_annotated</td>
<td>Selects custom-annotated tabular file format</td>
</tr>
<tr>
<td>Optional</td>
<td>active_only</td>
<td>freeform</td>
<td>Selects freeform file format</td>
</tr>
<tr>
<td>Optional</td>
<td>active_only</td>
<td>freeform</td>
<td>Selects freeform file format</td>
</tr>
<tr>
<td>Optional</td>
<td>active_only</td>
<td>freeform</td>
<td>Selects freeform file format</td>
</tr>
</tbody>
</table>

**Description**

The `import_build_points_file` allows the user to specify a file that contains a list of points and truth model responses used to construct a surrogate model. These can be used by all methods that (explicitly, e.g. surrogate-based optimization, or implicitly, e.g. efficient global optimization) operate on a surrogate. In particular, these points and responses are used in place of truth model evaluations to construct the initial surrogate. When used to construct surrogate models or emulators these are often called build points or training data.

**Default Behavior**

By default, methods do not import points from a file.
Usage Tips
Dakota parses input files without regard to whitespace, but the import_build_points_file must be in one of three formats:

- annotated (default)
- custom_annotated
- freeform

Examples

```plaintext
method
  polynomial_choas
  expansion_order = 4
  importBuild_points_file = 'dakota_uq_rosenbrock_pce_import.annot.pts.dat'
```

annotated

- Keywords Area
- method
- global_interval_est
- sbo
- import_build_points_file
- annotated

Selects annotated tabular file format

Topics
This keyword is related to the topics:

- file_formats

Specification

Alias: none
Argument(s): none
Default: annotated format

Description
An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior
By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips
To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify custom_annotated header eval_id.

Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

evironment
tabular_data
tabular_data_file = 'dakota_summary.dat'
annotated

Resulting tabular file:

<table>
<thead>
<tr>
<th>eval_id</th>
<th>interface</th>
<th>x1</th>
<th>x2</th>
<th>obj_fn</th>
<th>nln_ineq_con_1</th>
<th>nln_ineq_con_2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>NO_ID</td>
<td>0.9</td>
<td>1.1</td>
<td>0.0002</td>
<td>0.26</td>
<td>0.76</td>
</tr>
<tr>
<td>2</td>
<td>NO_ID</td>
<td>0.90009</td>
<td>1.1</td>
<td>0.00019964</td>
<td>0.2601620081</td>
<td>0.759955</td>
</tr>
<tr>
<td>3</td>
<td>NO_ID</td>
<td>0.89991</td>
<td>1.1</td>
<td>0.00020036</td>
<td>0.2598380081</td>
<td>0.760045</td>
</tr>
</tbody>
</table>

custom_annotated

Keywords Area

method

global_interval_est

sbo

import_build_points_file

custom_annotated

Selects custom-annotated tabular file format

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none

Argument(s): none

Default: annotated format
### Description

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

### Default Behavior

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

### Usage Tips

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

### Examples

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:

```environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
custom_annotated header eval_id
```

Resulting tabular file:

```
%eval_id x1 x2 obj_fn nln_ineq_con_1 nln_ineq_con_2
1 0.9 1.1 0.0002 0.26 0.76
2 0.90009 1.1 0.0001996404857 0.2601620081 0.759955
3 0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...```
6.2. METHOD

header

- Keywords Area
- method
- global_interval_est
- sbo
- import_build_points_file
- custom_annotated
- header

Enable header row in custom-annotated tabular file

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no header

**Description**

See description of parent custom_annotated

eval_id

- Keywords Area
- method
- global_interval_est
- sbo
- import_build_points_file
- custom_annotated
- eval_id

Enable evaluation ID column in custom-annotated tabular file

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no eval_id column

**Description**

See description of parent custom_annotated
interface_id

- Keywords Area
- method
- global_interval_est
- sbo
- import_build_points_file
- custom.annotated
- interface_id

Enable interface ID column in custom-annotated tabular file

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no interface_id column

**Description**

See description of parent custom.annotated

**freeform**

- Keywords Area
- method
- global_interval_est
- sbo
- import_build_points_file
- freeform

Selects freeform file format

**Topics**

This keyword is related to the topics:

- file.formats

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** annotated format
6.2. METHOD

Description

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior

The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips

• Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.
• When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
• In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).
• Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```
environment
  tabular_data
  tabular_data_file = 'dakota_summary.dat'
  freeform
```

Resulting tabular file:

```
  0.9  1.1  0.0002  0.26  0.76
  0.90009  1.1  0.0001996404857  0.2601620081  0.759955
  0.89991  1.1  0.0002003604863  0.2598380081  0.760045
  ...
```

active_only

• Keywords Area
• method
• global_interval_est
• sbo
• import_build_points_file
• active_only

Import only active variables from tabular data file

Topics

This keyword is related to the topics:

• file_formats
CHAPTER 6. KEYWORDS AREA

Speciﬁcation

**Alias:** none
**Argument(s):** none

**Description**

By default, files for tabular data imports are expected to contain columns for all variables, active and inactive. The keyword `active_only` indicates that the file to import contains only the active variables.

This option should only be used in contexts where the inactive variables have no influence, for example, building a surrogate over active variables, with the state variables held at nominal. It should not be used in more complex nested contexts, where the values of inactive variables are relevant to the function evaluations used to build the surrogate.

`export_approx_points_file`

- **Keywords Area**
- **method**
- **global_interval_est**
- **sbo**
- **export_approx_points_file**

Output file for evaluations of a surrogate model

**Specification**

**Alias:** `export_points_file`
**Argument(s):** STRING
**Default:** no point export to a file

<table>
<thead>
<tr>
<th>Required-/Optional</th>
<th>Description of Group Tabular Format (Group 1)</th>
<th>Dakota Keyword annotated</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional(Choose One)</td>
<td></td>
<td>custom_annotated</td>
<td>Selects custom-annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>freeform</td>
<td>Selects freeform file format</td>
</tr>
</tbody>
</table>

**Description**

The `export_approx_points_file` keyword allows the user to specify a file in which the points (input variable values) at which the surrogate model is evaluated and corresponding response values computed by the surrogate model will be written. The response values are the surrogate’s predicted approximation to the truth model responses at those points.
Usage Tips
Dakota exports tabular data in one of three formats:

- annotated (default)
- custom_annotated
- freeform

annotated
- Keywords Area
- method
- global_interval_est
- sbo
- export_approx_points_file
- annotated
  Selects annotated tabular file format

Topics
This keyword is related to the topics:

- file_formats

Specification
Alias: none
  Argument(s): none
  Default: annotated format

Description
An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior
By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips
- To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify custom_annotated header eval_id
- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.
Examples
Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```python
environment
tabular_data
  tabular_data_file = 'dakota_summary.dat'
annotated

Resulting tabular file:

<table>
<thead>
<tr>
<th>%eval_id</th>
<th>interface</th>
<th>x1</th>
<th>x2</th>
<th>obj_fn</th>
<th>nln_ineq_con_1</th>
<th>nln_ineq_con_2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>NO_ID</td>
<td>0.9</td>
<td>1.1</td>
<td>0.0002</td>
<td>0.26</td>
<td>0.76</td>
</tr>
<tr>
<td>2</td>
<td>NO_ID</td>
<td>0.9009</td>
<td>1.1</td>
<td>0.0001996404857</td>
<td>0.2601620081</td>
<td>0.759955</td>
</tr>
<tr>
<td>3</td>
<td>NO_ID</td>
<td>0.89991</td>
<td>1.1</td>
<td>0.0002003604863</td>
<td>0.2598380081</td>
<td>0.760045</td>
</tr>
</tbody>
</table>
...```

custom_annotated

- Keywords Area
- method
- global_interval_est
- sbo
- export_approx_points_file
- custom_annotated

Selects custom-annotated tabular file format

Topics
This keyword is related to the topics:

- file_formats

Specification
Alias: none
Argument(s): none
Default: annotated format

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>header</td>
<td>Enable header row in custom-annotated tabular file</td>
</tr>
</tbody>
</table>
6.2. METHOD

<table>
<thead>
<tr>
<th>Optional</th>
<th>eval_id</th>
<th>Enable evaluation ID column in custom-annotated tabular file</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>interface_id</td>
<td>Enable interface ID column in custom-annotated tabular file</td>
</tr>
</tbody>
</table>

### Description

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

#### Default Behavior

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

#### Usage Tips

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

#### Examples

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
custom_annotated header eval_id
```

Resulting tabular file:

```
%eval_id     x1     x2     obj_fn  nln_ineq_con_1  nln_ineq_con_2
1     0.9     1.1     0.0002  0.26    0.76
2     0.90009 1.1  0.0001996404857 0.2601620081 0.759955
3     0.89991 1.1  0.0002003604863 0.2598380081 0.760045
...
```

header
- Keywords Area
- method
- global_interval_est
CHAPTER 6. KEYWORDS AREA

- sbo
- export_approx_points_file
- custom.annotated
- header

Enable header row in custom-annotated tabular file

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no header

**Description**

See description of parent `custom.annotated`

**eval_id**

- **Keywords Area**
- method
- **global_interval_est**
- sbo
- **export_approx_points_file**
- **custom.annotated**
- eval_id

Enable evaluation ID column in custom-annotated tabular file

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no eval_id column

**Description**

See description of parent `custom.annotated`
6.2. METHOD

interface_id
- Keywords Area
- method
- global_interval_est
- sbo
- export_approx_points_file
- custom_annotated
- interface_id

Enable interface ID column in custom-annotated tabular file

Specification
Alias: none
Argument(s): none
Default: no interface_id column

Description
See description of parent custom_annotated

freeform
- Keywords Area
- method
- global_interval_est
- sbo
- export_approx_points_file
- freeform

Selects freeform file format

Topics
This keyword is related to the topics:
- file_formats

Specification
Alias: none
Argument(s): none
Default: annotated format
Description
A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior
The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips
- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples
Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
    tabular_data_file = 'dakota_summary.dat'
    freeform
Resulting tabular file:

    0.9    1.1    0.0002    0.26    0.76
    0.90009 1.1 0.0001996404857 0.2601620081 0.759955
    0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...
```

ego
- Keywords Area
- method
- global_interval_est
- ego

Use the Efficient Global Optimization method

Specification
Alias: none
Argument(s): none
6.2. METHOD

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>gaussian_process</td>
<td>Gaussian Process surrogate model</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>use_derivatives</td>
<td>Use derivative data to construct surrogate models</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>import_build_-points_file</td>
<td>File containing points you wish to use to build a surrogate</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>export_approx_-points_file</td>
<td>Output file for evaluations of a surrogate model</td>
</tr>
</tbody>
</table>

**Description**

In the case of ego, the efficient global optimization (EGO) method is used to calculate bounds. By default, the Surfpack GP (Kriging) model is used, but the Dakota implementation may be selected instead. If use_derivatives is specified the GP model will be built using available derivative data (Surfpack GP only).

See efficient_global for more information.

gaussian_process

- **Keywords Area**
- method
- global_interval_est
- ego
- gaussian_process

Gaussian Process surrogate model

**Specification**

**Alias:** kriging

**Argument(s):** none

**Default:** Surfpack Gaussian process
### Description

Use the Gaussian process (GP) surrogate from Surfpack, which is specified using the `surfpack` keyword.

An alternate version of GP surrogates was available in prior versions of Dakota. **For now, both versions are supported but the dakota version is deprecated and intended to be removed in a future release.**

**Known Issue:** When using discrete variables, there have been sometimes significant differences in surrogate behavior observed across computing platforms in some cases. The cause has not yet been fully diagnosed and is currently under investigation. In addition, guidance on appropriate construction and use of surrogates with discrete variables is under development. In the meantime, users should therefore be aware that there is a risk of inaccurate results when using surrogates with discrete variables.

### surfpack

- **Keywords Area**
- **method**
- **global_interval_est**
- **ego**
- **gaussian_process**
- **surfpack**

Use the Surfpack version of Gaussian Process surrogates

### Specification

**Alias:** none

**Argument(s):** none

### Description

This keyword specifies the use of the Gaussian process that is incorporated in our surface fitting library called Surfpack.

Several user options are available:

1. **Optimization methods:**

   Maximum Likelihood Estimation (MLE) is used to find the optimal values of the hyper-parameters governing the trend and correlation functions. By default the global optimization method DIRECT is used for MLE, but other options for the optimization method are available. See `optimization_method`.

   The total number of evaluations of the likelihood function can be controlled using the `max_trials` keyword followed by a positive integer. Note that the likelihood function does not require running the "truth" model, and is relatively inexpensive to compute.
6.2. METHOD

2. Trend Function:
   The GP models incorporate a parametric trend function whose purpose is to capture large-scale variations. See trend.

3. Correlation Lengths:
   Correlation lengths are usually optimized by Surfpack, however, the user can specify the lengths manually. See correlation lengths.

4. Ill-conditioning
   One of the major problems in determining the governing values for a Gaussian process or Kriging model is the fact that the correlation matrix can easily become ill-conditioned when there are too many input points close together. Since the predictions from the Gaussian process model involve inverting the correlation matrix, ill-conditioning can lead to poor predictive capability and should be avoided.
   Note that a sufficiently bad sample design could require correlation lengths to be so short that any interpolatory GP model would become inept at extrapolation and interpolation.
   The surfpack model handles ill-conditioning internally by default, but behavior can be modified using

5. Gradient Enhanced Kriging (GEK).
   The use_derivatives keyword will cause the Surfpack GP to be constructed from a combination of function value and gradient information (if available).
   See notes in the Theory section.

Theory

Gradient Enhanced Kriging
Incorporating gradient information will only be beneficial if accurate and inexpensive derivative information is available, and the derivatives are not infinite or nearly so. Here “inexpensive” means that the cost of evaluating a function value plus gradient is comparable to the cost of evaluating only the function value, for example gradients computed by analytical, automatic differentiation, or continuous adjoint techniques. It is not cost effective to use derivatives computed by finite differences. In tests, GEK models built from finite difference derivatives were also significantly less accurate than those built from analytical derivatives. Note that GEK’s correlation matrix tends to have a significantly worse condition number than Kriging for the same sample design.
This issue was addressed by using a pivoted Cholesky factorization of Kriging’s correlation matrix (which is a small sub-matrix within GEK’s correlation matrix) to rank points by how much unique information they contain. This reordering is then applied to whole points (the function value at a point immediately followed by gradient information at the same point) in GEK’s correlation matrix. A standard non-pivoted Cholesky is then applied to the reordered GEK correlation matrix and a bisection search is used to find the last equation that meets the constraint on the (estimate of) condition number. The cost of performing pivoted Cholesky on Kriging’s correlation matrix is usually negligible compared to the cost of the non-pivoted Cholesky factorization of GEK’s correlation matrix. In tests, it also resulted in more accurate GEK models than when pivoted Cholesky or whole-point-block pivoted Cholesky was performed on GEK’s correlation matrix.

dakota
- Keywords Area
- method
- global_interval_est
Select the built-in Gaussian Process surrogate

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

A second version of GP surrogates was available in prior versions of Dakota. **For now, both versions are supported but the dakota version is deprecated and intended to be removed in a future release.**

Historically these models were drastically different, but in Dakota 5.1, they became quite similar. They now differ in that the Surfpack GP has a richer set of features/options and tends to be more accurate than the Dakota version. Due to how the Surfpack GP handles ill-conditioned correlation matrices (which significantly contributes to its greater accuracy), the Surfpack GP can be a factor of two or three slower than Dakota’s. As of Dakota 5.2, the Surfpack implementation is the default in all contexts except Bayesian calibration. More details on the gaussian_process_dakota model can be found in [58].

Dakota’s GP deals with ill-conditioning in two ways. First, when it encounters a non-invertible correlation matrix it iteratively increases the size of a “nugget,” but in such cases the resulting approximation smooths rather than interpolates the data. Second, it has a `point_selection` option (default off) that uses a greedy algorithm to select a well-spaced subset of points prior to the construction of the GP. In this case, the GP will only interpolate the selected subset. Typically, one should not need point selection in trust-region methods because a small number of points are used to develop a surrogate within each trust region. Point selection is most beneficial when constructing with a large number of points, typically more than order one hundred, though this depends on the number of variables and spacing of the sample points.

This differs from the `point_selection` option of the Dakota GP which initially chooses a well-spaced subset of points and finds the correlation parameters that are most likely for that one subset.

**use_derivatives**

- Keywords Area
- method
- global_interval_est
- ego
- use_derivatives

Use derivative data to construct surrogate models

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** use function values only
6.2. METHOD

Description

The `use_derivatives` flag specifies that any available derivative information should be used in global approximation builds, for those global surrogate types that support it (currently, polynomial regression and the Surfpack Gaussian process).

However, its use with Surfpack Gaussian process is not recommended.

import_build_points_file

- Keywords Area
- method
- global_interval_est
- ego
- import_build_points_file

File containing points you wish to use to build a surrogate

Specification

Alias: import_points_file
Argument(s): STRING
Default: no point import from a file

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional/(Choose One)</td>
<td>Tabular Format (Group 1)</td>
<td>annotated</td>
<td>Selects annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>custom.annotated</td>
<td>Selects custom-annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>freeform</td>
<td>Selects freeform file format</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>active_only</td>
<td>Import only active variables from tabular data file</td>
</tr>
</tbody>
</table>

Description

The `import_build_points_file` allows the user to specify a file that contains a list of points and truth model responses used to construct a surrogate model. These can be used by all methods that (explicitly, e.g. surrogate-based optimization, or implicitly, e.g. efficient global optimization) operate on a surrogate. In particular, these points and responses are used in place of truth model evaluations to construct the initial surrogate. When used to construct surrogate models or emulators these are often called build points or training data.

Default Behavior

By default, methods do not import points from a file.
Usage Tips
Dakota parses input files without regard to whitespace, but the import_build_points_file must be in one of three formats:

- annotated (default)
- custom_annotated
- freeform

Examples

```python
method
    polynomial_chaos
    expansion_order = 4
    import_build_points_file = 'dakota_uq_rosenbrock_pce_import.annot.pts.dat'
```

annotated

- Keywords Area
- method
- global_interval_est
- ego
- import_build_points_file
- annotated

Selects annotated tabular file format

Topics
This keyword is related to the topics:

- file_formats

Specification

Alias: none
Argument(s): none
Default: annotated format

Description
An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior
By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips
6.2. METHOD

- To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify `custom_annotated` header eval_id

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to `annotated` format, though `freeform` remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the `freeform` option.

Examples

Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```python
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
annotated

Resulting tabular file:
```
<table>
<thead>
<tr>
<th>%eval_id</th>
<th>interface</th>
<th>x1</th>
<th>x2</th>
<th>obj_fn</th>
<th>nln_ineq_con_1</th>
<th>nln_ineq_con_2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>NO_ID</td>
<td>0.9</td>
<td>1.1</td>
<td>0.0002</td>
<td>0.26</td>
<td>0.76</td>
</tr>
<tr>
<td>2</td>
<td>NO_ID</td>
<td>0.90009</td>
<td>1.1</td>
<td>0.0001996404857</td>
<td>0.2601620081</td>
<td>0.759955</td>
</tr>
<tr>
<td>3</td>
<td>NO_ID</td>
<td>0.89991</td>
<td>1.1</td>
<td>0.0002003604863</td>
<td>0.2598380081</td>
<td>0.760045</td>
</tr>
<tr>
<td>...</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
```

- `custom_annotated`

  - Keywords Area
  - method
  - global_interval_est
  - ego
  - import_build_points_file
  - `custom_annotated`

  Selects custom-annotated tabular file format

Topics

This keyword is related to the topics:

- `file_formats`

Specification

**Alias:** none

**Argument(s):** none

**Default:** annotated format
### Description

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

#### Default Behavior

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

#### Usage Tips

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

#### Examples

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface-id), and data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
custom_annotated header eval_id
```

Resulting tabular file:

```
%eval_id  x1  x2  obj_fn  nln_ineq_con_1  nln_ineq_con_2
1  0.9  1.1  0.0002  0.26  0.76
2  0.90009  1.1  0.0001996404857  0.2601620081  0.759955
3  0.89991  1.1  0.0002003604863  0.2598380081  0.760045
...```
6.2. METHOD

header
- Keywords Area
- method
- global_interval_est
- ego
- import_build_points_file
- custom_annotated
- header

Enable header row in custom-annotated tabular file

Specification
Alias: none
Argument(s): none
Default: no header

Description
See description of parent custom_annotated

eval_id
- Keywords Area
- method
- global_interval_est
- ego
- import_build_points_file
- custom_annotated
- eval_id

Enable evaluation ID column in custom-annotated tabular file

Specification
Alias: none
Argument(s): none
Default: no eval_id column

Description
See description of parent custom_annotated
interface_id

- Keywords Area
- method
- global_interval_est
- ego
- import_build_points_file
- custom.annotated
- interface_id

Enable interface ID column in custom-annotated tabular file

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no interface_id column

**Description**

See description of parent custom.annotated

**freeform**

- Keywords Area
- method
- global_interval_est
- ego
- import_build_points_file
- freeform

Selects freeform file format

**Topics**

This keyword is related to the topics:

- file.formats

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** annotated format
6.2. METHOD

Description
A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior
The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips
- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples
Export a freeform tabular file containing only data for variables and responses. Input file fragment:
```plaintext
evironment
tabular_data
  tabular_data_file = 'dakota_summary.dat'
  freeform
```
Resulting tabular file:
```
0.9     1.1     0.0002     0.26     0.76
0.90009 1.1 0.0001996404857 0.2601620081 0.759955
0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...
```

active_only
- Keywords Area
- method
- global_interval_est
- ego
- import_build_points_file
- active_only

Import only active variables from tabular data file

Topics
This keyword is related to the topics:
- file_formats
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none
  Argument(s): none

Description

By default, files for tabular data imports are expected to contain columns for all variables, active and inactive. The keyword \texttt{active\_only} indicates that the file to import contains only the active variables.

This option should only be used in contexts where the inactive variables have no influence, for example, building a surrogate over active variables, with the state variables held at nominal. It should not be used in more complex nested contexts, where the values of inactive variables are relevant to the function evaluations used to build the surrogate.

\texttt{export\_approx\_points\_file}

- Keywords Area
- method
- \texttt{global\_interval\_est}
- ego
- \texttt{export\_approx\_points\_file}

Output file for evaluations of a surrogate model

 Specification

Alias: \texttt{export\_points\_file}
  Argument(s): STRING
  Default: no point export to a file

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional(Choose One)</td>
<td>Tabular Format (Group 1)</td>
<td>annotated</td>
<td>Selects annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>\texttt{custom_annotated}</td>
<td>Selects custom-annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>\texttt{freeform}</td>
<td>Selects freeform file format</td>
</tr>
</tbody>
</table>

Description

The \texttt{export\_approx\_points\_file} keyword allows the user to specify a file in which the points (input variable values) at which the surrogate model is evaluated and corresponding response values computed by the surrogate model will be written. The response values are the surrogate’s predicted approximation to the truth model responses at those points.
Usage Tips
Dakota exports tabular data in one of three formats:

- annotated (default)
- custom_annotated
- freeform

annotated
- Keywords Area
- method
- global_interval_est
- ego
- export_approx_points_file
- annotated
Selects annotated tabular file format

Topics
This keyword is related to the topics:

- fileFormats

Specification
Alias: none

Argument(s): none
Default: annotated format

Description
An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior
By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips
- To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify custom_annotated header eval_id
- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.
CHAPTER 6. KEYWORDS AREA

Examples

Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

environment
    tabular_data
        tabular_data_file = 'dakota_summary.dat'
    annotated

Resulting tabular file:

%eval_id interface x1 x2 obj_fn nln_ineq_con_1 nln_ineq_con_2
1 NO_ID 0.9 1.1 0.0002 0.26 0.76
2 NO_ID 0.90009 1.1 0.0001996404857 0.2601620081 0.759955
3 NO_ID 0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...

custom_annotated

- Keywords Area
- method
- global_interval_est
- ego
- export_approx_points_file
- custom_annotated

Selects custom-annotated tabular file format

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none

Argument(s): none

Default: annotated format

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>header</td>
<td></td>
<td>Enable header row in custom-annotated tabular file</td>
</tr>
</tbody>
</table>
### Description

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, `eval_id` column, and `interface_id` column appear in the tabular file, thus bridging freeform and (fully) annotated.

#### Default Behavior

The `annotated` format is the default for tabular export/import. To control which header row and columns are in the input/output, specify `custom_annotated`, followed by options, in the relevant export/import context.

#### Usage Tips

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to `annotated` format, though `freeform` remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the `freeform` option.

#### Examples

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and `eval_id` (no `interface_id`), and data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
custom_annotated header eval_id
```

Resulting tabular file:

<table>
<thead>
<tr>
<th>%eval_id</th>
<th>x1</th>
<th>x2</th>
<th>obj_fn</th>
<th>nln_ineq_con_1</th>
<th>nln_ineq_con_2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.9</td>
<td>1.1</td>
<td>0.0002</td>
<td>0.26</td>
<td>0.76</td>
</tr>
<tr>
<td>2</td>
<td>0.90009</td>
<td>1.1</td>
<td>0.0001996404857</td>
<td>0.2601620081</td>
<td>0.7599555</td>
</tr>
<tr>
<td>3</td>
<td>0.89991</td>
<td>1.1</td>
<td>0.0002003604863</td>
<td>0.2598380081</td>
<td>0.760045</td>
</tr>
<tr>
<td>...</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

#### Keywords Area

- `method`
- `global_interval_est`
• ego
• export_approx_points_file
• custom.annotated
• header

Enable header row in custom-annotated tabular file

**Specification**

Alias: none
Argument(s): none
Default: no header

**Description**

See description of parent `custom.annotated`

eval_id

• Keywords Area
• method
• global_interval_est
• ego
• export_approx_points_file
• custom.annotated
• eval_id

Enable evaluation ID column in custom-annotated tabular file

**Specification**

Alias: none
Argument(s): none
Default: no eval_id column

**Description**

See description of parent `custom.annotated`
6.2. METHOD

interface_id

• Keywords Area
• method
• global_interval_est
• ego
• export_approx_points_file
• custom_annotated
• interface_id

Enable interface ID column in custom-annotated tabular file

Specification

Alias: none

Argument(s): none

Default: no interface_id column

Description

See description of parent custom_annotated

freeform

• Keywords Area
• method
• global_interval_est
• ego
• export_approx_points_file
• freeform

Selects freeform file format

Topics

This keyword is related to the topics:

• file_formats

Specification

Alias: none

Argument(s): none

Default: annotated format
Description

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior

The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips

- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
freeform
```

Resulting tabular file:

```plaintext
0.9 1.1 0.0002 0.26 0.76
0.90009 1.1 0.0001996404857 0.2601620081 0.759955
0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...```

ea

- Keywords Area
- method
- global_interval_est

Use an evolutionary algorithm

Specification

Alias: none
Argument(s): none
6.2. **METHOD**

**Description**

In this approach, the evolutionary algorithm from Coliny, `coliny_ea`, is used to perform the interval optimization with no surrogate model involved. Again, this option of `ea` can support interval optimization over discrete variables.

**lhs**

- **Keywords Area**
- **method**
- **global_interval_est**
- **lhs**

Uses Latin Hypercube Sampling (LHS) to sample variables

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

The `lhs` keyword invokes Latin Hypercube Sampling as the means of drawing samples of uncertain variables according to their probability distributions. This is a stratified, space-filling approach that selects variable values from a set of equi-probable bins.

**Default Behavior**

Latin Hypercube Sampling is the default sampling mode in most contexts (exception: multilevel_sampling). To explicitly specify LHS in the Dakota input file, the `lhs` keyword must appear in conjunction with the `sample_type` keyword.

**Usage Tips**

Latin Hypercube Sampling is very robust and can be applied to any problem. It is fairly effective at estimating the mean of model responses and linear correlations with a reasonably small number of samples relative to the number of variables.

**Examples**

```dakota
method
  sampling
    sample_type lhs
    samples = 20
```

**rng**

- **Keywords Area**
- **method**
- **global_interval_est**
- **rng**

Selection of a random number generator
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): none

Default: Mersenne twister (mt19937)

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required (Choose One)</td>
<td></td>
<td>mt19937</td>
<td>Generates random numbers using the Mersenne twister</td>
</tr>
<tr>
<td>rnum2</td>
<td></td>
<td></td>
<td>Generates pseudo-random numbers using the Pecos package</td>
</tr>
</tbody>
</table>

Description

The rng keyword is used to indicate a choice of random number generator.

Default Behavior

If specified, the rng keyword must be accompanied by either rnum2 (pseudo-random numbers) or mt19937 (random numbers generated by the Mersenne twister). Otherwise, mt19937, the Mersenne twister is used by default.

Usage Tips

The default is recommended, as the Mersenne twister is a higher quality random number generator.

Examples

```
method
  sampling
    sample_type lhs
    samples = 10
    seed = 98765
    rng rnum2
```

mt19937

- Keywords Area
- method
- global_interval_est
- rng
- mt19937

Generates random numbers using the Mersenne twister

Specification

Alias: none

Argument(s): none
6.2. METHOD

Description
The mt19937 keyword directs Dakota to use the Mersenne twister to generate random numbers. Additional information can be found on wikipedia: http://en.wikipedia.org/wiki/Mersenne_twister.

Default Behavior
mt19937 is the default random number generator. To specify it explicitly in the Dakota input file, however, it must be specified in conjunction with the rng keyword.

Usage Tips
Use of the Mersenne twister random number generator (mt19937) is recommended.

Examples
method sampling
  sample_type lhs
  samples = 10
  seed = 98765
  rng mt19937

rnum2
  • Keywords Area
  • method
  • global_interval_est
  • rng
  • rnum2
Generates pseudo-random numbers using the Pecos package

Specification
Alias: none
Argument(s): none

Description
The rnum2 keyword directs Dakota to use pseudo-random numbers generated by the Pecos package.

Default Behavior
rnum2 is not used by default. To change this behavior, it must be specified in conjunction with the rng keyword.

Usage Tips
Use of the Mersenne twister random number generator (mt19937) is recommended over rnum2.

Examples
method sampling
  sample_type lhs
  samples = 10
  seed = 98765
  rng rnum2
model_pointer

- Keywords Area
- method
- global_interval_est
- model_pointer

Identifier for model block to be used by a method

Topics

This keyword is related to the topics:

- block_pointer

Specification

Alias: none

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)

Description

The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.

Usage Tips

When doing advanced analyses that involve using multiple methods and multiple models, defining a model_pointer for each method is imperative.

See block_pointer for details about pointers.

Examples

```python
environment
tabular_graphics_data
method_pointer = 'UQ'

method
id_method = 'UQ'
model_pointer = 'SURR'
sampling,
  samples = 10
  seed = 98765 rng rnum2
  response_levels = 0.1 0.2 0.6
  0.1 0.2 0.6
  0.1 0.2 0.6
sample_type lhs
distribution cumulative

model
id_model = 'SURR'
```
6.2. METHOD

```
surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
id_method = 'DACE'
model_pointer = 'DACE_M'
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = 'DACE_M'
single
interface_pointer = 'I1'

variables
uniform_uncertain = 2
lower_bounds = 0. 0.
upper_bounds = 1. 1.
descriptors = 'x1' 'x2'

interface
id_interface = 'I1'
system asynch evaluation_concurrency = 5
analysis_driver = 'text_book'

responses
response_functions = 3
no_gradients
no_hessians
```

6.2.59 bayes_calibration

- Keywords Area
- method
- bayes_calibration

Bayesian calibration

Topics

This keyword is related to the topics:

- bayesian_calibration
- package_queso

Specification

Alias: nond_bayes_calibration

<table>
<thead>
<tr>
<th>Argument(s):</th>
<th>none</th>
<th>Required/- Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Required (Choose One)</td>
<td>Group 1</td>
<td>queso</td>
<td>Markov Chain Monte Carlo algorithms from the QUESO package</td>
<td></td>
<td></td>
</tr>
<tr>
<td>-----------------------</td>
<td>---------</td>
<td>-------</td>
<td>----------------------------------------------------------</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>gpmsa</td>
<td>(Experimental) Gaussian Process Models for Simulation Analysis (GPMSA) Bayesian calibration</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>wasabi</td>
<td>(Experimental Method) Non-MCMC Bayesian inference using interval analysis</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>dream</td>
<td>DREAM (DiffeRential Evolution Adaptive Metropolis)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>experimental_design</td>
<td>(Experimental) Adaptively select experimental designs for iterative Bayesian updating</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>calibrate_error_multipliers</td>
<td>Calibrate hyper-parameter multipliers on the observation error covariance</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>burn_in_samples</td>
<td>Manually specify the burn in period for the MCMC chain.</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>-------------------</td>
<td>------------------------------------------</td>
<td>--------------------------------------------------------</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>posterior_stats</td>
<td>Compute information-theoretic metrics on posterior parameter distribution</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>model_discrepancy</td>
<td>(Experimental) Post-calibration calculation of model discrepancy correction</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>sub_sampling_period</td>
<td>Specify a sub-sampling of the MCMC chain</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>probability_levels</td>
<td>Specify probability levels at which to compute credible and prediction intervals</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>convergence_tolerance</td>
<td>Stopping criterion based on convergence of the objective function or statistics</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>max_iterations</td>
<td>Number of iterations allowed for optimizers and adaptive UQ methods</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Description

Bayesian calibration methods take prior information on parameter values (in the form of prior distributions) and observational data (e.g. from experiments) and infer posterior distributions on the parameter values. When the computational simulation is then executed with samples from the posterior parameter distributions, the results that are produced are consistent with (“agree with”) the experimental data. Calibrating parameters from a computational simulation model requires a likelihood function that specifies the likelihood of observing a particular observation given the model and its associated parameterization; Dakota assumes a Gaussian likelihood function. The algorithms that produce the posterior distributions on model parameters are most commonly Monte Carlo Markov Chain (MCMC) sampling algorithms. MCMC methods require many samples, often tens of thousands, so in the case of model calibration, often emulators of the computational simulation are used. For more details on the algorithms underlying the methods, see the Dakota User’s manual.

Dakota has four classes of Bayesian calibration methods: QUESO/DRAM, GPMSA, DREAM, and WASABI.

1. The QUESO methods use components from the QUESO library (Quantification of Uncertainty for Estimation, Simulation, and Optimization) developed at The University of Texas at Austin. Dakota uses its DRAM (Delayed Rejected Adaptive Metropolis) algorithm, and variants, for the MCMC sampling.

2. GPMSA (Gaussian Process Models for Simulation Analysis) is an approach developed at Los Alamos National Laboratory and Dakota currently uses the QUESO implementation. It constructs Gaussian process models to emulate the expensive computational simulation as well as model discrepancy. GPMSA also has extensive features for calibration, such as the capability to include a model discrepancy term and the capability to model functional data such as time series data. This is an experimental capability and not all features are available in Dakota yet.

3. DREAM (DiffeRential Evolution Adaptive Metropolis) is a method that runs multiple different chains simultaneously for global exploration, and automatically tunes the proposal covariance during the process by a self-adaptive randomized subspace sampling. [86].

4. WASABI: Non-MCMC Bayesian inference via interval analysis

Usage Tips

The Bayesian capabilities are under active development. At this stage, the QUESO methods in Dakota are the most advanced and robust, followed by DREAM, followed by GPMSA and WASABI which are not yet ready for production use.

Note that as of Dakota 6.2, the field responses and associated field data may be used with QUESO and DREAM. That is, the user can specify field simulation data and field experiment data, and Dakota will interpolate and provide the proper residuals to the Bayesian calibration.

queso

- Keywords Area
- method
- bayes_calibration
- queso

Markov Chain Monte Carlo algorithms from the QUESO package
6.2. METHOD

Topics

This keyword is related to the topics:

- bayesian_calibration
- package_queso

Specification

Alias: none  
Argument(s): none

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>chain_samples</td>
<td>chain_samples</td>
<td>Number of Markov Chain Monte Carlo posterior samples</td>
</tr>
<tr>
<td>Optional</td>
<td>seed</td>
<td>seed</td>
<td>Seed of the random number generator</td>
</tr>
<tr>
<td>Optional</td>
<td>emulator</td>
<td>emulator</td>
<td>Use an emulator or surrogate model to evaluate the likelihood function</td>
</tr>
<tr>
<td>Optional</td>
<td>standardized_space</td>
<td>standardized_space</td>
<td>Perform Bayesian inference in standardized probability space</td>
</tr>
<tr>
<td>Optional</td>
<td>logit_transform</td>
<td>logit_transform</td>
<td>Utilize the logit transformation to reduce sample rejection for bounded domains</td>
</tr>
<tr>
<td>Optional</td>
<td>export_chain-points_file</td>
<td>export_chain-points_file</td>
<td>Export the MCMC chain to the specified filename</td>
</tr>
<tr>
<td>Optional</td>
<td>dram</td>
<td>dram</td>
<td>Use the DRAM MCMC algorithm</td>
</tr>
</tbody>
</table>

Optional (Choose One) MCMC algorithm type (Group 1)
### Description

The *queso* method supports the following MCMC algorithms: DRAM (Delayed Rejection Adaptive Metropolis), delayed rejection (DR) only, adaptive metropolis (AM) only, pure Metropolis Hastings (MH)s, and multilevel (M-L).

When calibrating fast-running simulation models, use of an emulator is not typically warranted. For slower models, using an emulator model in the MCMC sampling will greatly improve the speed, since the Monte Carlo Markov Chain will generate thousands of samples on the emulator instead of the real simulation code. An emulator may be specified with the keyword `emulator`, followed by a `gaussian_process` emulator, a `pce` emulator (polynomial chaos expansion), or a `sc` emulator (stochastic collocation). For the `gaussian_process` emulator, the user must specify whether to use the `surfpack` or `dakota` version of the Gaussian process. The user can define the number of samples `build_samples` from which the emulator should be built. It is also possible to build the Gaussian process from points read in from the `import_points_file` and to export approximation-based sample evaluations using `export_points_file`. For `pce` or `sc`, the user can define a `sparse_grid_level`.

There are a variety of ways the user can specify the proposal covariance matrix which is very important in

<table>
<thead>
<tr>
<th>Keyword</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>delayed_rejection</code></td>
<td>Use the Delayed Rejection MCMC algorithm</td>
</tr>
<tr>
<td><code>adaptive_metropolis</code></td>
<td>Use the Adaptive Metropolis MCMC algorithm</td>
</tr>
<tr>
<td><code>metropolis_hastings</code></td>
<td>Use the Metropolis-Hastings MCMC algorithm</td>
</tr>
<tr>
<td><code>multilevel</code></td>
<td>Use the multilevel MCMC algorithm.</td>
</tr>
<tr>
<td><code>rng</code></td>
<td>Selection of a random number generator</td>
</tr>
<tr>
<td><code>pre_solve</code></td>
<td>Perform deterministic optimization for MAP before Bayesian calibration</td>
</tr>
<tr>
<td><code>proposal_covariance</code></td>
<td>Defines the technique used to generate the MCMC proposal covariance.</td>
</tr>
</tbody>
</table>
governing the samples generated in the chain. The proposal covariance specifies the covariance structure of a multivariate normal distribution. The user can specify proposal covariance, followed by derivatives, prior, values, or filename. The derivative specification involves forming the Hessian of the misfit function (the negative log likelihood). When derivative information is available inexpensively (e.g. from an emulator), the derived-based proposal covariance forms a more accurate proposal distribution, resulting in lower rejection rates and faster chain mixing. The prior setting involves constructing the proposal from the variance of the prior distributions of the parameters being calibrated. When specifying the proposal covariance with values or from a file, the user can choose to specify only the diagonals of the covariance matrix with diagonal or to specify the full covariance matrix with matrix.

There are two other controls for QUESO. The pre_solve option enables the user to start the chain at an optimal point, the Maximum A Posteriori (MAP) point. This is the point in parameter space that maximizes the log posterior, (defined as the log-likelihood minus the log_prior). A deterministic optimization method is used to obtain the MAP point, and the MCMC chain is then started at the best point found in the optimization. The second factor is a logit_transform, which performs an internal variable transformation from bounded domains to unbounded domains in order to reduce sample rejection due to an out-of-bounds condition.

Note that as of Dakota 6.2, the field data capability may be used with QUESO. That is, the user can specify field simulation data and field experiment data, and Dakota will interpolate and provide the proper residuals to the Bayesian calibration.

**chain_samples**

- **Keywords** Area
- **method**
- **bayes_calibration**
- **queso**
- **chain_samples**

Number of Markov Chain Monte Carlo posterior samples

**Specification**

* Alias: samples
  * **Argument(s):** INTEGER
  * **Default:** method-dependent

**Description**

The chain_samples keyword indicates the number of draws from the posterior distribution to perform. When an emulator is active, this will be the number of samples on the constructed surrogate model.

**Default Behavior**

The default number of chain samples is method-dependent. QUESO methods use 48576. DREAM uses (number of generations) x (number of chains).

**Usage Tips**

MCMC methods typically require a large number of chain samples to converge, often thousands to millions.
CHAPTER 6. KEYWORDS AREA

Examples

method
    bayes_calibration queso
    chain_samples = 20000

seed
    • Keywords Area
    • method
    • bayes_calibration
    • queso
    • seed

Seed of the random number generator

Specification

Alias: none
    Argument(s): INTEGER
    Default: system-generated (non-repeatable)

Description

The random seed control provides a mechanism for making a stochastic method repeatable. That is, the use of the same random seed in identical studies will generate identical results.

    Default Behavior
    If not specified, the seed is randomly generated.

    Expected Output
    If seed is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

    Usage Tips
    If a stochastic study was run without seed specified, and the user later wishes to repeat the study using the same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen. That value can then be added to the Dakota input file.

Examples

method
    sampling
    sample_type lhs
    samples = 10
    seed = 15347

emulator

    • Keywords Area
    • method
    • bayes_calibration
6.2. METHOD

- queso
- emulator

Use an emulator or surrogate model to evaluate the likelihood function

**Specification**

**Alias:** none

**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required (Choose One)</td>
<td>emulator type (Group 1)</td>
<td>gaussian_process</td>
<td>Gaussian Process surrogate model</td>
</tr>
<tr>
<td></td>
<td></td>
<td>pce</td>
<td>Polynomial Chaos Expansion surrogate model</td>
</tr>
<tr>
<td></td>
<td></td>
<td>sc</td>
<td>Stochastic Collocation polynomial surrogate model</td>
</tr>
<tr>
<td>Optional</td>
<td>use_derivatives</td>
<td></td>
<td>Use derivative data to construct surrogate models</td>
</tr>
</tbody>
</table>

**Description**

This keyword describes the type of emulator used when calculating the likelihood function for the Bayesian calibration. The emulator can be a Gaussian process, polynomial chaos expansion, or stochastic collocation.

- **gaussian_process**
  - Keywords Area
  - method
  - bayes_calibration
  - queso
  - emulator
  - gaussian_process
    Gaussian Process surrogate model

**Specification**

**Alias:** kriging

**Argument(s):** none

**Default:** Surfpack Gaussian process
CHAPTER 6. KEYWORDS AREA

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required (Choose One)</td>
<td></td>
<td>surfpack</td>
<td>Use the Surfpack version of Gaussian Process surrogates</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>dakota</td>
<td>Select the built in Gaussian Process surrogate</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>build_samples</td>
<td>Number of initial model evaluations used in build phase</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>posterior_adaptive</td>
<td>Adapt emulator model to increase accuracy in high posterior probability regions</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>import_build_points_file</td>
<td>File containing points you wish to use to build a surrogate</td>
</tr>
</tbody>
</table>

Description

Use the Gaussian process (GP) surrogate from Surfpack, which is specified using the `surfpack` keyword.

An alternate version of GP surrogates was available in prior versions of Dakota. For now, both versions are supported but the `dakota` version is deprecated and intended to be removed in a future release.

Known Issue: When using discrete variables, there have been sometimes significant differences in surrogate behavior observed across computing platforms in some cases. The cause has not yet been fully diagnosed and is currently under investigation. In addition, guidance on appropriate construction and use of surrogates with discrete variables is under development. In the meantime, users should therefore be aware that there is a risk of inaccurate results when using surrogates with discrete variables.

surfpack
- Keywords Area
- method
- bayes_calibration
- queso
- emulator
- gaussian_process
- surfpack

Use the Surfpack version of Gaussian Process surrogates
6.2. METHOD

Specification

Alias: none
Argument(s): none

Description

This keyword specifies the use of the Gaussian process that is incorporated in our surface fitting library called Surfpack.

Several user options are available:

1. Optimization methods:
   Maximum Likelihood Estimation (MLE) is used to find the optimal values of the hyper-parameters governing the trend and correlation functions. By default the global optimization method DIRECT is used for MLE, but other options for the optimization method are available. See optimization method.

   The total number of evaluations of the likelihood function can be controlled using the max_trials keyword followed by a positive integer. Note that the likelihood function does not require running the "truth" model, and is relatively inexpensive to compute.

2. Trend Function:
   The GP models incorporate a parametric trend function whose purpose is to capture large-scale variations. See trend.

3. Correlation Lengths:
   Correlation lengths are usually optimized by Surfpack, however, the user can specify the lengths manually. See correlation_lengths.

4. Ill-conditioning
   One of the major problems in determining the governing values for a Gaussian process or Kriging model is the fact that the correlation matrix can easily become ill-conditioned when there are too many input points close together. Since the predictions from the Gaussian process model involve inverting the correlation matrix, ill-conditioning can lead to poor predictive capability and should be avoided.

   Note that a sufficiently bad sample design could require correlation lengths to be so short that any interpolatory GP model would become inept at extrapolation and interpolation.

   The surfpack model handles ill-conditioning internally by default, but behavior can be modified using 5. Gradient Enhanced Kriging (GEK).

   The use_derivatives keyword will cause the Surfpack GP to be constructed from a combination of function value and gradient information (if available).

   See notes in the Theory section.

Theory

Gradient Enhanced Kriging

Incorporating gradient information will only be beneficial if accurate and inexpensive derivative information is available, and the derivatives are not infinite or nearly so. Here "inexpensive" means that the cost of evaluating a function value plus gradient is comparable to the cost of evaluating only the function value, for example gradients computed by analytical, automatic differentiation, or continuous adjoint techniques. It is not cost effective to use derivatives computed by finite differences. In tests, GEK models built from finite difference derivatives were also
significantly less accurate than those built from analytical derivatives. Note that GEK’s correlation matrix tends to have a significantly worse condition number than Kriging for the same sample design.

This issue was addressed by using a pivoted Cholesky factorization of Kriging’s correlation matrix (which is a small sub-matrix within GEK’s correlation matrix) to rank points by how much unique information they contain. This reordering is then applied to whole points (the function value at a point immediately followed by gradient information at the same point) in GEK’s correlation matrix. A standard non-pivoted Cholesky is then applied to the reordered GEK correlation matrix and a bisection search is used to find the last equation that meets the constraint on the (estimate of) condition number. The cost of performing pivoted Cholesky on Kriging’s correlation matrix is usually negligible compared to the cost of the non-pivoted Cholesky factorization of GEK’s correlation matrix. In tests, it also resulted in more accurate GEK models than when pivoted Cholesky or whole-point-block pivoted Cholesky was performed on GEK’s correlation matrix.

dakota

- Keywords Area
- method
- bayes_calibration
- queso
- emulator
- gaussian_process
- dakota

Select the built in Gaussian Process surrogate

**Specification**

*Alias*: none

*Argument(s)*: none

**Description**

A second version of GP surrogates was available in prior versions of Dakota. **For now, both versions are supported but the dakota version is deprecated and intended to be removed in a future release.**

Historically these models were drastically different, but in Dakota 5.1, they became quite similar. They now differ in that the Surfpack GP has a richer set of features/options and tends to be more accurate than the Dakota version. Due to how the Surfpack GP handles ill-conditioned correlation matrices (which significantly contributes to its greater accuracy), the Surfpack GP can be a factor of two or three slower than Dakota’s. As of Dakota 5.2, the Surfpack implementation is the default in all contexts except Bayesian calibration.

More details on the gaussian_process dakota model can be found in[58].

Dakota’s GP deals with ill-conditioning in two ways. First, when it encounters a non-invertible correlation matrix it iteratively increases the size of a "nugget," but in such cases the resulting approximation smooths rather than interpolates the data. Second, it has a point_selection option (default off) that uses a greedy algorithm to select a well-spaced subset of points prior to the construction of the GP. In this case, the GP will only interpolate the selected subset. Typically, one should not need point selection in trust-region methods because a small number of points are used to develop a surrogate within each trust region. Point selection is most beneficial when constructing with a large number of points, typically more than order one hundred, though this depends on the number of variables and spacing of the sample points.
6.2. METHOD

This differs from the point_selection option of the Dakota GP which initially chooses a well-spaced subset of points and finds the correlation parameters that are most likely for that one subset.

\texttt{build_samples}

- Keywords Area
- method
- bayes_calibration
- queso
- emulator
- gaussian_process
- build_samples

Number of initial model evaluations used in build phase

**Specification**

Alias: none

**Argument(s):** INTEGER

**Description**

The number of build points or training points used in the initial phase of an algorithm or model construction. Typically these are the initial set of data points used to construct (train) a surrogate model (emulator). If the number of \texttt{build_samples} is less than the minimum number of points required to build the surrogate, Dakota will augment the samples to obtain the minimum required.

**Examples**

Perform GP-based adaptive importance sampling, building the GP with 100 points and then performing 100 approximate evaluations to evaluate the probability.

```plaintext
method
  gpais
    build_samples = 100
    samples_on_emulator = 100
    max_iterations = 5
    response_levels = -1.065
```

**posterior_adaptive**

- Keywords Area
- method
- bayes_calibration
- queso
CHAPTER 6. KEYWORDS AREA

- emulator
- gaussian_process
- posterior_adaptive

Adapt emulator model to increase accuracy in high posterior probability regions

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

Following an emulator-based MCMC process, this option refines the emulator by selecting points in regions of high posterior probability, performing truth evaluations at these points, updating the emulator, and reperforming the MCMC process. The adaptation is continued until the maximum number of iterations is exceeded or the convergence tolerance is met.

**Examples**

```plaintext
bayes_calibration queso
  chain_samples = 2000 seed = 348
delayed_rejection
  emulator
gaussian_process surfpack build_samples = 30
  posterior_adaptive max_iterations = 10
  proposal_covariance derivatives

import_build_points_file

- Keywords Area
- method
- bayes_calibration
- queso
- emulator
- gaussian_process
- import_build_points_file

File containing points you wish to use to build a surrogate

**Specification**

**Alias:** import_points_file

**Argument(s):** STRING

**Default:** no point import from a file
### Description

The `import_build_points_file` allows the user to specify a file that contains a list of points and truth model responses used to construct a surrogate model. These can be used by all methods that (explicitly, e.g. surrogate-based optimization, or implicitly, e.g. efficient global optimization) operate on a surrogate. In particular, these points and responses are used in place of truth model evaluations to construct the initial surrogate. When used to construct surrogate models or emulators these are often called build points or training data.

**Default Behavior**

By default, methods do not import points from a file.

**Usage Tips**

Dakota parses input files without regard to whitespace, but the `import_build_points_file` must be in one of three formats:

- annotated (default)
- custom.annotated
- freeform

**Examples**

```dakota
method
    polynomial_chaos
    expansion_order = 4
    import_build_points_file = 'dakota_uq_rosenbrock_pce_import.annot.pts.dat'
```

**annotated**

- Keywords Area
- method
- bayes_calibration
- queso
Topics
This keyword is related to the topics:

- file formats

Specification
Alias: none
Argument(s): none
Default: annotated format

Description
An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior
By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips
- To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify custom annotated header eval_id
- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples
Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```
environment
  tabular_data
    tabular_data_file = 'dakota_summary.dat'
    annotated

Resulting tabular file:
%eval_id interface x1  x2  obj_fn nln_ineq_con_1 nln_ineq_con_2
1 NO_ID 0.9 1.1 0.0002 0.26 0.76
2 NO_ID 0.90009 1.1 0.0001996404857 0.2601620081 0.759955
3 NO_ID 0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...
```
6.2. METHOD

custom_annotated

- Keywords Area
- method
- bayes_calibration
- queso
- emulator
- gaussian_process
- import_build.points_file
- custom_annotated

Selects custom-annotated tabular file format

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none

Argument(s): none

Default: annotated format

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>header</td>
<td>Enable header row in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>eval_id</td>
<td>Enable evaluation ID column in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>interface_id</td>
<td>Enable interface ID column in custom-annotated tabular file</td>
</tr>
</tbody>
</table>
Description

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

Default Behavior

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

Usage Tips

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:

```plaintext
environment
  tabular_data
    tabular_data_file = 'dakota_summary.dat'
    custom_annotated header eval_id
```

Resulting tabular file:

```
%eval_id x1 x2 obj_fn nln_ineq_con_1 nln_ineq_con_2
1 0.9 1.1 0.0002 0.26 0.76
2 0.90009 1.1 0.0001996404857 0.2601620081 0.759955
3 0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...```

header

- Keywords Area
  - method
    - bayes_calibration
  - qeso
  - emulator
    - gaussian_process
    - import_build_points_file
    - custom_annotated
    - header

Enable header row in custom-annotated tabular file
6.2. METHOD

Specification

Alias: none
  Argument(s): none
  Default: no header

Description

See description of parent custom_annotated

eval_id
  • Keywords Area
  • method
  • bayes_calibration
  • queso
  • emulator
  • gaussian_process
  • import_build_points_file
  • custom_annotated
  • eval_id

Enable evaluation ID column in custom-annotated tabular file

Specification

Alias: none
  Argument(s): none
  Default: no eval_id column

Description

See description of parent custom_annotated

interface_id
  • Keywords Area
  • method
  • bayes_calibration
  • queso
  • emulator
  • gaussian_process
• import_build_points_file

• custom.annotated

• interface_id

Enable interface ID column in custom-annotated tabular file

**Specification**

Alias: none

Argument(s): none

Default: no interface_id column

**Description**

See description of parent custom.annotated

**freeform**

• Keywords Area

• method

• bayes_calibration

• queso

• emulator

• gaussian_process

• import_build_points_file

• freeform

Selects freeform file format

**Topics**

This keyword is related to the topics:

• file_formats

**Specification**

Alias: none

Argument(s): none

Default: annotated format
6.2. METHOD

Description

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior

The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips

- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```python
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
freeform
```

Resulting tabular file:

```
0.9  1.1  0.0002  0.26  0.76
0.90009  1.1  0.0001996404857  0.2601620081  0.759955
0.89991  1.1  0.0002003604863  0.2598380081  0.760045
...
```

active_only

- Keywords Area
- method
- bayes_calibration
- queo
- emulator
- gaussian_process
- import_build_points_file
- active_only

Import only active variables from tabular data file
CHAPTER 6. KEYWORDS AREA

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none

Argument(s): none

Description

By default, files for tabular data imports are expected to contain columns for all variables, active and inactive. The keyword `active_only` indicates that the file to import contains only the active variables.

This option should only be used in contexts where the inactive variables have no influence, for example, building a surrogate over active variables, with the state variables held at nominal. It should not be used in more complex nested contexts, where the values of inactive variables are relevant to the function evaluations used to build the surrogate.

pce

- Keywords Area
- method
- bayes_calibration
- queso
- emulator
- pce

Polynomial Chaos Expansion surrogate model

Specification

Alias: none

Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required (Choose One)</td>
<td>sparse_grid_level_sequence</td>
<td>sparse_grid_level_sequence</td>
<td>Level to use in sparse grid integration or interpolation</td>
</tr>
</tbody>
</table>
6.2. METHOD

<table>
<thead>
<tr>
<th>expansion_order_sequence</th>
<th>The (initial) order of a polynomial expansion</th>
</tr>
</thead>
<tbody>
<tr>
<td>orthogonal_least_interpolation</td>
<td>Build a polynomial chaos expansion from simulation samples using orthogonal least interpolation.</td>
</tr>
</tbody>
</table>

**Description**

Selects a polynomial chaos expansion (PCE) surrogate model to use in the Bayesian likelihood calculations. When using PCE as a surrogate within the Bayesian framework, the PCE coefficients can be computed either from integration using a sparse grid or from regression using a random/unstructured data set.

**See Also**

These keywords may also be of interest:

- polynomial_chaos
- sparse_grid_level_sequence

- Keywords Area
- method
- bayes_calibration
- queso
- emulator
- pce
- sparse_grid_level_sequence

Level to use in sparse grid integration or interpolation

**Specification**

- **Alias:** none
- **Argument(s):** INTEGERLIST

**Description**

Multi-dimensional integration by the Smolyak sparse grid method (specified with sparse_grid_level and, optionally, dimension_preference). The underlying one-dimensional integration rules are the same as for the tensor-product quadrature case; however, the default rule selection is nested for sparse grids (Genz-Keister for normals/transformed normals and Gauss-Patterson for uniforms/transformed uniforms). This default can be overridden with an explicit non_nested specification (resulting in Gauss-Hermite for normals/transformed normals.
and Gauss-Legendre for uniforms/transformed uniforms). As for tensor quadrature, the dimension_preference specification enables the use of anisotropic sparse grids (refer to the PCE description in the User’s Manual for the anisotropic index set constraint definition). Similar to anisotropic tensor grids, the dimension with greatest preference will have resolution at the full sparse_grid_level and all other dimension resolutions will be reduced in proportion to their reduced preference. For PCE with either isotropic or anisotropic sparse grids, a summation of tensor-product expansions is used, where each anisotropic tensor-product quadrature rule underlying the sparse grid construction results in its own anisotropic tensor-product expansion as described in case 1. These anisotropic tensor-product expansions are summed into a sparse PCE using the standard Smolyak summation (again, refer to the User’s Manual for additional details). As for quadrature_order, the sparse_grid_level specification admits an array input for enabling specification of multiple grid resolutions used by certain advanced solution methodologies.

**Usage Tips**

This keyword can be used when using sparse grid integration to calculate PCE coefficients or when generating samples for sparse grid collocation.

For most use cases, this keyword will specify a single integer level. In more advanced UQ studies with hierarchical models, the list of integers can apply to different models and/or model levels

```
expansion_order_sequence
```

- **Keywords Area**
- **method**
- **bayes_calibration**
- **queso**
- **emulator**
- **pce**
- **expansion_order_sequence**

The (initial) order of a polynomial expansion

**Specification**

**Alias:** none

**Argument(s):** INTEGERLIST

<table>
<thead>
<tr>
<th>Required/-Optional Required</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Group</strong></td>
<td><strong>Group 1</strong></td>
<td><strong>collocation_points_sequence</strong></td>
<td>Number of collocation points to estimate PCE coefficients</td>
</tr>
</tbody>
</table>
6.2. METHOD

| Optional | collocation_ratio | Set the number of points used to build a PCE via regression to be proportional to the number of terms in the expansion. |
| Optional | cross_validation | Use cross validation to choose the 'best' polynomial order of a polynomial chaos expansion. |
| Optional | posterior_adaptive | Adapt emulator model to increase accuracy in high posterior probability regions |
| Optional | import_build-points_file | File containing points you wish to use to build a surrogate |

Description

When the expansion order for a polynomial chaos expansion is specified, the coefficients may be computed by integration based on random samples or by regression using either random or sub-sampled tensor product quadrature points.

Multidimensional integration by Latin hypercube sampling (specified with `expansion_samples`). In this case, the expansion order $p$ cannot be inferred from the numerical integration specification and it is necessary to provide an `expansion_order` to specify $p$ for a total-order expansion.

Linear regression (specified with either `collocation_points` or `collocation_ratio`). A total-order expansion is used and must be specified using `expansion_order` as described in the previous option. To avoid requiring the user to calculate $N$ from $n$ and $p$, the `collocation_ratio` allows for specification of a constant factor applied to $N$ (e.g., `collocation_ratio = 2` produces samples $= 2N$). In addition, the default linear relationship with $N$ can be overridden using a real-valued exponent specified using `ratio_order`. In this case, the number of samples becomes $cN^o$ where $c$ is the `collocation_ratio` and $o$ is the `ratio_order`. The `use_derivatives` flag informs the regression approach to include derivative matching equations (limited to gradients at present) in the least squares solutions, enabling the use of fewer collocation points for a given expansion order and dimension (number of points required becomes $\frac{cN^o}{n+1}$). When admissible, a constrained least squares approach is employed in which response values are first reproduced exactly and error in reproducing response derivatives is minimized. Two collocation grid options are supported: the default is Latin hypercube sampling ("point collocation"), and an alternate approach of "probabilistic collocation" is also available through inclusion of the `tensor_grid` keyword. In this alternate case, the collocation grid is defined using a subset of tensor-product quadrature points: the order of the tensor-product grid is selected as one more than the expansion order in each dimension (to avoid sampling at roots of the basis polynomials) and then the tensor multi-index is uniformly sampled to generate a non-repeated subset of tensor quadrature points.
If \texttt{collocation\_points} or \texttt{collocation\_ratio} is specified, the PCE coefficients will be determined by regression. If no regression specification is provided, appropriate defaults are defined. Specifically SVD-based least-squares will be used for solving over-determined systems and under-determined systems will be solved using LASSO. For the situation when the number of function values is smaller than the number of terms in a PCE, but the total number of samples including gradient values is greater than the number of terms, the resulting over-determined system will be solved using equality constrained least squares. Technical information on the various methods listed below can be found in the Linear regression section of the Theory Manual. Some of the regression methods (OMP, LASSO, and LARS) are able to produce a set of possible PCE coefficient vectors (see the Linear regression section in the Theory Manual). If cross validation is inactive, then only one solution, consistent with the \texttt{noise\_tolerance}, will be returned. If cross validation is active, Dakota will choose between possible coefficient vectors found internally by the regression method across the set of expansion orders (1,...,\texttt{expansion\_order}) and the set of specified noise tolerances and return the one with the lowest cross validation error indicator.

**Usage Tips**

For most use cases, this keyword will specify a single integer order. In more advanced UQ studies with hierarchical models, the list of integers can apply to different models and/or model levels.

\begin{verbatim}
  collocation\_points\_sequence
  \hspace{0.5cm} Keyword: Keywords Area
  \hspace{0.5cm} Method
  \hspace{0.5cm} bayes\_calibration
  \hspace{0.5cm} queso
  \hspace{0.5cm} emulator
  \hspace{0.5cm} pce
  \hspace{0.5cm} expansion\_order\_sequence
  \hspace{0.5cm} collocation\_points\_sequence

  Number of collocation points to estimate PCE coefficients
\end{verbatim}

**Specification**

Alias: none

\texttt{Argument(s): INTEGERLIST}

**Description**

Specify the number of collocation points used to estimate PCE coefficients using regression or orthogonal-least-interpolation.

**Usage Tips**

For most use cases, this keyword will specify a single integer number of points. In more advanced UQ studies with hierarchical models, the list of integers can apply to different models and/or model levels.
collocation_ratio

- Keywords Area
- method
- bayes_calibration
- qeso
- emulator
- pce
- expansion_order_sequence
- collocation_ratio

Set the number of points used to build a PCE via regression to be proportional to the number of terms in the expansion.

**Specification**

**Alias:** none

**Argument(s):** REAL

**Description**

Set the number of points used to build a PCE via regression to be proportional to the number of terms in the expansion. To avoid requiring the user to calculate N from n and p, the collocation_ratio allows for specification of a constant factor applied to N (e.g., collocation_ratio = 2. produces samples = 2N). In addition, the default linear relationship with N can be overridden using a real-valued exponent specified using ratio_order. In this case, the number of samples becomes $cN^o$ where $c$ is the collocation_ratio and $o$ is the ratio_order. The use_derivatives flag informs the regression approach to include derivative matching equations (limited to gradients at present) in the least squares solutions, enabling the use of fewer collocation points for a given expansion order and dimension (number of points required becomes $\frac{cN^o}{n+1}$).

cross_validation

- Keywords Area
- method
- bayes_calibration
- qeso
- emulator
- pce
- expansion_order_sequence
- cross_validation

Use cross validation to choose the ‘best’ polynomial order of a polynomial chaos expansion.
CHAPTER 6. KEYWORDS AREA

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

Use cross validation to choose the 'best' polynomial degree of a polynomial chaos expansion. 10 fold cross validation is used to estimate the cross validation error of a total-order polynomial expansion for orders 1 through to order. The order chosen is the one that produces the lowest cross validation error. If there are not enough points to perform 10 fold cross validation then one-at-a-time cross validation will be performed.

**Examples**

```
bayes_calibration queso
chain_samples = 2000 seed = 348
delayed_rejection
emulator
gaussian_process surfpack build_samples = 30
posterior_adaptive max_iterations = 10
proposal_covariance derivatives
```
6.2. METHOD

import_build_points_file

- Keywords Area
- method
- bayes_calibration
- queso
- emulator
- pce
- expansion_order_sequence
- import_build_points_file

File containing points you wish to use to build a surrogate

Specification

Alias: import_points_file

Argument(s): STRING

Default: no point import from a file

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional/Choose One</td>
<td>Tabular Format (Group 1)</td>
<td>annotated</td>
<td>Selects annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>custom_annotated</td>
<td>Selects custom-annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>freeform</td>
<td>Selects freeform file format</td>
</tr>
<tr>
<td>Optional</td>
<td>active_only</td>
<td>Import only active variables from tabular data file</td>
<td></td>
</tr>
</tbody>
</table>

Description

The import_build_points_file allows the user to specify a file that contains a list of points and truth model responses used to construct a surrogate model. These can be used by all methods that (explicitly, e.g. surrogate-based optimization, or implicitly, e.g. efficient global optimization) operate on a surrogate. In particular, these points and responses are used in place of truth model evaluations to construct the initial surrogate. When used to construct surrogate models or emulators these are often called build points or training data.

Default Behavior

By default, methods do not import points from a file.

Usage Tips

Dakota parses input files without regard to whitespace, but the import_build_points_file must be in one of three formats:
• annotated (default)
• custom_annotated
• freeform

Examples
method
  polynomial_grammar
  expansion_order = 4
  import_build_points_file = 'dakota_uq_rosenbrock_pce_import.annot.pts.dat'

annotated
• Keywords Area
• method
• bayes_calibration
• qeso
• emulator
• pce
• expansion_order_sequence
• import_build_points_file
• annotated

Selects annotated tabular file format

Topics
This keyword is related to the topics:
• file_formats

Specification
Alias: none
  Argument(s): none
  Default: annotated format

Description
An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior
By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips
6.2. METHOD

- To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify `custom_annotated header eval_id`

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to `annotated format`, though `freeform` remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the `freeform` option.

### Examples

Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```
environment
  tabular_data
    tabular_data_file = 'dakota_summary.dat'
    annotated

Resulting tabular file:
```

<table>
<thead>
<tr>
<th>eval_id</th>
<th>interface</th>
<th>x1</th>
<th>x2</th>
<th>obj_fn</th>
<th>nln_ineq_con_1</th>
<th>nln_ineq_con_2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 NO_ID</td>
<td></td>
<td>0.9</td>
<td>1.1</td>
<td>0.0002</td>
<td>0.26</td>
<td>0.76</td>
</tr>
<tr>
<td>2 NO_ID</td>
<td></td>
<td>0.90009</td>
<td>1.1</td>
<td>0.0001996404857</td>
<td>0.2601620081</td>
<td>0.759955</td>
</tr>
<tr>
<td>3 NO_ID</td>
<td></td>
<td>0.89991</td>
<td>1.1</td>
<td>0.0002003604863</td>
<td>0.2598380081</td>
<td>0.760045</td>
</tr>
<tr>
<td>...</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### custom_annotated

- Keywords Area

- method

- bayes_calibration

- queso

- emulator

- pce

- expansion_order_sequence

- import_build_points_file

- custom_annotated

Selects custom-annotated tabular file format

### Topics

This keyword is related to the topics:

- file_formats

### Specification

**Alias:** none

**Argument(s):** none

**Default:** annotated format
Description

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

Default Behavior

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

Usage Tips

• Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

• When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

• Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:

```
environment
  tabular_data
    tabular_data_file = 'dakota_summary.dat'
    custom_annotated header eval_id
```

Resulting tabular file:

```
%eval_id  x1  x2  obj_fn  nln_ineq_con_1  nln_ineq_con_2
1 0.9 1.1 0.0002 0.26 0.76
2 0.90009 1.1 0.0001996404857 0.2601620081 0.759955
3 0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...```
6.2. METHOD

header
- Keywords Area
- method
- bayes_calibration
- `qeso`
- emulator
- `pce`
- `expansion_order_sequence`
- import_build_points_file
- custom_annotated
- `header`

Enable header row in custom-annotated tabular file

**Specification**

Alias: none
Argument(s): none
Default: no header

**Description**

See description of parent `custom_annotated`

eval_id
- Keywords Area
- method
- bayes_calibration
- `qeso`
- emulator
- `pce`
- `expansion_order_sequence`
- import_build_points_file
- custom_annotated
- `eval_id`

Enable evaluation ID column in custom-annotated tabular file
CHAPTER 6. KEYWORDS AREA

**Specification**

Alias: none  
Argument(s): none  
**Default:** no eval_id column  

**Description**

See description of parent `custom.annotated`

```plaintext
interface_id
  • Keywords Area
  • method
  • bayes_calibration
  • quo
  • emulator
  • pce
  • expansion_order_sequence
  • import_build_points_file
  • custom.annotated
  • interface_id

Enable interface ID column in custom-annotated tabular file
```

**Specification**

Alias: none  
Argument(s): none  
**Default:** no interface_id column  

**Description**

See description of parent `custom.annotated`

```plaintext
freeform
  • Keywords Area
  • method
  • bayes_calibration
  • quo
  • emulator
```
6.2. METHOD

- `pce`
- `expansion_order_sequence`
- `import_build_points_file`
- `freeform`

Selects freeform file format

Topics

This keyword is related to the topics:

- `file_formats`

Specification

Alias: none

Argument(s): none

Default: annotated format

Description

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior

The annotated format is the default for tabular export/import. To change this behavior, specify `freeform` in the relevant export/import context.

Usage Tips

- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though `freeform` remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- In `freeform`, the `num_rows` x `num_cols` total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the `freeform` option.

Examples

Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```
environment
    tabular_data
        tabular_data_file = 'dakota_summary.dat'
        freeform
```

Resulting tabular file:

```
0.9 1.1 0.0002 0.26 0.76
0.90009 1.1 0.0001996404857 0.2601620081 0.759955
0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...
```
active_only

- Keywords Area
- method
- bayes_calibration
- queso
- emulator
- pce
- expansion_order_sequence
- import_build_points_file
- active_only

Import only active variables from tabular data file

Topics

This keyword is related to the topics:
- file_formats

Specification

Alias: none

Argument(s): none

Description

By default, files for tabular data imports are expected to contain columns for all variables, active and inactive. The keyword active_only indicates that the file to import contains only the active variables.

This option should only be used in contexts where the inactive variables have no influence, for example, building a surrogate over active variables, with the state variables held at nominal. It should not be used in more complex nested contexts, where the values of inactive variables are relevant to the function evaluations used to build the surrogate.

orthogonal_least_interpolation

- Keywords Area
- method
- bayes_calibration
- queso
- emulator
- pce
- orthogonal_least_interpolation

Build a polynomial chaos expansion from simulation samples using orthogonal least interpolation.
6.2. METHOD

Specification

Alias: none

Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required</td>
<td>collocation_points-sequence</td>
<td>posterior_adaptive</td>
<td>Number of collocation points to estimate PCE coefficients</td>
</tr>
<tr>
<td>Optional</td>
<td>import_build-points_file</td>
<td></td>
<td>Adapt emulator model to increase accuracy in high posterior probability regions</td>
</tr>
</tbody>
</table>

Description

Build a polynomial chaos expansion from simulation samples using orthogonal least interpolation. Unlike the other regression methods expansion_order cannot be set. OLI will produce the lowest degree polynomial that interpolates the data

collocation_points_sequence

- Keywords Area
- method
- bayes_calibration
- qeso
- emulator
- pce
- orthogonal_least_interpolation
- collocation_points_sequence

Number of collocation points to estimate PCE coefficients

Specification

Alias: none

Argument(s): INTEGERLIST
Description

Specify the number of collocation points used to estimate PCE coefficients using regression or orthogonal-least-interpolation.

Usage Tips

For most use cases, this keyword will specify a single integer number of points. In more advanced UQ studies with hierarchical models, the list of integers can apply to different models and/or model levels

```
posterior_adaptive
```

- Keywords Area
- method
- bayes_calibration
- queso
- emulator
- pce
- orthogonal_least_interpolation
- posterior_adaptive

Adapt emulator model to increase accuracy in high posterior probability regions

Specification

Alias: none

Argument(s): none

Description

Following an emulator-based MCMC process, this option refines the emulator by selecting points in regions of high posterior probability, performing truth evaluations at these points, updating the emulator, and reperforming the MCMC process. The adaptation is continued until the maximum number of iterations is exceeded or the convergence tolerance is met.

Examples

```
bayes_calibration queso
chain_samples = 2000 seed = 348
delayed_rejection
emulator
gaussian_process surfpack build_samples = 30
posterior_adaptive max_iterations = 10
proposal_covariance derivatives
```
import_build_points_file

- Keywords Area
- method
- bayes_calibration
- queso
- emulator
- pce
- orthogonal_least_interpolation
- import_build_points_file

File containing points you wish to use to build a surrogate

Specification

Alias: import_points_file
Argument(s): STRING
Default: no point import from a file

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional/Choose One</td>
<td>Tabular Format (Group 1)</td>
<td>annotated</td>
<td>Selects annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>custom_annotated</td>
<td>Selects custom-annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>freeform</td>
<td>Selects freeform file format</td>
</tr>
</tbody>
</table>

| Optional          | active_only          | Import only active variables from tabular data file |

Description

The import_build_points_file allows the user to specify a file that contains a list of points and truth model responses used to construct a surrogate model. These can be used by all methods that (explicitly, e.g. surrogate-based optimization, or implicitly, e.g. efficient global optimization) operate on a surrogate. In particular, these points and responses are used in place of truth model evaluations to construct the initial surrogate. When used to construct surrogate models or emulators these are often called build points or training data.

Default Behavior
By default, methods do not import points from a file.

Usage Tips
Dakota parses input files without regard to whitespace, but the import_build_points_file must be in one of three formats:
• annotated (default)
• custom_annotated
• freeform

Examples

method
  polynomial_choas
    expansion_order = 4
    import_build_points_file = 'dakota_uq_rosenbrock_pce_import.annot.pts.dat'

annotated
• Keywords Area
• method
• bayes_calibration
• queso
• emulator
• pce
• orthogonal_least_interpolation
• import_build_points_file
• annotated

Selects annotated tabular file format

Topics

This keyword is related to the topics:

• file_formats

Specification

Alias: none
  Argument(s): none
  Default: annotated format

Description

An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior

By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips
6.2. **METHOD**

- To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify `custom.annotated` header eval id.
- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

### Examples

Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```python
environment
    tabular_data
    tabular_data_file = ‘dakota_summary.dat’
    annotated
```

Resulting tabular file:

```plaintext
%eval_id interface x1 x2 obj_fn nln_ineq_con_1 nln_ineq_con_2
1   NO_ID 0.9 1.1 0.0002 0.26 0.76
2   NO_ID 0.90009 1.1 0.0001996404857 0.2601620081 0.759955
3   NO_ID 0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...```

`custom.annotated`

- Keywords Area
- method
- bayes_calibration
- queso
- emulator
- pce
- orthogonal_least_interpolation
- import_build_points_file
- custom.annotated

Selects custom-annotated tabular file format

### Topics

This keyword is related to the topics:

- file_formats

### Specification

**Alias:** none  
**Argument(s):** none  
**Default:** annotated format
### Description

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

**Default Behavior**

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

**Usage Tips**

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

### Examples

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
custom_annotated header eval_id
```

Resulting tabular file:

```
%eval_id  x1   x2  obj_fn nln_ineq_con_1 nln_ineq_con_2
1    0.9  1.1   0.0002  0.26  0.76
2    0.90009 1.1 0.0001996404857 0.2601620081 0.759955
3    0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...
```
6.2. METHOD

header
• Keywords Area
• method
• bayes_calibration
• queso
• emulator
• pce
• orthogonal_least_interpolation
• import_build_points_file
• custom.annotated
• header

Enable header row in custom-annotated tabular file

Specification
Alias: none
Argument(s): none
Default: no header

Description
See description of parent custom.annotated

eval.id
• Keywords Area
• method
• bayes_calibration
• queso
• emulator
• pce
• orthogonal_least_interpolation
• import_build_points_file
• custom.annotated
• eval.id

Enable evaluation ID column in custom-annotated tabular file
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): none

Default: no eval_id column

Description

See description of parent custom_annotated

interface_id

- Keywords Area
- method
- bayes_calibration
- qeso
- emulator
- pce
- orthogonal_least_interpolation
- import_build_points_file
- custom_annotated
- interface_id

Enable interface ID column in custom-annotated tabular file

Specification

Alias: none

Argument(s): none

Default: no interface_id column

Description

See description of parent custom_annotated

freeform

- Keywords Area
- method
- bayes_calibration
- qeso
- emulator
6.2. **METHOD**

- pce
- orthogonal_least_interpolation
- import_build_points_file
- freeform

Selects freeform file format

**Topics**

This keyword is related to the topics:

- file_formats

**Specification**

*Alias:* none

*Argument(s):* none

*Default:* annotated format

**Description**

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

**Default Behavior**

The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

**Usage Tips**

- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

**Examples**

Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```environment
tabular_data
  tabular_data_file = 'dakota_summary.dat'
  freeform
```

Resulting tabular file:

```plaintext
0.9 1.1 0.0002 0.26 0.76
0.9009 1.1 0.0001996404857 0.2601620081 0.759955
0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...```
The `active_only` keyword is used to indicate that the file to import contains only the active variables. This option should only be used in contexts where the inactive variables have no influence, for example, building a surrogate over active variables, with the state variables held at nominal. It should not be used in more complex nested contexts, where the values of inactive variables are relevant to the function evaluations used to build the surrogate.

**Topics**

This keyword is related to the topics:

- `file_formats`

**Specification**

*Alias:* none  
*Argument(s):* none

**Description**

By default, files for tabular data imports are expected to contain columns for all variables, active and inactive. The keyword `active_only` indicates that the file to import contains only the active variables.

Stochastic Collocation polynomial surrogate model
6.2. METHOD

Specification

Alias: none

<table>
<thead>
<tr>
<th>Required/-Optional Required</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>sparse_grid_level_sequence</td>
<td>Level to use in sparse grid integration or interpolation</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Description

Selects stochastic collocation (SC) model to use in the Bayesian likelihood calculations. When using SC as a surrogate within the Bayesian framework, the build points (training points) for the stochastic collocation are constructed from a sparse grid.

See Also

These keywords may also be of interest:

- stoch_collocation

  sparse_grid_level_sequence

  - Keywords Area
  - method
  - bayes_calibration
  - queeso
  - emulator
  - sc
  - sparse_grid_level_sequence

  Level to use in sparse grid integration or interpolation

Specification

Alias: none

Argument(s): INTEGERLIST
CHAPTER 6. KEYWORDS AREA

Description
Multi-dimensional integration by the Smolyak sparse grid method (specified with sparse_grid_level and, optionally, dimension_preference). The underlying one-dimensional integration rules are the same as for the tensor-product quadrature case; however, the default rule selection is nested for sparse grids (Genz-Keister for normals/transformed normals and Gauss-Patterson for uniforms/transformed uniforms). This default can be overridden with an explicit non_nested specification (resulting in Gauss-Hermite for normals/transformed normals and Gauss-Legendre for uniforms/transformed uniforms). As for tensor quadrature, the dimension_preference specification enables the use of anisotropic sparse grids (refer to the PCE description in the User’s Manual for the anisotropic index set constraint definition). Similar to anisotropic tensor grids, the dimension with greatest preference will have resolution at the full sparse_grid_level and all other dimension resolutions will be reduced in proportion to their reduced preference. For PCE with either isotropic or anisotropic sparse grids, a summation of tensor-product expansions is used, where each anisotropic tensor-product quadrature rule underlying the sparse grid construction results in its own anisotropic tensor-product expansion as described in case 1. These anisotropic tensor-product expansions are summed into a sparse PCE using the standard Smolyak summation (again, refer to the User’s Manual for additional details). As for quadrature_order, the sparse_grid_level specification admits an array input for enabling specification of multiple grid resolutions used by certain advanced solution methodologies.

Usage Tips
This keyword can be used when using sparse grid integration to calculate PCE coefficients or when generating samples for sparse grid collocation.

For most use cases, this keyword will specify a single integer level. In more advanced UQ studies with hierarchical models, the list of integers can apply to different models and/or model levels

use_derivatives

- Keywords Area
- method
- bayes_calibration
- queso
- emulator
- use_derivatives

Use derivative data to construct surrogate models

Specification
Alias: none
Argument(s): none
Default: use function values only

Description
The use_derivatives flag specifies that any available derivative information should be used in global approximation builds, for those global surrogate types that support it (currently, polynomial regression and the Surfpack Gaussian process).

However, its use with Surfpack Gaussian process is not recommended.
**6.2. METHOD**

**standardized_space**
- Keywords Area
- method
- bayes_calibration
- qeso
- standardized_space

Perform Bayesian inference in standardized probability space

**Specification**

*Alias:* none

*Argument(s):* none

**Description**

This option transforms the inference process (MCMC sampling and any emulator model management) into a standardized probability space.

The variable transformations performed are as described in `askey`.

**Default Behavior**

The default for the Gaussian process and no emulator options is to perform inference in the original probability space (no transformation). Polynomial chaos and stochastic collocation emulators, on the other hand, are always formed in standardized probability space, such that the inference process is also performed in this standardized space.

**Expected Output**

The user will see the truth model evaluations performed in the original space, whereas any method diagnostics relating to the MCMC samples (e.g., QUESO data in the outputData directory) will report points and response data (response gradients and Hessians, if present, will differ but response values will not) that correspond to the transformed space.

**Usage Tips**

Selecting `standardized_space` generally has the effect of scaling the random variables to be of comparable magnitude, which can improve the efficiency of the Bayesian inference process.

**Examples**

```plaintext
method, bayes_calibration qeso
    samples = 2000 seed = 348
dram
standardized_space
```

**logit_transform**
- Keywords Area
- method
- bayes_calibration
• logit_transform

Utilize the logit transformation to reduce sample rejection for bounded domains

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

The logit transformation performs an internal variable transformation from bounded domains to unbounded domains in order to reduce sample rejection due to an out-of-bounds condition.

**Default Behavior**

This option is experimental at present, and is therefore defaulted off.

**Usage Tips**

This option can be helpful when regions of high posterior density exist in the corners of a multi-dimensional bounded domain. In these cases, it may be difficult to generate feasible samples from the proposal density, such that transformation to unbounded domains may greatly reduce sample rejection rates.

**Examples**

```plaintext
method, bayes_calibration queso
samples = 2000 seed = 348
dram
logit_transform
```

**export_chain_points_file**

• **Keywords Area**

• **method**

• **bayes_calibration**

• **queso**

• **export_chain_points_file**

Export the MCMC chain to the specified filename

**Specification**

**Alias:** none

**Argument(s):** STRING

**Default:** chain export to default filename
Optional (Choose One) | Tabular Format (Group 1) | annotated | Selects annotated tabular file format
---|---|---|---
| custom_annotated | Selects custom-annotated tabular file format
| freeform | Selects freeform file format

### Description
The filename to which the final MCMC posterior chain will be exported.

**Default Behavior** No export to file.

**Expected Output**
A tabular data file will be produced in the specified format (annotated by default) containing samples from the posterior distribution.

**Usage Tips**
**Additional Discussion**

- **annotated**
  - Keywords Area
  - method
  - bayes_calibration
  - queso
  - export_chain_points_file
  - annotated

Selects annotated tabular file format

### Topics
This keyword is related to the topics:

- file_formats

### Specification
**Alias:** none
**Argument(s):** none
**Default:** annotated
CHAPTER 6. KEYWORDS AREA

Description

An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior

By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips

- To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify custom_annotated header eval_id

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```plaintext
evironment
    tabular_data
        tabular_data_file = 'dakota_summary.dat'
        annotated

Resulting tabular file:

%eval_id interface      x1  x2   obj_fn  nln_ineq_con_1  nln_ineq_con_2
1  NO_ID                0.9 1.1 0.0002  0.26         0.76
2  NO_ID               0.90009 1.1 0.00019964048570.26016200810.759955
3  NO_ID               0.89991 1.1 0.00020036048630.25983800810.760045
...

custom_annotated

- Keywords Area

- method

- bayes_calibration

- queso

- export_chain_points_file

- custom_annotated

Selects custom-annotated tabular file format
6.2. METHOD

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none

Argument(s): none

<p>| Required/- | Description of | Dakota Keyword | Dakota Keyword |</p>
<table>
<thead>
<tr>
<th>Optional</th>
<th>Group</th>
<th></th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>header</td>
<td></td>
<td>Enable header row in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td>eval_id</td>
<td></td>
<td>Enable evaluation ID column in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td>interface_id</td>
<td></td>
<td>Enable interface ID column in custom-annotated tabular file</td>
</tr>
</tbody>
</table>

Description

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

Default Behavior

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom.annotated, followed by options, in the relevant export/import context.

Usage Tips

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:
environment
  tabular_data
    tabular_data_file = 'dakota_summary.dat'
    custom_annotated header eval_id

Resulting tabular file:

<table>
<thead>
<tr>
<th>%eval_id</th>
<th>x1</th>
<th>x2</th>
<th>obj_fn</th>
<th>nln_ineq_con_1</th>
<th>nln_ineq_con_2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.9</td>
<td>1.1</td>
<td>0.0002</td>
<td>0.26</td>
<td>0.76</td>
</tr>
<tr>
<td>2</td>
<td>0.90009</td>
<td>1.1</td>
<td>0.0001996404857</td>
<td>0.2601620081</td>
<td>0.759955</td>
</tr>
<tr>
<td>3</td>
<td>0.89991</td>
<td>1.1</td>
<td>0.0002003604863</td>
<td>0.2598380081</td>
<td>0.760045</td>
</tr>
<tr>
<td>...</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

header

- Keywords Area
- method
- bayes_calibration
- queso
- export_chain_points_file
- custom_annotated
- header

Enable header row in custom-annotated tabular file

Specification

Alias: none
Argument(s): none

Description

See description of parent custom_annotated

eval_id

- Keywords Area
- method
- bayes_calibration
- queso
- export_chain_points_file
- custom_annotated
- eval_id

Enable evaluation ID column in custom-annotated tabular file
6.2. METHOD

Specification

Alias: none
Argument(s): none

Description

See description of parent custom_annotated

interface_id

- Keywords Area
- method
- bayes_calibration
- queso
- export_chain_points_file
- custom_annotated
- interface_id

Enable interface ID column in custom-annotated tabular file

Specification

Alias: none
Argument(s): none

Description

See description of parent custom_annotated

freeform

- Keywords Area
- method
- bayes_calibration
- queso
- export_chain_points_file
- freeform

Selects freeform file format

Topics

This keyword is related to the topics:

- file_formats
CHAPTER 6. KEYWORDS AREA

**Specification**

Alias: none  
**Argument(s):** none  
**Default:** annotated

**Description**

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

**Default Behavior**

The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

**Usage Tips**

- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

**Examples**

Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
freeform
```

Resulting tabular file:

```
0.9 1.1 0.0002 0.26 0.76
0.90009 1.1 0.0001996404857 0.2601620081 0.759955
0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...```

dram

- **Keywords Area**
- **method**
- **bayes_calibration**
- **queso**
- **dram**

Use the DRAM MCMC algorithm
6.2. METHOD

Topics
This keyword is related to the topics:

- bayesian_calibration

Specification
Alias: none
Argument(s): none
Default: dram

Description
The type of Markov Chain Monte Carlo used. This keyword specifies the use of DRAM, (Delayed Rejection Adaptive Metropolis)[39].

Default Behavior
Five MCMC algorithm variants are supported: dram, delayed_rejection, adaptive_metropolis, metropolis_hastings, and multilevel. The default is dram.

Usage Tips
If the user knows very little about the proposal covariance, using dram is a recommended strategy. The proposal covariance is adaptively updated, and the delayed rejection may help improve low acceptance rates.

Examples
```
method,
    bayes_calibration queso
    dram
    samples = 10000 seed = 348
```
Description

This keyword specifies the use of the Delayed Rejection algorithm in which there can be a delay in rejecting samples from the chain. That is, the "DR" part of DRAM is used but the "AM" part is not, rather a regular Metropolis-Hastings algorithm is used.

Default Behavior

Five MCMC algorithm variants are supported: dram, delayed_rejection, adaptive_metropolis, metropolis_hastings, and multilevel. The default is dram.

Usage Tips

If the user knows something about the proposal covariance or the proposal covariance is informed through derivative information, using delayed_rejection is preferred over dram: the proposal covariance is already being informed by derivative information and the adaptive metropolis is not necessary.

Examples

```
method,
    bayes_calibration queso
    delayed_rejection
    samples = 10000 seed = 348
```

See Also

These keywords may also be of interest:

- proposal_covariance

adaptive_metropolis

- Keywords Area
- method
- bayes_calibration
- queso
- adaptive_metropolis

Use the Adaptive Metropolis MCMC algorithm

Topics

This keyword is related to the topics:

- bayesian_calibration

Specification

Alias: none
Argument(s): none
Default: dram
6.2. METHOD

Description

This keyword specifies the use of the Adaptive Metropolis algorithm. That is, the "AM" part of DRAM is used but the "DR" part is not: specifying this keyword activates only the Adaptive Metropolis part of the MCMC algorithm, in which the covariance of the proposal density is updated adaptively.

**Default Behavior**

Five MCMC algorithm variants are supported: dram, delayed_rejection, adaptive_metropolis, metropolis_hastings, and multilevel. The default is dram.

**Usage Tips**

If the user knows very little about the proposal covariance, but doesn’t want to incur the cost of using full dram with both delayed rejection and adaptive metropolis, specifying only adaptive_metropolis offers a good strategy.

**Examples**

```plaintext
method,
  bayes_calibration queso
  adaptive_metropolis
  samples = 10000 seed = 348

metropolis_hastings

  • Keywords Area
  • method
  • bayes_calibration
  • queso
  • metropolis_hastings

  Use the Metropolis-Hastings MCMC algorithm
```

**Topics**

This keyword is related to the topics:

- bayesian_calibration

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** dram

**Description**

This keyword specifies the use of a Metropolis-Hastings algorithm for the MCMC chain generation. This means there is no delayed rejection and no adaptive proposal covariance updating as in DRAM.

**Default Behavior**

Five MCMC algorithm variants are supported: dram, delayed_rejection, adaptive_metropolis, metropolis_hastings, and multilevel. The default is dram.
**Usage Tips**
If the user wants to use Metropolis-Hastings, possibly as a comparison to the other methods which involve more chain adaptation, this is the MCMC type to use.

**Examples**
```
method,
  bayes_calibration queso
  metropolis_hastings
  samples = 10000 seed = 348
```

**multilevel**
- Keywords Area
- method
- bayes_calibration
- queso
- multilevel

Use the multilevel MCMC algorithm.

**Topics**
This keyword is related to the topics:
- bayesian_calibration

**Specification**
**Alias:** none
**Argument(s):** none
**Default:** dram

**Description**
Selects the multilevel algorithm described in[70].

**Default Behavior**
Five MCMC algorithm variants are supported: dram, delayed_rejection, adaptive_metropolis, metropolis_hastings, and multilevel. The default is dram.

**Usage Tips**
The multilevel algorithm is a more experimental algorithm than the other MCMC approaches mentioned above. It works well in cases where the prior can be "evolved" to a posterior in a structured way. Currently, the multilevel option is not in production form.

**Examples**
```
method,
  bayes_calibration queso
  multilevel
  samples = 10000 seed = 348
```
6.2. METHOD

rng

- **Keywords Area**
- method
- bayes_calibration
- queso
- rng

Selection of a random number generator

**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** Mersenne twister (mt19937)

<p>| Required/- | Description of | Dakota Keyword | Dakota Keyword Description |</p>
<table>
<thead>
<tr>
<th>Optional Required (Choose One)</th>
<th>Group</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>mt19937</td>
<td>Generates random numbers using the Mersenne twister</td>
</tr>
<tr>
<td></td>
<td></td>
<td>rnum2</td>
<td>Generates pseudo-random numbers using the Pecos package</td>
</tr>
</tbody>
</table>

**Description**

The `rng` keyword is used to indicate a choice of random number generator.

**Default Behavior**

If specified, the `rng` keyword must be accompanied by either `rnum2` (pseudo-random numbers) or `mt19937` (random numbers generated by the Mersenne twister). Otherwise, `mt19937`, the Mersenne twister is used by default.

**Usage Tips**

The default is recommended, as the Mersenne twister is a higher quality random number generator.

**Examples**

```plaintext
method
sampling
  sample_type lhs
  samples = 10
  seed = 98765
  rng rnum2
```
**mt19937**

- **Keywords Area**
- method
- bayes_calibration
- queso
- rng
- mt19937

Generates random numbers using the Mersenne twister

**Specification**

**Alias:** none  
**Argument(s):** none

**Description**

The *mt19937* keyword directs Dakota to use the Mersenne twister to generate random numbers. Additional information can be found on wikipedia: [http://en.wikipedia.org/wiki/Mersenne_twister](http://en.wikipedia.org/wiki/Mersenne_twister).

**Default Behavior**

*mt19937* is the default random number generator. To specify it explicitly in the Dakota input file, however, it must be specified in conjunction with the *rng* keyword.

**Usage Tips**

Use of the Mersenne twister random number generator (*mt19937*) is recommended.

**Examples**

```dakota
method
  sampling
    sample_type lhs
    samples = 10
    seed = 98765
    rng mt19937
```

**rnum2**

- **Keywords Area**
- method
- bayes_calibration
- queso
- rng
- rnum2

Generates pseudo-random numbers using the Pecos package
6.2. METHOD

Specification

Alias: none
Argument(s): none

Description

The rnum2 keyword directs Dakota to use pseudo-random numbers generated by the Pecos package.

Default Behavior

rnum2 is not used by default. To change this behavior, it must be specified in conjunction with the rng keyword.

Usage Tips

Use of the Mersenne twister random number generator (mt19937) is recommended over rnum2.

Examples

method
  sampling
    sample_type lhs
    samples = 10
    seed = 98765
    rng rnum2

pre_solve

- Keywords Area
- method
- bayes_calibration
- queo
- pre_solve

Perform deterministic optimization for MAP before Bayesian calibration

Specification

Alias: none
Argument(s): none
Default: nip pre-solve for emulators

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>sqp</td>
<td>Group 1</td>
<td></td>
<td>Uses a sequential quadratic programming method for underlying optimization</td>
</tr>
</tbody>
</table>
CHAPTER 6. KEYWORDS AREA

<table>
<thead>
<tr>
<th>Keyword</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>nip</td>
<td>Uses a nonlinear interior point method for underlying optimization</td>
</tr>
<tr>
<td>none</td>
<td>Deactivates MAP pre-solve prior to initiating the MCMC process.</td>
</tr>
</tbody>
</table>

**Description**

When specified, Dakota will perform a deterministic derivative-based optimization to maximize the log posterior (minimize the negative log posterior = misfit - log prior + constant normalization factors). The Markov chain in Bayesian calibration will subsequently be started at the best point found in the optimization (the MAP point), which can eliminate the need for "burn in" of the chain in which some initial portion of the chain is discarded. Note that both optimization methods available (sqp and nip) require derivatives of the negative log posterior, either first-order in the case of SQP (with quasi-Newton Hessians from secant updates) or second-order in the case of full-Newton NIP (with explicit Hessian use). The derivatives will be computed from the same model used for the MCMC process; e.g. if an emulator is used, the emulator derivatives will be used, otherwise they will be based on the user’s model specification for the model.

It is important to clarify that the use of the Hessian of the negative log posterior within a full Newton solver does not strictly require Hessians from the model response quantities of interest (QoIs). Rather, the Hessian of the negative log posterior is formed from an exact Hessian of the negative log prior and a misfit Hessian that can be either exact or approximated: the full misfit Hessian can be formed using QoI residuals, gradients, and Hessians or the Gauss-Newton approximate misfit Hessian can be formed using only QoI gradients [6]. This Hessian composition is configured automatically based on MAP solver selection and the emulator’s or simulation model’s support for derivatives.

**Default Behavior** The default MAP pre-solve behavior depends on the use of an emulator model within the inference process.

If there is an emulator (for which derivatives are easily computed), then the MAP pre-solve is active by default and a full Newton NIP formulation is selected if OPT++ is available. The default use of a MAP pre-solve can be overridden using "pre_solve none" and the default selection of OPT++ full Newton NIP can be replaced with NPSOL SQP using "pre_solve sqp." Depending on the emulator’s support for derivatives of the simulated QoI (gradients for dakota GP and stochastic collocation; gradients and Hessians for surfpack GP and polynomial chaos), the contribution of the misfit Hessian to the Hessian of the negative log posterior will be computed either using the full misfit Hessian or its Gauss-Newton approximation (refer to Bayesian chapter in[6]).

If no emulator model is specified, then the pre-solve is bypassed by default and the MCMC chain is initiated from user-specified (or default) initial value for the prior distributions of the random variables. This default can be overridden by specifying "pre_solve nip" for a full Newton NIP solution or "pre_solve sqp" for an NPSOL SQP solution. Both MAP pre-solve approaches require QoI gradients from the simulation model, and the full Newton approach can further leverage QoI Hessians when available (though not required due to the Gauss-Newton approximation, as explained previously).

**Expected Output** When pre-solve is enabled, the output will include a deterministic optimization, followed by a Bayesian calibration. The final results will include the MAP point as well as posterior statistics from the MCMC chain. The MAP point that is reported is the point with highest posterior probability spanning both the pre-solve and the subsequent MCMC chain; it will most commonly reflect the end state of the pre-solve, although it can reflect subsequent improvements from the chain evolution, should they occur.
6.2. METHOD

Examples

```plaintext
method
bayes_calibration queso
samples = 2000 seed = 348
delayed_rejection
emulator
  pce sparse_grid_level = 2
  pre_solve nip # default for emulators

sqp

- Keywords Area
- method
- bayes_calibration
- queso
- pre_solve
- sqp

Uses a sequential quadratic programming method for underlying optimization

Specification

Alias: none
Argument(s): none

Description

Many uncertainty quantification methods solve a constrained optimization problem under the hood. The sqp keyword directs Dakota to use a sequential quadratic programming method to solve that problem. A sequential quadratic programming solves a sequence of linearly constrained quadratic optimization problems to arrive at the solution to the optimization problem.

nip

- Keywords Area
- method
- bayes_calibration
- queso
- pre_solve
- nip

Uses a nonlinear interior point method for underlying optimization
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none
  Argument(s): none

Description

Many uncertainty quantification methods solve a constrained optimization problem under the hood. The nip keyword directs Dakota to use a nonlinear interior point to solve that problem. A nonlinear interior point method traverses the interior of the feasible region to arrive at the solution to the optimization problem.

none
  • Keywords Area
  • method
  • bayes_calibration
  • queso
  • pre_solve
  • none

Deactivates MAP pre-solve prior to initiating the MCMC process.

Specification

Alias: none
  Argument(s): none

Description

Pre-solving for the maximum a posteriori probability (MAP) point could be undesirable when testing MCMC performance or too expensive to pursue in some settings. The option "none" provides an override that deactivates the pre-solve option for cases where it would normally be active by default (e.g., for emulator models).

proposal_covariance
  • Keywords Area
  • method
  • bayes_calibration
  • queso
  • proposal_covariance

Defines the technique used to generate the MCMC proposal covariance.
6.2. METHOD

Topics

This keyword is related to the topics:

- bayesian_calibration

Specification

Alias: none

Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required (Choose One)</td>
<td>Group 1</td>
<td>derivatives</td>
<td>Use derivatives to inform the MCMC proposal covariance.</td>
</tr>
<tr>
<td>prior</td>
<td>Uses the covariance of the prior distributions to define the MCMC proposal covariance.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>values</td>
<td>Specifies matrix values to use as the MCMC proposal covariance.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>filename</td>
<td>Uses a file to import a user-specified MCMC proposal covariance.</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Description

The proposal covariance is used to define a multivariate normal (MVN) jumping distribution used to create new points within a Markov chain. That is, a new point in the chain is determined by sampling within a MVN probability density with prescribed covariance that is centered at the current chain point. The accuracy of the proposal covariance has a significant effect on rejection rates and the efficiency of chain mixing.

Default Behavior

The default proposal covariance is prior when no emulator is present; derivatives when an emulator is present.

Expected Output

The effect of the proposal covariance is reflected in the MCMC chain values and the rejection rates, which can be seen in the diagnostic outputs from the QUESO solver within the QuesoDiagnostics directory.

Usage Tips
When derivative information is available inexpensively (e.g., from an emulator model), the derived-based proposal covariance forms a more accurate proposal distribution, resulting in lower rejection rates and faster chain mixing.

**derivatives**

- **Keywords Area**
- **method**
- **bayes_calibration**
- **queso**
- **proposal_covariance**
- **derivatives**

Use derivatives to inform the MCMC proposal covariance.

**Topics**

This keyword is related to the topics:

- **bayesian_calibration**

**Specification**

**Alias:** none  
**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>Group</td>
<td></td>
<td>Description</td>
</tr>
<tr>
<td>Optional</td>
<td>proposal_updates</td>
<td>restarts the MCMC chain with updated derivative-based proposal covariance.</td>
<td></td>
</tr>
</tbody>
</table>

**Description**

This keyword selection results in definition of the MCMC proposal covariance from the Hessian of the misfit function (negative log likelihood), where this Hessian is defined from either a Gauss-Newton approximation (using only first derivatives of the calibration terms) or a full Hessian (using values, first derivatives, and second derivatives of the calibration terms). If this Hessian is indeterminate, it will be corrected as described in [6].

**Default Behavior** The default is prior based proposal covariance. This is a more advanced option that exploits structure in the form of the likelihood.

**Expected Output**

When derivatives are specified for defining the proposal covariance, the misfit Hessian and its inverse (the MVN proposal covariance) will be output to the standard output stream.

**Usage Tips**
6.2. METHOD

The full Hessian of the misfit is used when either supported by the emulator in use (for PCE and surfpack GP, but not SC or dakota GP) or by the user’s response specification (Hessian type is not "no_hessians"), in the case of no emulator. When this full Hessian is indefinite and cannot be inverted to form the proposal covariance, fallback to the positive semi-definite Gauss-Newton Hessian is employed.

Since this proposal covariance is locally accurate, it should be updated periodically using the proposal_updates option. While the adaptive metropolis option can be used in combination with derivative-based preconditioning, it is generally preferable to instead increase the proposal update frequency due to the improved local accuracy of this approach.

Examples

```plaintext
method
    bayes_calibration queso
        samples = 2000 seed = 348
        delayed_rejection
        emulator pce sparse_grid_level = 2
        proposal_covariance derivatives # default proposal_updates

proposal_updates

• Keywords Area
• method
• bayes_calibration
• queso
• proposal_covariance
• derivatives
• proposal_updates

Restarts the MCMC chain with updated derivative-based proposal covariance.

Specification

Alias: none

Argument(s): INTEGER

Description

When employing derivative-based proposal covariance, this specification defines the number of restarts that are performed during the course of the total sample size of the MCMC chain. For each restart, a new chain is initiated from the final point in the previous acceptance chain using updated proposal covariance corresponding to the derivatives values at the new starting point.

Default Behavior

If proposal_updates is not specified, then the default frequency for restarting the chain with updated proposal covariance is every 100 samples.

Expected Output

Each restarted chain will generate a new QUESO header and sampling summary, and the chain diagnostics will be appended within the outputData directory.

Usage Tips
proposal_updates should be tailored to the size of the total chain, accounting for the relative expense of derivative-based proposal updates.

**Examples**

```plaintext
method,
  bayes_calibration queso
  samples = 2000 seed = 348
  delayed_rejection
  emulator pce sparse_grid_level = 2
  proposal_covariance derivatives
    proposal_updates = 50 # restarted chains, each with 40 new points
```

**prior**

- Keywords Area
- method
- bayes_calibration
- queso
- proposal_covariance
- prior

Uses the covariance of the prior distributions to define the MCMC proposal covariance.

**Topics**

This keyword is related to the topics:

- bayesian_calibration

**Specification**

Alias: none

**Argument(s):** none

**Description**

This keyword selection results in definition of the MCMC proposal covariance from the covariance of the prior distributions. This covariance is currently assumed to be diagonal without correlation.

**Default Behavior**

This is the default proposal_covariance option.

**Usage Tips**

Since this proposal covariance is defined globally, the chain does not need to be periodically restarted using local updates to this proposal. However, it is usually effective to adapt the proposal using one of the adaptive metropolis MCMC options.
6.2. METHOD

Examples

```plaintext
method,    
    bayes_calibration queso
    samples = 2000 seed = 348
    dram
    proposal_covariance prior

values

- Keywords Area
- method
- bayes_calibration
- queso
- proposal_covariance
- values

Specifies matrix values to use as the MCMC proposal covariance.

Specification

Alias: none

<table>
<thead>
<tr>
<th>Required/- Required/ Optional</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>diagona One</td>
<td></td>
<td>diagonal</td>
<td>Specifies the diagonal matrix format when specifying a user-specified proposal covariance.</td>
</tr>
<tr>
<td>matrix</td>
<td></td>
<td>matrix</td>
<td>Specifies the full matrix format when specifying a user-specified proposal covariance.</td>
</tr>
</tbody>
</table>

Description

This keyword selection results in definition of the MCMC proposal covariance from user-specified matrix values. The matrix input format must be declared as either a full matrix or a matrix diagonal.

Default Behavior

This option is not the default, and generally implies special a priori knowledge from the user.

Usage Tips

This option is not supported for the case of transformations to standardized probability space.
Examples

method,
    bayes_calibration queso
    samples = 1000 seed = 348
dram
    proposal_covariance
    values ... # See leaf nodes for required format option

diagonal

- Keywords Area
- method
- bayes_calibration
- queso
- proposal_covariance
- values
- diagonal

Specifies the diagonal matrix format when specifying a user-specified proposal covariance.

Specification

Alias: none
  Argument(s): none

Description

When specifying the MCMC proposal covariance in an input file, this keyword declares the use of a diagonal matrix format, i.e., the user only provides the (positive) values along the diagonal.

Examples

method,
    bayes_calibration queso
    samples = 1000 seed = 348
dram
    proposal_covariance
    values 1.0e6 1.0e-1
6.2. METHOD

- values
- matrix

Specifies the full matrix format when specifying a user-specified proposal covariance.

Specification

Alias: none
Argument(s): none

Description

When specifying the MCMC proposal covariance in an input file, this keyword declares the use of a full matrix format, i.e., the user provides all values of the matrix, not just the diagonal. The matrix must be symmetric, positive-definite.

Examples

```
method,
bayes_calibration queso
samples = 1000 seed = 348
dram
proposal_covariance
  matrix values 1.0 0.1
    0.1 2.0
```

filename

- Keywords Area
- method
- bayes_calibration
- queso
- proposal_covariance
- filename

Uses a file to import a user-specified MCMC proposal covariance.

Specification

Alias: none
Argument(s): STRING
## Description

This keyword selection results in definition of the MCMC proposal covariance from importing data a user-specified filename. This import must be declared as either a full matrix or a matrix diagonal.

### Default Behavior

This option is not the default, and generally implies special a priori knowledge from the user.

### Usage Tips

This option is not supported for the case of transformations to standardized probability space.

## Examples

```plaintext
method,
  bayes_calibration queso
  samples = 1000 seed = 348
  dram
  proposal_covariance
    filename ... # See leaf nodes for required format option
```

### diagonal

- Keywords Area
- method
- bayes_calibration
- queso
- proposal_covariance
- filename
- diagonal

Specifies the diagonal matrix format when importing a user-specified proposal covariance.
6.2. METHOD

Specification

Alias: none
  Argument(s): none

Description

When importing the MCMC proposal covariance from a user-specified filename, this keyword declares the use of a diagonal matrix format, i.e., the user only provides the (positive) values along the diagonal.

Examples

```
method, bayes_calibration queso
  samples = 1000 seed = 348
dram
  proposal_covariance
    diagonal filename 'dakota_cantilever_queso.diag.dat'
```

```
matrix
  Keywords Area
  method
  bayes_calibration
  queso
  proposal_covariance
  filename
  matrix
```

Specifies the full matrix format when importing a user-specified proposal covariance.

Specification

Alias: none
  Argument(s): none

Description

When importing the MCMC proposal covariance from a user-specified filename, this keyword declares the use of a full matrix format, i.e., the user provides all values of the matrix, not just the diagonal. The matrix must be symmetric, positive-definite.

Examples

```
method, bayes_calibration queso
  samples = 1000 seed = 348
dram
  proposal_covariance
    matrix filename 'dakota_cantilever_queso.matrix.dat'
```


**gpmsa**
- **Keywords Area**
- **method**
- **bayes.calibration**
- **gpmsa**

(Experimental) Gaussian Process Models for Simulation Analysis (GPMSA) Bayesian calibration

**Topics**
This keyword is related to the topics:
- **package_queso**
- **bayesian_calibration**

**Specification**

**Alias:** none

**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>chain_samples</td>
<td>Number of Markov Chain Monte Carlo posterior samples</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>seed</td>
<td>Seed of the random number generator</td>
</tr>
<tr>
<td>Required</td>
<td></td>
<td>build_samples</td>
<td>Number of initial model evaluations used in build phase</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>import_build_points_file</td>
<td>File containing points you wish to use to build a surrogate</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>standardized_space</td>
<td>Perform Bayesian inference in standardized probability space</td>
</tr>
</tbody>
</table>
6.2. Method

<table>
<thead>
<tr>
<th>Optional</th>
<th>logit_transform</th>
<th>Utilize the logit transformation to reduce sample rejection for bounded domains</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>gpmsa_normalize</td>
<td>Enable GPMSA-internal normalization</td>
</tr>
<tr>
<td>Optional</td>
<td>export_chain-points_file</td>
<td>Export the MCMC chain to the specified filename</td>
</tr>
<tr>
<td>Optional (Choose One)</td>
<td>dram</td>
<td>Use the DRAM MCMC algorithm</td>
</tr>
<tr>
<td>Optional</td>
<td>delayed_rejection</td>
<td>Use the Delayed Rejection MCMC algorithm</td>
</tr>
<tr>
<td>Optional</td>
<td>adaptive-metropolis</td>
<td>Use the Adaptive Metropolis MCMC algorithm</td>
</tr>
<tr>
<td>Optional</td>
<td>metropolis-hastings</td>
<td>Use the Metropolis--Hastings MCMC algorithm</td>
</tr>
<tr>
<td>Optional</td>
<td>rng</td>
<td>Selection of a random number generator</td>
</tr>
<tr>
<td>Optional</td>
<td>proposal-covariance</td>
<td>Defines the technique used to generate the MCMC proposal covariance.</td>
</tr>
</tbody>
</table>
### Description

GPMSA (Gaussian Process Models for Simulation Analysis) is a surrogate-based Markov Chain Monte Carlo Bayesian calibration method. Dakota’s GPMSA is an experimental capability and not ready for production use at this time.

Central to GPMSA is the construction of a Gaussian Process emulator from simulation runs collected at various settings of input parameters. The emulator is a statistical model of the system response, and it is used to incorporate the observational data to improve system predictions and constrain or calibrate the unknown parameters. The GPMSA code draws heavily on the theory developed in the seminal Bayesian calibration paper by Kennedy and O’Hagan [55]. The particular approach in GPMSA was developed by the Los Alamos National Laboratory statistics group and documented in [48]. Dakota’s GPMSA capability comes from the QUESO package developed at UT Austin.

**Usage Tips:**

Configuring GPMSA essentially involves identifying the simulation build data, the experiment data, the calibration and configuration (state) variables, and any necessary algorithm controls. The GP surrogate model is automatically constructed internal to the algorithm and need not be specified through Dakota input.

Dakota’s GPMSA implementation is not intended for production use. There are a number of known limitations, including:

- Only works for scalar and multivariate responses, not field responses. Field responses will be treated as a single multi-variate response set. Consequently, simulation and experiment data must have the same dimensions.

- When build data is not imported a design of experiments will be conducted over all calibration and scenario variables present.

- Experiment data is required (one cannot pose the simulation data as a set of residuals with the assumption of 0-valued experiments).

- Output and diagnostics are limited. Advanced users will need to examine QUESO output files (potentially written in a transformed scaled space) in the QuesoDiagnostic directory

### Examples

The following input file fragment illustrates GPMSA-based Bayesian calibration of 3 $\beta$ variables with a uniform prior, with 3 configuration (scenario) variables $x$. A total of 60 simulation build points are provided in `sim_data.dat`, which contains columns for each $\beta$, followed by each $x$, and then the simulation response ‘lin’. Each row of the experiment data file `y_exp_with_var.dat` contains the values of the 3 $x$ variables, followed by the value of ‘lin’ and its observation error (variance).

```
method
  bayes_calibration gpmsa
  chain_samples 1000
  seed 2460
build_samples 60
  import_build_points_file 'sim_data.dat' freeform
export_chain_points_file 'posterior.dat'
burn_in_samples = 100 sub_sampling_period = 2
```
6.2. METHOD

posterior_stats kl

variables
uniform_uncertain 3
upper_bounds 0.4500 -0.1000 0.4000
initial_point 0.2750 -0.3000 0.1000
lower_bounds -0.1000 -0.5000 -0.2000
descriptors ‘beta0’ ‘beta1’ ‘beta2’

continuous_state 3
upper_bounds 3 * 1.0
initial_state 3 * 0.5
lower_bounds 3 * 0.0
descriptors ‘x0’ ‘x1’ ‘x2’

responses
descriptors ‘lin’
calibration_terms 1
calibration_data_file ‘y_exp_with_var.dat’
freeform
num_experiments 5
num_config_variables 3
variance_type ‘scalar’
no_gradients
no_hessians

chain_samples

• Keywords Area
• method
• bayes_calibration
• gpmsa
• chain_samples

Number of Markov Chain Monte Carlo posterior samples

Specification

Alias: samples
Argument(s): INTEGER
Default: method-dependent

Description

The chain_samples keyword indicates the number of draws from the posterior distribution to perform. When an emulator is active, this will be the number of samples on the constructed surrogate model.

Default Behavior

The default number of chain samples is method-dependent. QUESO methods use 48576. DREAM uses (number of generations) x (number of chains).

Usage Tips

MCMC methods typically require a large number of chain samples to converge, often thousands to millions.
**Examples**

```
method
    bayes_calibration queso
    chain_samples = 20000
```

**seed**

- **Keywords Area**
- **method**
- **bayes_calibration**
- **gpmsa**
- **seed**

Seed of the random number generator

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** system-generated (non-repeatable)

**Description**

The random **seed** control provides a mechanism for making a stochastic method repeatable. That is, the use of the same random seed in identical studies will generate identical results.

**Default Behavior**

If not specified, the seed is randomly generated.

**Expected Output**

If **seed** is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

**Usage Tips**

If a stochastic study was run without **seed** specified, and the user later wishes to repeat the study using the same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen. That value can then be added to the Dakota input file.

**Examples**

```
method
    sampling
        sample_type lhs
        samples = 10
        seed = 15347
```

**build_samples**

- **Keywords Area**
- **method**
- **bayes_calibration**
6.2. **METHOD**

- gpmsa
- build_samples

Number of initial model evaluations used in build phase

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Description**

The number of build points or training points used in the initial phase of an algorithm or model construction. Typically these are the initial set of data points used to construct (train) a surrogate model (emulator). If the number of build samples is less than the minimum number of points required to build the surrogate, Dakota will augment the samples to obtain the minimum required.

**Examples**

Perform GP-based adaptive importance sampling, building the GP with 100 points and then performing 100 approximate evaluations to evaluate the probability.

```
method gpais
  build_samples = 100
  samples_on_emulator = 100
  max_iterations = 5
  response_levels = -1.065
```

**import_build_points_file**

- Keywords Area
- method
- bayes_calibration
- gpmsa

File containing points you wish to use to build a surrogate

**Specification**

**Alias:** import_points_file

**Argument(s):** STRING

**Default:** no point import from a file

<table>
<thead>
<tr>
<th>Required/- Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

## Description

The `import_build_points_file` allows the user to specify a file that contains a list of points and truth model responses used to construct a surrogate model. These can be used by all methods that (explicitly, e.g. surrogate-based optimization, or implicitly, e.g. efficient global optimization) operate on a surrogate. In particular, these points and responses are used in place of truth model evaluations to construct the initial surrogate. When used to construct surrogate models or emulators these are often called build points or training data.

### Default Behavior

By default, methods do not import points from a file.

### Usage Tips

Dakota parses input files without regard to whitespace, but the `import_build_points_file` must be in one of three formats:

- annotated (default)
- custom_annotated
- freeform

### Examples

```dakota
method polynomial_chaos
  expansion_order = 4
  import_build_points_file = 'dakota_uq_rosenbrock_pce_import.annot.pts.dat'
```

### annotated

- Keywords Area
- method
- bayes_calibration
- gpmsa
- import_build_points_file
- annotated

Selects annotated tabular file format

<table>
<thead>
<tr>
<th>Optional (Choose One)</th>
<th>Tabular Format (Group 1)</th>
<th>annotated</th>
<th>Selects annotated tabular file format</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>custom_annotated</td>
<td>Selects custom-annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>freeform</td>
<td>Selects freeform file format</td>
</tr>
</tbody>
</table>
**6.2. METHOD**

**Topics**

This keyword is related to the topics:

- file_formats

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** annotated format

**Description**

An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

**Default Behavior**

By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

**Usage Tips**

- To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify custom_annotated header eval_id

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

**Examples**

Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
tabular_data_file = ‘dakota_summary.dat’
annotated
```

Resulting tabular file:

```
%eval_id interface x1   x2       obj_fn nln_ineq_con_1 nln_ineq_con_2
1 NO_ID   0.9   1.1 0.0002 0.26 0.76
2 NO_ID   0.90009 1.1 0.0001996404857 0.2601620081 0.759955
3 NO_ID   0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...```
### custom_annotated

- Keywords Area
- method
- bayes_calibration
- gpmsa
- import_build_points_file
- custom_annotated

Selects custom-annotated tabular file format

### Topics

This keyword is related to the topics:

- file_formats

### Specification

**Alias:** none  
**Argument(s):** none  
**Default:** annotated format

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of</th>
<th>Dakota Keyword</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>Group</td>
<td>header</td>
</tr>
<tr>
<td>Optional</td>
<td>eval_id</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>interface_id</td>
<td></td>
</tr>
</tbody>
</table>

**Default Behavior**

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

**Default Behavior**
6.2. METHOD

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

Usage Tips

• Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

• When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

• Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
custom_annotated header eval_id
```

Resulting tabular file:

```
%eval_id x1   x2   obj_fn nln_ineq_con_1 nln_ineq_con_2
1       0.9   1.1   0.0002   0.26    0.76
2       0.90009 1.1 0.0001996404857 0.2601620081 0.759955
3       0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...
```

header

• Keywords Area

• method

• bayes_calibration

• gpmsa

• import_build_points_file

• custom_annotated

• header

Enable header row in custom-annotated tabular file

Specification

Alias: none

Argument(s): none

Default: no header

Description

See description of parent custom_annotated
eval_id

- Keywords Area
- method
- bayes_calibration
- gpmsa
- import_build_points_file
- custom_annotated
- eval_id

Enable evaluation ID column in custom-annotated tabular file

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no eval_id column

**Description**

See description of parent *custom_annotated*

interface_id

- Keywords Area
- method
- bayes_calibration
- gpmsa
- import_build_points_file
- custom_annotated
- interface_id

Enable interface ID column in custom-annotated tabular file

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no interface_id column

**Description**

See description of parent *custom_annotated*
6.2. METHOD

freeform

• Keywords Area

• method

• bayes_calibration

• gpmsa

• import_build_points_file

• freeform

Selects freeform file format

Topics

This keyword is related to the topics:

• file_formats

Specification

Alias: none

Argument(s): none

Default: annotated format

Description

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior

The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips

• Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.

• When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

• In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).

• Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.
Examples
Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
  tabular_data_file = 'dakota_summary.dat'
freeform

Resulting tabular file:

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>0.9</td>
<td>1.1</td>
<td>0.002</td>
<td>0.26</td>
<td>0.76</td>
</tr>
<tr>
<td>0.90009</td>
<td>1.1</td>
<td>0.0001996404857</td>
<td>0.2601620081</td>
<td>0.759955</td>
</tr>
<tr>
<td>0.89991</td>
<td>1.1</td>
<td>0.0002003604863</td>
<td>0.2598380081</td>
<td>0.760045</td>
</tr>
</tbody>
</table>
```

standardized_space

- **Keywords Area**
- **method**
- **bayes_calibration**
- **gpmsa**
- **standardized_space**

Perform Bayesian inference in standardized probability space

Specification

**Alias:** none

**Argument(s):** none

Description

This option transforms the inference process (MCMC sampling and any emulator model management) into a standardized probability space.

The variable transformations performed are as described in `askey`.

**Default Behavior**

The default for the Gaussian process and no emulator options is to perform inference in the original probability space (no transformation). Polynomial chaos and stochastic collocation emulators, on the other hand, are always formed in standardized probability space, such that the inference process is also performed in this standardized space.

**Expected Output**

The user will see the truth model evaluations performed in the original space, whereas any method diagnostics relating to the MCMC samples (e.g., QUESO data in the outputData directory) will report points and response data (response gradients and Hessians, if present, will differ but response values will not) that correspond to the transformed space.

**Usage Tips**

Selecting `standardized_space` generally has the effect of scaling the random variables to be of comparable magnitude, which can improve the efficiency of the Bayesian inference process.
6.2. METHOD

Examples

```plaintext
method, bayes_calibration queso
    samples = 2000 seed = 348
    dram
    standardized_space

logit_transform

- Keywords Area
- method
- bayes_calibration
- gpmsa
- logit_transform

Utilize the logit transformation to reduce sample rejection for bounded domains

Specification

Alias: none
Argument(s): none

Description

The logit transformation performs an internal variable transformation from bounded domains to unbounded domains in order to reduce sample rejection due to an out-of-bounds condition.

Default Behavior

This option is experimental at present, and is therefore defaulted off.

Usage Tips

This option can be helpful when regions of high posterior density exist in the corners of a multi-dimensional bounded domain. In these cases, it may be difficult to generate feasible samples from the proposal density, such that transformation to unbounded domains may greatly reduce sample rejection rates.

Examples

```plaintext
method, bayes_calibration queso
    samples = 2000 seed = 348
    dram
    logit_transform

gpmsa_normalize

- Keywords Area
- method
- bayes_calibration
- gpmsa
- gpmsa_normalize

Enable GPMSA-internal normalization
**Specification**

Alias: none  
Argument(s): none

**Description**

Normalize variables and data (surrogate model build and experiment) when constructing the underlying Gaussian Process emulator. When specified, this option will normalize calibration parameters and configuration (scenario) variables based on the min/max of the build data. It will normalize simulation and experiment data by the mean and variance of the simulation build data.

**Default Behavior**  No GPMSA-specific scaling used.

**Examples**

```
method
  bayes_calibration gpmsa
  chain_samples 1000
  seed 2460
  ...
  gpmsa_normalize
```

```plaintext
export_chain_points_file
```

- Keywords Area
- method
- bayes_calibration
- gpmsa
- export_chain_points_file

Export the MCMC chain to the specified filename

**Specification**

Alias: none  
Argument(s): STRING  
Default: chain export to default filename
6.2. METHOD

| freeform | Selects freeform file format |

**Description**

The filename to which the final MCMC posterior chain will be exported.

*Default Behavior*  No export to file.

**Expected Output**

A tabular data file will be produced in the specified format (annotated by default) containing samples from the posterior distribution.

**Usage Tips**

**Additional Discussion**

annotated

- **Keywords Area**
- method
- bayes_calibration
- gpmsa
- export_chain_points_file
- annotated

Selects annotated tabular file format

**Topics**

This keyword is related to the topics:

- file_formats

**Specification**

*Alias:* none

*Argument(s):* none

*Default:* annotated

**Description**

An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

*Default Behavior*

By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

*Usage Tips*
• To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify `custom_annotated`
  header eval_id

• Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to
  annotated format, though freeform remains an option.

• When importing tabular data, a warning will be generated if a specific number of data are expected, but
  extra is found and an error generated when there is insufficient data.

• Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns,
and data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
annotated
```

Resulting tabular file:

```
%eval_id  interface  x1   x2   obj_fn  nln_ineq_con_1  nln_ineq_con_2
1  NO_ID  0.9   1.1  0.0002  0.26   0.76
2  NO_ID  0.90009  1.1  0.0001996404857  0.2601620081  0.759955
3  NO_ID  0.89991  1.1  0.0002003604863  0.2598380081  0.760045
...```

`custom_annotated`

• Keywords Area
• method
• bayes_calibration
• gpmsa
• export_chain_points_file
• custom_annotated

Selects custom-annotated tabular file format

Topics

This keyword is related to the topics:

• file_formats

Specification

Alias: none

Argument(s): none
6.2. METHOD

| Required/- | Description of | Dakota Keyword | Dakota Keyword Description |
| Optional | Group | header | Enable header row in custom-annotated tabular file |
| eval_id | Enable evaluation ID column in custom-annotated tabular file |
| interface_id | Enable interface ID column in custom-annotated tabular file |

**Description**

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

**Default Behavior**

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

**Usage Tips**

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

**Examples**

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
custom_annotated header eval_id
```

Resulting tabular file:

```plaintext
%eval_id  x1  x2  obj_fn  nln_ineq_con_1  nln_ineq_con_2
1  0.9  1.1  0.0002  0.26  0.76
2  0.90009  1.1  0.0001996404857  0.2601620081  0.759955
3  0.89991  1.1  0.0002003604863  0.2598380081  0.760045
...```


header

- Keywords Area
- method
- bayes_calibration
- gpmsa
- export_chain_points_file
- custom_annotated
- header

Enable header row in custom-annotated tabular file

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

See description of parent `custom_annotated`

- `eval_id`

- Keywords Area
- method
- bayes_calibration
- gpmsa
- export_chain_points_file
- custom_annotated
- `eval_id`

Enable evaluation ID column in custom-annotated tabular file

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

See description of parent `custom_annotated`
6.2. METHOD

interface\_id

- Keywords Area
- method
- bayes\_calibration
- gpmsa
- export\_chain\_points\_file
- custom\_annotated
- interface\_id

Enable interface ID column in custom-annotated tabular file

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

See description of parent custom\_annotated

**freeform**

- Keywords Area
- method
- bayes\_calibration
- gpmsa
- export\_chain\_points\_file
- freeform

Selects freeform file format

**Topics**

This keyword is related to the topics:

- file\_formats

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** annotated
CHAPTER 6. KEYWORDS AREA

Description

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior

The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips

• Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.

• When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

• In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).

• Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export a freeform tabular file containing only data for variables and responses. Input file fragment:

environment
tabular_data
tabular_data_file = ‘dakota_summary.dat’
freeform

Resulting tabular file:

0.9 1.1 0.0002 0.26 0.76
0.90009 1.1 0.0001996404857 0.2601620081 0.759955
0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...

dram

• Keywords Area

• method

• bayes_calibration

• gpmsa

• dram

Use the DRAM MCMC algorithm

Topics

This keyword is related to the topics:

• bayesian_calibration
6.2. METHOD

Specification

Alias: none
  Argument(s): none
  Default: dram

Description

The type of Markov Chain Monte Carlo used. This keyword specifies the use of DRAM, (Delayed Rejection Adaptive Metropolis)[39].

Default Behavior

Five MCMC algorithm variants are supported: dram, delayed_rejection, adaptive_metropolis, metropolis_hastings, and multilevel. The default is dram.

Usage Tips

If the user knows very little about the proposal covariance, using dram is a recommended strategy. The proposal covariance is adaptively updated, and the delayed rejection may help improve low acceptance rates.

Examples

```plaintext
method,
  bayes_calibration queso
  dram
  samples = 10000 seed = 348
```

delayed_rejection

- Keywords Area
- method
- bayes_calibration
- gpmsa
- delayed_rejection

Use the Delayed Rejection MCMC algorithm

Topics

This keyword is related to the topics:

- bayesian_calibration

Specification

Alias: none
  Argument(s): none
  Default: dram
CHAPTER 6. KEYWORDS AREA

Description

This keyword specifies the use of the Delayed Rejection algorithm in which there can be a delay in rejecting samples from the chain. That is, the "DR" part of DRAM is used but the "AM" part is not, rather a regular Metropolis-Hastings algorithm is used.

Default Behavior

Five MCMC algorithm variants are supported: dram, delayed_rejection, adaptive_metropolis, metropolis_hastings, and multilevel. The default is dram.

Usage Tips

If the user knows something about the proposal covariance or the proposal covariance is informed through derivative information, using delayed_rejection is preferred over dram: the proposal covariance is already being informed by derivative information and the adaptive metropolis is not necessary.

Examples

```
method,
    bayes_calibration queso
delayed_rejection
samples = 10000 seed = 348
```

See Also

These keywords may also be of interest:

- proposal_covariance

adaptive_metropolis

- Keywords Area
- method
- bayes_calibration
- gpmsa
- adaptive_metropolis

Use the Adaptive Metropolis MCMC algorithm

Topics

This keyword is related to the topics:

- bayesian_calibration

Specification

Alias: none
Argument(s): none
Default: dram
6.2. METHOD

Description

This keyword specifies the use of the Adaptive Metropolis algorithm. That is, the "AM" part of DRAM is used but the "DR" part is not: specifying this keyword activates only the Adaptive Metropolis part of the MCMC algorithm, in which the covariance of the proposal density is updated adaptively.

Default Behavior

Five MCMC algorithm variants are supported: dram, delayed_rejection, adaptive_metropolis, metropolis_hastings, and multilevel. The default is dram.

Usage Tips

If the user knows very little about the proposal covariance, but doesn’t want to incur the cost of using full dram with both delayed rejection and adaptive metropolis, specifying only adaptive_metropolis offers a good strategy.

Examples

```plaintext
method, 
   bayes_calibration queso 
      adaptive_metropolis 
         samples = 10000 seed = 348
```

Metropolis_hastings

- Keywords Area
- method
- bayes_calibration
- gpmsa
- metropolis_hastings

Use the Metropolis-Hastings MCMC algorithm

Topics

This keyword is related to the topics:

- bayesian_calibration

Specification

Alias: none
Argument(s): none
Default: dram

Description

This keyword specifies the use of a Metropolis-Hastings algorithm for the MCMC chain generation. This means there is no delayed rejection and no adaptive proposal covariance updating as in DRAM.

Default Behavior

Five MCMC algorithm variants are supported: dram, delayed_rejection, adaptive_metropolis, metropolis_hastings, and multilevel. The default is dram.
CHAPTER 6. KEYWORDS AREA

Usage Tips
If the user wants to use Metropolis-Hastings, possibly as a comparison to the other methods which involve more chain adaptation, this is the MCMC type to use.

Examples

```method,
  bayes_calibration queso
  metropolis_hastings
  samples = 10000 seed = 348
```

rng

- Keywords Area
- method
- bayes_calibration
- gpmsa
- rng

Selection of a random number generator

Specification

Alias: none
Argument(s): none
Default: Mersenne twister (mt19937)

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>mt19937</td>
<td>Generates random numbers using the Mersenne twister</td>
<td></td>
</tr>
<tr>
<td>Required</td>
<td>Choose One</td>
<td>rnum2</td>
<td>Generates pseudo-random numbers using the Pecos package</td>
</tr>
</tbody>
</table>

Description

The `rng` keyword is used to indicate a choice of random number generator.

Default Behavior
If specified, the `rng` keyword must be accompanied by either `rnum2` (pseudo-random numbers) or `mt19937` (random numbers generated by the Mersenne twister). Otherwise, `mt19937`, the Mersenne twister is used by default.

Usage Tips
The default is recommended, as the Mersenne twister is a higher quality random number generator.
6.2. METHOD

Examples

```dakota
method sampling
  sample_type lhs
  samples = 10
  seed = 98765
  rng rnum2

mt19937
  • Keywords Area
  • method
  • bayes_calibration
  • gpmsa
  • rng
  • mt19937

Generates random numbers using the Mersenne twister
```

Specification

Alias: none
  Argument(s): none

Description

The mt19937 keyword directs Dakota to use the Mersenne twister to generate random numbers. Additional information can be found on wikipedia: http://en.wikipedia.org/wiki/Mersenne_twister.

Default Behavior

mt19937 is the default random number generator. To specify it explicitly in the Dakota input file, however, it must be specified in conjunction with the rng keyword.

Usage Tips

Use of the Mersenne twister random number generator (mt19937) is recommended.

Examples

```dakota
method sampling
  sample_type lhs
  samples = 10
  seed = 98765
  rng mt19937

rnum2
  • Keywords Area
  • method
  • bayes_calibration
```
**Keywords Area**

- gpmsa
- rng
- rnum2

Generates pseudo-random numbers using the Pecos package

**Specification**

**Alias**: none

**Argument(s)**: none

**Description**

The `rnum2` keyword directs Dakota to use pseudo-random numbers generated by the Pecos package.

**Default Behavior**

`rnum2` is not used by default. To change this behavior, it must be specified in conjunction with the `rng` keyword.

**Usage Tips**

Use of the Mersenne twister random number generator (`mt19937`) is recommended over `rnum2`.

**Examples**

```plaintext
method sampling
  sample_type lhs
  samples = 10
  seed = 98765
  rng rnum2

proposal_covariance
```

**Topics**

This keyword is related to the topics:

- bayesian_calibration

**Specification**

**Alias**: none

**Argument(s)**: none
6.2. METHOD

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required (Choose One)</td>
<td>Group 1</td>
<td>derivatives</td>
<td>Use derivatives to inform the MCMC proposal covariance.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>prior</td>
<td>Uses the covariance of the prior distributions to define the MCMC proposal covariance.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>values</td>
<td>Specifies matrix values to use as the MCMC proposal covariance.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>filename</td>
<td>Uses a file to import a user-specified MCMC proposal covariance.</td>
</tr>
</tbody>
</table>

**Description**

The proposal covariance is used to define a multivariate normal (MVN) jumping distribution used to create new points within a Markov chain. That is, a new point in the chain is determined by sampling within a MVN probability density with prescribed covariance that is centered at the current chain point. The accuracy of the proposal covariance has a significant effect on rejection rates and the efficiency of chain mixing.

**Default Behavior**

The default proposal covariance is `prior` when no emulator is present; `derivatives` when an emulator is present.

**Expected Output**

The effect of the proposal covariance is reflected in the MCMC chain values and the rejection rates, which can be seen in the diagnostic outputs from the QUESO solver within the `QuesoDiagnostics` directory.

**Usage Tips**

When derivative information is available inexpensively (e.g., from an emulator model), the derived-based proposal covariance forms a more accurate proposal distribution, resulting in lower rejection rates and faster chain mixing.

- **derivatives**
  - **Keywords Area**
  - **method**
  - **bayes_calibration**
• gpmsa
• proposal_covariance
• derivatives

Use derivatives to inform the MCMC proposal covariance.

Topics

This keyword is related to the topics:

• bayesian_calibration

Specification

Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>proposal_updates</td>
<td>Restarts the MCMC chain with updated derivative-based proposal covariance.</td>
</tr>
</tbody>
</table>

Description

This keyword selection results in definition of the MCMC proposal covariance from the Hessian of the misfit function (negative log likelihood), where this Hessian is defined from either a Gauss-Newton approximation (using only first derivatives of the calibration terms) or a full Hessian (using values, first derivatives, and second derivatives of the calibration terms). If this Hessian is indeterminate, it will be corrected as described in[6]

Default Behavior  The default is prior based proposal covariance. This is a more advanced option that exploits structure in the form of the likelihood.

Expected Output

When derivatives are specified for defining the proposal covariance, the misfit Hessian and its inverse (the MVN proposal covariance) will be output to the standard output stream.

Usage Tips

The full Hessian of the misfit is used when either supported by the emulator in use (for PCE and surfpack GP, but not SC or dakota GP) or by the user’s response specification (Hessian type is not ”no_hessians”), in the case of no emulator. When this full Hessian is indefinite and cannot be inverted to form the proposal covariance, fallback to the positive semi-definite Gauss-Newton Hessian is employed.

Since this proposal covariance is locally accurate, it should be updated periodically using the proposal_updates option. While the adaptive metropolis option can be used in combination with derivative-based preconditioning, it is generally preferable to instead increase the proposal update frequency due to the improved local accuracy of this approach.
6.2. METHOD

Examples

method,
    bayes_calibration queso
    samples = 2000 seed = 348
delayed_rejection
eulimator pce sparse_grid_level = 2
    proposal_covariance derivatives # default proposal_updates

    proposal_updates
    • Keywords Area
    • method
    • bayes_calibration
    • gpmsa
    • proposal_covariance
    • derivatives
    • proposal_updates

Restarts the MCMC chain with updated derivative-based proposal covariance.

Specification

Alias: none
    Argument(s): INTEGER

Description

When employing derivative-based proposal covariance, this specification defines the number of restarts that are performed during the course of the total sample size of the MCMC chain. For each restart, a new chain is initiated from the final point in the previous acceptance chain using updated proposal covariance corresponding to the derivatives values at the new starting point.

Default Behavior

If proposal_updates is not specified, then the default frequency for restarting the chain with updated proposal covariance is every 100 samples.

Expected Output

Each restarted chain will generate a new QUESO header and sampling summary, and the chain diagnostics will be appended within the outputData directory.

Usage Tips

proposal_updates should be tailored to the size of the total chain, accounting for the relative expense of derivative-based proposal updates.

Examples

method,
    bayes_calibration queso
    samples = 2000 seed = 348
delayed_rejection
eulimator pce sparse_grid_level = 2
    proposal_covariance derivatives
    proposal_updates = 50 # restarted chains, each with 40 new points
prior

- Keywords Area
- method
- bayes_calibration
- gpmsa
- proposal_covariance
- prior

Uses the covariance of the prior distributions to define the MCMC proposal covariance.

Topics
This keyword is related to the topics:

- bayesian_calibration

Specification
Alias: none
Argument(s): none

Description
This keyword selection results in definition of the MCMC proposal covariance from the covariance of the prior distributions. This covariance is currently assumed to be diagonal without correlation.

Default Behavior
This is the default proposal_covariance option.

Usage Tips
Since this proposal covariance is defined globally, the chain does not need to be periodically restarted using local updates to this proposal. However, it is usually effective to adapt the proposal using one of the adaptive metropolis MCMC options.

Examples

```plaintext
method,
  bayes_calibration queso
  samples = 2000 seed = 348
  dram
  proposal_covariance prior
```

values

- Keywords Area
- method
- bayes_calibration
- gpmsa
• proposal_covariance
• values

Specifies matrix values to use as the MCMC proposal covariance.

Specification

Alias: none

Argument(s): REALLIST

<table>
<thead>
<tr>
<th>Required/-Optional Required/Group (Choose One)</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>diagonal</td>
<td>Specifies the diagonal matrix format when specifying a user-specified proposal covariance.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>matrix</td>
<td>Specifies the full matrix format when specifying a user-specified proposal covariance.</td>
</tr>
</tbody>
</table>

Description

This keyword selection results in definition of the MCMC proposal covariance from user-specified matrix values. The matrix input format must be declared as either a full matrix or a matrix diagonal.

Default Behavior

This option is not the default, and generally implies special a priori knowledge from the user.

Usage Tips

This option is not supported for the case of transformations to standardized probability space.

Examples

```
method,
  bayes_calibration queso
  samples = 1000 seed = 348
  dram
  proposal_covariance
    values ... # See leaf nodes for required format option
```

diagonal

• Keywords Area
• method
• bayes_calibration
CHAPTER 6. KEYWORDS AREA

- gpmsa
- proposal_covariance
- values
- diagonal

Specifies the diagonal matrix format when specifying a user-specified proposal covariance.

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

When specifying the MCMC proposal covariance in an input file, this keyword declares the use of a diagonal matrix format, i.e., the user only provides the (positive) values along the diagonal.

**Examples**

```plaintext
method,
  bayes_calibration queso
  samples = 1000 seed = 348
dram
  proposal_covariance
diagonal values 1.0e6 1.0e-1
```

**matrix**

- Keywords Area
- method
- bayes_calibration
- gpmsa
- proposal_covariance
- values
- matrix

Specifies the full matrix format when specifying a user-specified proposal covariance.

**Specification**

**Alias:** none

**Argument(s):** none
6.2. METHOD

Description

When specifying the MCMC proposal covariance in an input file, this keyword declares the use of a full matrix format, i.e., the user provides all values of the matrix, not just the diagonal. The matrix must be symmetric, positive-definite.

Examples

```
method,
   bayes_calibration queso
   samples = 1000 seed = 348
   dram
   proposal_covariance
      matrix values 1.0 0.1
      0.1 2.0
```

**filename**

- Keywords Area
- method
- bayes_calibration
- gpmsa
- proposal_covariance
- filename

Uses a file to import a user-specified MCMC proposal covariance.

Specification

**Alias:** none  
**Argument(s):** STRING

<table>
<thead>
<tr>
<th>Required/-Optional Required(Choose One)</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>diagonal</td>
<td></td>
<td>diagonal</td>
<td>Specifies the diagonal matrix format when importing a user-specified proposal covariance.</td>
</tr>
</tbody>
</table>
matrix

Specifies the full matrix format when importing a user-specified proposal covariance.

Description

This keyword selection results in definition of the MCMC proposal covariance from importing data a user-specified filename. This import must be declared as either a full matrix or a matrix diagonal.

Default Behavior

This option is not the default, and generally implies special a priori knowledge from the user.

Usage Tips

This option is not supported for the case of transformations to standardized probability space.

Examples

```
method,
  bayes_calibration queso
  samples = 1000 seed = 348
dram
  proposal_covariance
    filename ... # See leaf nodes for required format option
```

diagonal

• Keywords Area
• method
• bayes_calibration
• gpmsa
• proposal_covariance
• filename
• diagonal

Specifies the diagonal matrix format when importing a user-specified proposal covariance.

Specification

Alias: none
Argument(s): none

Description

When importing the MCMC proposal covariance from a user-specified filename, this keyword declares the use of a diagonal matrix format, i.e., the user only provides the (positive) values along the diagonal.
6.2. Method

Examples

```
method,
  bayes_calibration queso
  samples = 1000 seed = 348
dram
  proposal_covariance
diagonal filename 'dakota_cantilever_queso.diag.dat'
```

**matrix**

- **Keywords Area**
- **method**
- **bayes_calibration**
- **gpmsa**
- **proposal_covariance**
- **filename**
- **matrix**

Specifies the full matrix format when importing a user-specified proposal covariance.

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

When importing the MCMC proposal covariance from a user-specified filename, this keyword declares the use of a full matrix format, i.e., the user provides all values of the matrix, not just the diagonal. The matrix must be symmetric, positive-definite.

**Examples**

```
method,
  bayes_calibration queso
  samples = 1000 seed = 348
dram
  proposal_covariance
  matrix filename 'dakota_cantilever_queso.matrix.dat'
```

**options_file**

- **Keywords Area**
- **method**
- **bayes Calibration**
- **gpmsa**
- **options_file**

File containing advanced GPMSA options
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): STRING

Description

Allow power users to override default GPMSA options such as hyper-parameter priors.

Default Behavior
No advanced options used.

Usage Tips
Known limitation: When using an options file, QUESO/GPMSA base environment settings from Dakota will be bypassed. It is therefore necessary to set any relevant Dakota defaults in the options file.

Examples

```bash
# FILE: dakota_gpmsa.opts

# Base QUESO Environment options
eval_verbosity = 2
env_subDisplayFileName = QuesoDiagnostics/display
env_subDisplayAllowedSet = 0 1
eval_seed = 2460

# GPMSA Options
gpmsa_emulator_precision_shape = 2.0
gpmsa_emulator_precision_scale = 0.2
gpmsa_emulator_correlation_strength_alpha = 1.0
gpmsa_emulator_correlation_strength_beta = 0.1
gpmsa_discrepancy_precision_shape = 1.0
gpmsa_discrepancy_precision_scale = 1e4
gpmsa_discrepancy_correlation_strength_alpha = 1.0
gpmsa_discrepancy_correlation_strength_beta = 0.1
gpmsa_emulator_data_precision_shape = 3.0
gpmsa_emulator_data_precision_scale = 333.333
```

wasabi

- Keywords Area
- method
- bayes_calibration
- wasabi

(Experimental Method) Non-MCMC Bayesian inference using interval analysis

Specification

Alias: none

Argument(s): none

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table showing the required/optional status, description of group, Dakota keyword, and description of Dakota keyword.
Description

Offers an alternative to Markov Chain Monte Carlo-based Bayesian inference. This is a nascent capability, not yet ready for production use.

Usage Guidelines: The WASABI method requires an emulator model.

Attention: While the emulator specification for WASABI includes the keyword posterior_adaptive, it is not yet operational.

Examples

method
CHAPTER 6. KEYWORDS AREA

```
bayes_calibration
   wasabi

seed
   
   Keywords Area
   
   method
   
   bayes_calibration
   
   wasabi
   
   seed
   
   Seed of the random number generator

Specification

Alias: none

Argument(s): INTEGER

Default: system-generated (non-repeatable)

Description

The random seed control provides a mechanism for making a stochastic method repeatable. That is, the use of the same random seed in identical studies will generate identical results.

Default Behavior

If not specified, the seed is randomly generated.

Expected Output

If seed is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

Usage Tips

If a stochastic study was run without seed specified, and the user later wishes to repeat the study using the same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen. That value can then be added to the Dakota input file.

Examples

```
method
   sampling
       sample_type lhs
       samples = 10
       seed = 15347
```

emulator

   Keywords Area
   
   method
   
   bayes_calibration
   
   wasabi
6.2. METHOD

- emulator

Use an emulator or surrogate model to evaluate the likelihood function

**Specification**

**Alias:** none

**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Required (Choose One)</strong></td>
<td>emulator type (Group 1)</td>
<td>gaussian_process</td>
<td>Gaussian Process surrogate model</td>
</tr>
<tr>
<td></td>
<td></td>
<td>pce</td>
<td>Polynomial Chaos Expansion surrogate model</td>
</tr>
<tr>
<td></td>
<td></td>
<td>sc</td>
<td>Stochastic Collocation polynomial surrogate model</td>
</tr>
</tbody>
</table>

**Optional**

|                       | use_derivatives       | Use derivative data to construct surrogate models |

**Description**

This keyword describes the type of emulator used when calculating the likelihood function for the Bayesian calibration. The emulator can be a Gaussian process, polynomial chaos expansion, or stochastic collocation.

**gaussian_process**

- Keywords Area
- method
- bayes_calibration
- wasabi
- emulator
- gaussian_process

Gaussian Process surrogate model

**Specification**

**Alias:** kriging

**Argument(s):** none

**Default:** Surfpack Gaussian process
**CHAPTER 6. KEYWORDS AREA**

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Required</strong> (Choose One)</td>
<td><strong>Group 1</strong></td>
<td>surfpack</td>
<td>Use the Surfpack version of Gaussian Process surrogates</td>
</tr>
<tr>
<td></td>
<td></td>
<td>dakota</td>
<td>Select the built in Gaussian Process surrogate</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>build_samples</td>
<td>Number of initial model evaluations used in build phase</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>posterior_adaptive</td>
<td>Adapt emulator model to increase accuracy in high posterior probability regions</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>import_build_points_file</td>
<td>File containing points you wish to use to build a surrogate</td>
</tr>
</tbody>
</table>

**Description**

Use the Gaussian process (GP) surrogate from Surfpack, which is specified using the `surfpack` keyword. An alternate version of GP surrogates was available in prior versions of Dakota. **For now, both versions are supported but the dakota version is deprecated and intended to be removed in a future release.**

*Known Issue:* When using discrete variables, there have been sometimes significant differences in surrogate behavior observed across computing platforms in some cases. The cause has not yet been fully diagnosed and is currently under investigation. In addition, guidance on appropriate construction and use of surrogates with discrete variables is under development. In the meantime, users should therefore be aware that there is a risk of inaccurate results when using surrogates with discrete variables.

**surfpack**

- Keywords Area
- method
- bayes_calibration
- wasabi
- emulator
- gaussian_process
- surfpack

Use the Surfpack version of Gaussian Process surrogates
6.2. METHOD

Specification

Alias: none
Argument(s): none

Description

This keyword specifies the use of the Gaussian process that is incorporated in our surface fitting library called Surfpack.

Several user options are available:

1. Optimization methods:
   Maximum Likelihood Estimation (MLE) is used to find the optimal values of the hyper-parameters governing the trend and correlation functions. By default the global optimization method DIRECT is used for MLE, but other options for the optimization method are available. See optimization_method.
   The total number of evaluations of the likelihood function can be controlled using the max_trials keyword followed by a positive integer. Note that the likelihood function does not require running the "truth" model, and is relatively inexpensive to compute.

2. Trend Function:
   The GP models incorporate a parametric trend function whose purpose is to capture large-scale variations. See trend.

3. Correlation Lengths:
   Correlation lengths are usually optimized by Surfpack, however, the user can specify the lengths manually. See correlation_lengths.

4. Ill-conditioning
   One of the major problems in determining the governing values for a Gaussian process or Kriging model is the fact that the correlation matrix can easily become ill-conditioned when there are too many input points close together. Since the predictions from the Gaussian process model involve inverting the correlation matrix, ill-conditioning can lead to poor predictive capability and should be avoided.
   Note that a sufficiently bad sample design could require correlation lengths to be so short that any interpolatory GP model would become inept at extrapolation and interpolation.
   The surfpack model handles ill-conditioning internally by default, but behavior can be modified using

5. Gradient Enhanced Kriging (GEK).
   The use_derivatives keyword will cause the Surfpack GP to be constructed from a combination of function value and gradient information (if available).
   See notes in the Theory section.

Theory

Gradient Enhanced Kriging

Incorporating gradient information will only be beneficial if accurate and inexpensive derivative information is available, and the derivatives are not infinite or nearly so. Here "inexpensive" means that the cost of evaluating a function value plus gradient is comparable to the cost of evaluating only the function value, for example gradients computed by analytical, automatic differentiation, or continuous adjoint techniques. It is not cost effective to use derivatives computed by finite differences. In tests, GEK models built from finite difference derivatives were also
significantly less accurate than those built from analytical derivatives. Note that GEK’s correlation matrix tends to have a significantly worse condition number than Kriging for the same sample design.

This issue was addressed by using a pivoted Cholesky factorization of Kriging’s correlation matrix (which is a small sub-matrix within GEK’s correlation matrix) to rank points by how much unique information they contain. This reordering is then applied to whole points (the function value at a point immediately followed by gradient information at the same point) in GEK’s correlation matrix. A standard non-pivoted Cholesky is then applied to the reordered GEK correlation matrix and a bisection search is used to find the last equation that meets the constraint on the (estimate of) condition number. The cost of performing pivoted Cholesky on Kriging’s correlation matrix is usually negligible compared to the cost of the non-pivoted Cholesky factorization of GEK’s correlation matrix. In tests, it also resulted in more accurate GEK models than when pivoted Cholesky or whole-point-block pivoted Cholesky was performed on GEK’s correlation matrix.

**dakota**
- **Keywords Area**
- **method**
- **bayes_calibration**
- **wasabi**
- **emulator**
- **gaussian_process**
- **dakota**

Select the built-in Gaussian Process surrogate

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

A second version of GP surrogates was available in prior versions of Dakota. **For now, both versions are supported but the dakota version is deprecated and intended to be removed in a future release.**

Historically these models were drastically different, but in Dakota 5.1, they became quite similar. They now differ in that the Surfpack GP has a richer set of features/options and tends to be more accurate than the Dakota version. Due to how the Surfpack GP handles ill-conditioned correlation matrices (which significantly contributes to its greater accuracy), the Surfpack GP can be a factor of two or three slower than Dakota’s. As of Dakota 5.2, the Surfpack implementation is the default in all contexts except Bayesian calibration.

More details on the **gaussian_process** dakota model can be found in[58].

Dakota’s GP deals with ill-conditioning in two ways. First, when it encounters a non-invertible correlation matrix it iteratively increases the size of a “nugget,” but in such cases the resulting approximation smooths rather than interpolates the data. Second, it has a `point_selection` option (default off) that uses a greedy algorithm to select a well-spaced subset of points prior to the construction of the GP. In this case, the GP will only interpolate the selected subset. Typically, one should not need point selection in trust-region methods because a small number of points are used to develop a surrogate within each trust region. Point selection is most beneficial when constructing with a large number of points, typically more than one hundred, though this depends on the number of variables and spacing of the sample points.
This differs from the point_selection option of the Dakota GP which initially chooses a well-spaced subset of points and finds the correlation parameters that are most likely for that one subset.

**build_samples**

- Keywords Area
- method
- bayes_calibration
- wasabi
- emulator
- gaussian_process
- build_samples

Number of initial model evaluations used in build phase

**Specification**

Alias: none

**Argument(s):** INTEGER

**Description**

The number of build points or training points used in the initial phase of an algorithm or model construction. Typically these are the initial set of data points used to construct (train) a surrogate model (emulator). If the number of build_samples is less than the minimum number of points required to build the surrogate, Dakota will augment the samples to obtain the minimum required.

**Examples**

Perform GP-based adaptive importance sampling, building the GP with 100 points and then performing 100 approximate evaluations to evaluate the probability.

```plaintext
method
   gpais
   build_samples = 100
   samples_on_emulator = 100
   max_iterations = 5
   response_levels = -1.065
```

**posterior_adaptive**

- Keywords Area
- method
- bayes_calibration
- wasabi
• emulator
• gaussian_process
• posterior_adaptive

Adapt emulator model to increase accuracy in high posterior probability regions

**Specification**

**Alias:** none  
**Argument(s):** none

**Description**

Following an emulator-based MCMC process, this option refines the emulator by selecting points in regions of high posterior probability, performing truth evaluations at these points, updating the emulator, and reperforming the MCMC process. The adaptation is continued until the maximum number of iterations is exceeded or the convergence tolerance is met.

**Examples**

```latex
bayes_calibration queso  
  chain_samples = 2000 seed = 348  
  delayed_rejection  
  emulator  
    gaussian_process surfpack build_samples = 30  
    posterior_adaptive max_iterations = 10  
    proposal_covariance derivatives

import_build_points_file
```

** Specification**

**Alias:** import_build_points_file  
**Argument(s):** STRING  
**Default:** no point import from a file

**Keyword Area**

**Method**

• bayes_calibration
• wasabi
• emulator
• gaussian_process

File containing points you wish to use to build a surrogate

**Specification**

**Alias:** import_points_file  
**Argument(s):** STRING  
**Default:** no point import from a file
### Description

The `import_build_points_file` allows the user to specify a file that contains a list of points and truth model responses used to construct a surrogate model. These can be used by all methods that (explicitly, e.g. surrogate-based optimization, or implicitly, e.g. efficient global optimization) operate on a surrogate. In particular, these points and responses are used in place of truth model evaluations to construct the initial surrogate. When used to construct surrogate models or emulators these are often called build points or training data.

**Default Behavior**

By default, methods do not import points from a file.

**Usage Tips**

Dakota parses input files without regard to whitespace, but the `import_build_points_file` must be in one of three formats:

- `annotated` (default)
- `custom_annotated`
- `freeform`

**Examples**

```plaintext
method
  polynomial_chaos
    expansion_order = 4
  import_build_points_file = 'dakota_uq_rosenbrock_pce_import.annot.pts.dat'

annotated

  • Keywords Area
  • method
  • bayes_calibration
  • wasabi
```
• emulator
• gaussian_process
• import_build_points_file
• annotated
Selects annotated tabular file format

Topics
This keyword is related to the topics:
• file_formats

Specification
Alias: none
Argument(s): none
Default: annotated format

Description
An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior
By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips
• To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify custom.annotated header eval_id
• Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
• When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
• Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples
Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```plaintext
environment
  tabular_data
  tabular_data_file = 'dakota_summary.dat'
  annotated

Resulting tabular file:
%eval_id interface x1 x2 obj_fn nln_ineq_con_1 nln_ineq_con_2
1 NO_ID 0.9 1.1 0.0002 0.26 0.76
2 NO_ID 0.90009 1.1 0.0001996404857 0.2601620081 0.759955
3 NO_ID 0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...```
6.2. METHOD

custom_annotated

- Keywords Area
- method
- bayes_calibration
- wasabi
- emulator
- gaussian_process
- import_build_points_file
- custom_annotated

Selects custom-annotated tabular file format

**Topics**

This keyword is related to the topics:

- file_formats

**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** annotated format

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>header</td>
<td>eval_id</td>
<td>Enable evaluation ID column in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td>interface_id</td>
<td></td>
<td>Enable interface ID column in custom-annotated tabular file</td>
</tr>
</tbody>
</table>
CHAPTER 6. KEYWORDS AREA

Description

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

Default Behavior

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

Usage Tips

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
custom_annotated header eval_id
```

Resulting tabular file:

```
%eval_id x1 x2 obj_fn nln_ineq_con_1 nln_ineq_con_2
1 0.9 1.1 0.0002 0.26 0.76
2 0.90009 1.1 0.0001996404857 0.2601620081 0.759955
3 0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...
```

header

- Keywords Area
- method
- bayes_calibration
- wasabi
- emulator
- gaussian_process
- import_build_points_file
- custom_annotated
- header

Enable header row in custom-annotated tabular file
6.2. METHOD

Specification

Alias: none
Argument(s): none
Default: no header

Description

See description of parent custom_annotated

eval_id

- Keywords Area
- method
- bayes_calibration
- wasabi
- emulator
- gaussian_process
- import_build_points_file
- custom_annotated
- eval_id

Enable evaluation ID column in custom-annotated tabular file

Specification

Alias: none
Argument(s): none
Default: no eval_id column

Description

See description of parent custom_annotated

interface_id

- Keywords Area
- method
- bayes_calibration
- wasabi
- emulator
- gaussian_process
CHAPTER 6. KEYWORDS AREA

- import
- build
- points_file

- custom.annotated

- interface_id

Enable interface ID column in custom-annotated tabular file

**Specification**

**Alias:** none

- **Argument(s):** none
- **Default:** no interface_id column

**Description**

See description of parent custom.annotated

**freeform**

- **Keywords Area**

- **method**

- **bayes_calibration**

- **wasabi**

- **emulator**

- **gaussian_process**

- **import.build.points_file**

- **freeform**

Selects freeform file format

**Topics**

This keyword is related to the topics:

- **fileformats**

**Specification**

**Alias:** none

- **Argument(s):** none
- **Default:** annotated format
6.2. METHOD

Description
A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior
The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips
- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples
Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```python
environment
tabular_data
  tabular_data_file = 'dakota_summary.dat'
  freeform
```

Resulting tabular file:

```plaintext
0.9 1.1 0.0002 0.26 0.76
0.90009 1.1 0.0001996404857 0.2601620081 0.759955
0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...
```

- active_only
  - Keywords Area
  - method
  - bayes_calibration
  - wasabi
  - emulator
  - gaussian_process
  - import_build_points_file
  - active_only

Import only active variables from tabular data file
Topics
This keyword is related to the topics:

- file_formats

Specification
Alias: none
Argument(s): none

Description
By default, files for tabular data imports are expected to contain columns for all variables, active and inactive. The keyword active_only indicates that the file to import contains only the active variables.

This option should only be used in contexts where the inactive variables have no influence, for example, building a surrogate over active variables, with the state variables held at nominal. It should not be used in more complex nested contexts, where the values of inactive variables are relevant to the function evaluations used to build the surrogate.

pce

- Keywords Area
- method
- bayes_calibration
- wasabi
- emulator
- pce

Polynomial Chaos Expansion surrogate model

Specification
Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required (Choose One)</td>
<td>Group 1</td>
<td>sparse_grid_level, sequence</td>
<td>Level to use in sparse grid integration or interpolation</td>
</tr>
</tbody>
</table>
6.2. METHOD

<table>
<thead>
<tr>
<th>expansion_order_sequence</th>
<th>The (initial) order of a polynomial expansion</th>
</tr>
</thead>
<tbody>
<tr>
<td>orthogonal_least_interpolation</td>
<td>Build a polynomial chaos expansion from simulation samples using orthogonal least interpolation.</td>
</tr>
</tbody>
</table>

**Description**

Selects a polynomial chaos expansion (PCE) surrogate model to use in the Bayesian likelihood calculations. When using PCE as a surrogate within the Bayesian framework, the PCE coefficients can be computed either from integration using a sparse grid or from regression using a random/unstructured data set.

**See Also**

These keywords may also be of interest:

- `polynomial_chaos`

**sparse_grid_level_sequence**

- `Keywords Area`
- `method`
- `bayes_calibration`
- `wasabi`
- `emulator`
- `pce`
- `sparse_grid_level_sequence`

Level to use in sparse grid integration or interpolation

**Specification**

**Alias:** none

**Argument(s):** INTEGERLIST

**Description**

Multi-dimensional integration by the Smolyak sparse grid method (specified with `sparse_grid_level` and, optionally, `dimension_preference`). The underlying one-dimensional integration rules are the same as for the tensor-product quadrature case; however, the default rule selection is nested for sparse grids (Genz-Keister for normals/transformed normals and Gauss-Patterson for uniforms/transformed uniforms). This default can be overridden with an explicit non_nested specification (resulting in Gauss-Hermite for normals/transformed normals for uniforms/transformed uniforms).
and Gauss-Legendre for uniforms/transformed uniforms). As for tensor quadrature, the dimension_preference specification enables the use of anisotropic sparse grids (refer to the PCE description in the User’s Manual for the anisotropic index set constraint definition). Similar to anisotropic tensor grids, the dimension with greatest preference will have resolution at the full sparse_grid_level and all other dimension resolutions will be reduced in proportion to their reduced preference. For PCE with either isotropic or anisotropic sparse grids, a summation of tensor-product expansions is used, where each anisotropic tensor-product quadrature rule underlying the sparse grid construction results in its own anisotropic tensor-product expansion as described in case 1. These anisotropic tensor-product expansions are summed into a sparse PCE using the standard Smolyak summation (again, refer to the User’s Manual for additional details). As for quadrature_order, the sparse_grid_level specification admits an array input for enabling specification of multiple grid resolutions used by certain advanced solution methodologies.

**Usage Tips**

This keyword can be used when using sparse grid integration to calculate PCE coefficients or when generating samples for sparse grid collocation.

For most use cases, this keyword will specify a single integer level. In more advanced UQ studies with hierarchical models, the list of integers can apply to different models and/or model levels.

**expansion_order_sequence**

- Keywords Area
- method
- bayes_calibration
- wasabi
- emulator
- pce
- expansion_order_sequence

The (initial) order of a polynomial expansion

**Specification**

**Alias:** none

**Argument(s):** INTEGERLIST

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required (Choose One)</td>
<td>collocation_points_sequence</td>
<td>Number of collocation points to estimate PCE coefficients</td>
<td></td>
</tr>
</tbody>
</table>
### Description

When the "expansion_order" for a polynomial chaos expansion is specified, the coefficients may be computed by integration based on random samples or by regression using either random or sub-sampled tensor product quadrature points.

Multidimensional integration by Latin hypercube sampling (specified with "expansion_samples"). In this case, the expansion order $p$ cannot be inferred from the numerical integration specification and it is necessary to provide an "expansion_order" to specify $p$ for a total-order expansion.

Linear regression (specified with either "collocation_points" or "collocation_ratio"). A total-order expansion is used and must be specified using "expansion_order" as described in the previous option. To avoid requiring the user to calculate $N$ from $n$ and $p$, the "collocation_ratio" allows for specification of a constant factor applied to $N$ (e.g., \( \text{collocation_ratio} = 2 \) produces $2N$). In addition, the default linear relationship with $N$ can be overridden using a real-valued exponent specified using "ratio_order". In this case, the number of samples becomes \( cN^o \) where $c$ is the "collocation_ratio" and $o$ is the "ratio_order". The "use_derivatives" flag informs the regression approach to include derivative matching equations (limited to gradients at present) in the least squares solutions, enabling the use of fewer collocation points for a given expansion order and dimension (number of points required becomes \( \frac{cN^o}{n+1} \)). When admissible, a constrained least squares approach is employed in which response values are first reproduced exactly and error in reproducing response derivatives is minimized. Two collocation grid options are supported: the default is Latin hypercube sampling ("point collocation"), and an alternate approach of "probabilistic collocation" is also available through inclusion of the "tensor_grid" keyword. In this alternate case, the collocation grid is defined using a subset of tensor-product quadrature points: the order of the tensor-product grid is selected as one more than the expansion order in each dimension (to avoid sampling at roots of the basis polynomials) and then the tensor multi-index is uniformly sampled to generate a non-repeated subset of tensor quadrature points.

<table>
<thead>
<tr>
<th>Method</th>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.2. METHOD</td>
<td>collocation_ratio</td>
<td>Set the number of points used to build a PCE via regression to be proportional to the number of terms in the expansion.</td>
</tr>
<tr>
<td>1471</td>
<td>cross_validation</td>
<td>Use cross validation to choose the 'best' polynomial order of a polynomial chaos expansion.</td>
</tr>
<tr>
<td>Optional</td>
<td>posterior_adaptive</td>
<td>Adapt emulator model to increase accuracy in high posterior probability regions.</td>
</tr>
<tr>
<td>Optional</td>
<td>import_build_points_file</td>
<td>File containing points you wish to use to build a surrogate.</td>
</tr>
</tbody>
</table>
If `collocation_points` or `collocation_ratio` is specified, the PCE coefficients will be determined by regression. If no regression specification is provided, appropriate defaults are defined. Specifically SVD-based least-squares will be used for solving over-determined systems and under-determined systems will be solved using LASSO. For the situation when the number of function values is smaller than the number of terms in a PCE, but the total number of samples including gradient values is greater than the number of terms, the resulting over-determined system will be solved using equality constrained least squares. Technical information on the various methods listed below can be found in the Linear regression section of the Theory Manual. Some of the regression methods (OMP, LASSO, and LARS) are able to produce a set of possible PCE coefficient vectors (see the Linear regression section in the Theory Manual). If cross validation is inactive, then only one solution, consistent with the `noise_tolerance`, will be returned. If cross validation is active, Dakota will choose between possible coefficient vectors found internally by the regression method across the set of expansion orders (1,...,expansion_order) and the set of specified noise tolerances and return the one with the lowest cross validation error indicator.

**Usage Tips**

For most use cases, this keyword will specify a single integer order. In more advanced UQ studies with hierarchical models, the list of integers can apply to different models and/or model levels.

`collocation_points_sequence`

- Keywords Area
- method
- bayes_calibration
- wasabi
- emulator
- pce
- `expansion_order_sequence`
- `collocation_points_sequence`

Number of collocation points to estimate PCE coefficients

### Specification

**Alias:** none

**Argument(s):** INTEGERLIST

### Description

Specify the number of collocation points used to estimate PCE coefficients using regression or orthogonal-least-interpolation.

**Usage Tips**

For most use cases, this keyword will specify a single integer number of points. In more advanced UQ studies with hierarchical models, the list of integers can apply to different models and/or model levels.
6.2. METHOD

• collocation_ratio
  • Keywords Area
  • method
  • bayes_calibration
  • wasabi
  • emulator
  • pce
  • expansion_order_sequence
  • collocation_ratio

Set the number of points used to build a PCE via regression to be proportional to the number of terms in the expansion.

**Specification**

**Alias:** none

**Argument(s):** REAL

**Description**

Set the number of points used to build a PCE via regression to be proportional to the number of terms in the expansion. To avoid requiring the user to calculate $N$ from $n$ and $p$, the collocation_ratio allows for specification of a constant factor applied to $N$ (e.g., collocation_ratio = 2. produces samples = 2N). In addition, the default linear relationship with $N$ can be overridden using a real-valued exponent specified using ratio_order. In this case, the number of samples becomes $cN^o$ where $c$ is the collocation_ratio and $o$ is the ratio_order. The use_derivatives flag informs the regression approach to include derivative matching equations (limited to gradients at present) in the least squares solutions, enabling the use of fewer collocation points for a given expansion order and dimension (number of points required becomes $\frac{cN^o}{n+1}$).

• cross_validation
  • Keywords Area
  • method
  • bayes_calibration
  • wasabi
  • emulator
  • pce
  • expansion_order_sequence
  • cross_validation

Use cross validation to choose the ‘best’ polynomial order of a polynomial chaos expansion.
CHAPTER 6. KEYWORDS AREA

**Specification**

**Alias:** none  
**Argument(s):** none

**Description**

Use cross validation to choose the 'best' polynomial degree of a polynomial chaos expansion. 10 fold cross validation is used to estimate the cross validation error of a total-order polynomial expansion for orders 1 through to order. The order chosen is the one that produces the lowest cross validation error. If there are not enough points to perform 10 fold cross validation then one-at-a-time cross validation will be performed.

**posterior_adaptive**

- Keywords Area
- method
- bayes_calibration
- wasabi
- emulator
- pce
- expansion_order_sequence
- posterior_adaptive

Adapt emulator model to increase accuracy in high posterior probability regions

**Specification**

**Alias:** none  
**Argument(s):** none

**Description**

Following an emulator-based MCMC process, this option refines the emulator by selecting points in regions of high posterior probability, performing truth evaluations at these points, updating the emulator, and reperforming the MCMC process. The adaptation is continued until the maximum number of iterations is exceeded or the convergence tolerance is met.

**Examples**

```
bayes_calibration queso
chain_samples = 2000 seed = 348
delayed_rejection
emulator
gaussian_process surfpack build_samples = 30
posterior_adaptive max_iterations = 10
proposal_covariance derivatives
```
import_build_points_file

- Keywords Area
- method
- bayes_calibration
- wasabi
- emulator
- pce
- expansion_order_sequence
- import_build_points_file

File containing points you wish to use to build a surrogate

### Specification

**Alias:** import_points_file  
**Argument(s):** STRING  
**Default:** no point import from a file

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional/Choose One</td>
<td>Tabular Format (Group 1)</td>
<td>annotated</td>
<td>Selects annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>custom_annotated</td>
<td>Selects custom-annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>freeform</td>
<td>Selects freeform file format</td>
</tr>
</tbody>
</table>

**Optional**

|                  | active_only | Import only active variables from tabular data file |

### Description

The `import_build_points_file` allows the user to specify a file that contains a list of points and truth model responses used to construct a surrogate model. These can be used by all methods that (explicitly, e.g. surrogate-based optimization, or implicitly, e.g. efficient global optimization) operate on a surrogate. In particular, these points and responses are used in place of truth model evaluations to construct the initial surrogate. When used to construct surrogate models or emulators these are often called build points or training data.

#### Default Behavior

By default, methods do not import points from a file.

#### Usage Tips

Dakota parses input files without regard to whitespace, but the `import_build_points_file` must be in one of three formats:
• annotated (default)
• custom.annotated
• freeform

Examples

method
  polynomial_choas
  expansion_order = 4
  import_build_points_file = 'dakota_uq_rosenbrock_pce_import.annot.pts.dat'

annotated
• Keywords Area
• method
• bayes_calibration
• wasabi
• emulator
• pce
• expansion_order_sequence
• import_build_points_file
• annotated

Selects annotated tabular file format

Topics
This keyword is related to the topics:
• file Formats

Specification
Alias: none
  Argument(s): none
  Default: annotated format

Description
An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior
By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips
6.2. METHOD

- To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify `custom_annotated` header eval_id
- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to `annotated` format, though `freeform` remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the `freeform` option.

Examples

Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```plaintext
environment
    tabular_data
        tabular_data_file = 'dakota_summary.dat'
        annotated

Resulting tabular file:
%eval_id interface x1 x2 obj_fn nln_ineq_con_1 nln_ineq_con_2
1 NO_ID 0.9 1.1 0.0002 0.26 0.76
2 NO_ID 0.90009 1.1 0.0001996404857 0.2601620081 0.759955
3 NO_ID 0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...
```

- `custom_annotated`
- Keywords Area
- method
- bayes_calibration
- wasabi
- emulator
- pce
- expansion_order_sequence
- import_build_points_file
- custom_annotated

Selects custom-annotated tabular file format

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none
Argument(s): none
Default: annotated format
### Description

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

**Default Behavior**

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

**Usage Tips**

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

**Examples**

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
  tabular_data_file = 'dakota_summary.dat'
custom_annotated header eval_id
```

Resulting tabular file:

```plaintext
%eval_id x1 x2 obj_fn nln_ineq_con_1 nln_ineq_con_2
1 0.9 1.1 0.0002 0.26 0.76
2 0.90009 1.1 0.0001996404857 0.2601620081 0.759955
3 0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...
6.2. METHOD

header

- Keywords Area
- method
- bayes_calibration
- wasabi
- emulator
- pce
- expansion_order_sequence
- import_build_points_file
- custom_annotated
- header

Enable header row in custom-annotated tabular file

**Specification**

Alias: none

Argument(s): none

Default: no header

**Description**

See description of parent custom_annotated

eval_id

- Keywords Area
- method
- bayes_calibration
- wasabi
- emulator
- pce
- expansion_order_sequence
- import_build_points_file
- custom_annotated
- eval_id

Enable evaluation ID column in custom-annotated tabular file
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): none

Default: no eval_id column

Description

See description of parent `custom_annotated`

```
interface_id

  Keywords Area
  method
  bayes_calibration
  wasabi
  emulator
  pce
  expansion_order_sequence
  import_build_points_file
  custom_annotated

Enable interface ID column in custom-annotated tabular file
```

Specification

Alias: none

Argument(s): none

Default: no interface_id column

Description

See description of parent `custom_annotated`

```
freeform

  Keywords Area
  method
  bayes_calibration
  wasabi
  emulator
```
6.2. METHOD

- pce
- expansion_order_sequence
- import_build_points_file
- freeform

Selects freeform file format

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none

Argument(s): none

Default: annotated format

Description

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior

The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips

- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```bash
environment
  tabular_data
    tabular_data_file = 'dakota_summary.dat'
    freeform

Resulting tabular file:

```

0.9 1.1 0.0002 0.26 0.76
0.90009 1.1 0.0001996404857 0.2601620081 0.759955
0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...
```
active_only
• Keywords Area
• method
• bayes_calibration
• wasabi
• emulator
• pce
• expansion_order_sequence
• import_build_points_file
• active_only
Import only active variables from tabular data file

Topics
This keyword is related to the topics:
• file_formats

Specification
Alias: none
Argument(s): none

Description
By default, files for tabular data imports are expected to contain columns for all variables, active and inactive. The keyword `active_only` indicates that the file to import contains only the active variables.

This option should only be used in contexts where the inactive variables have no influence, for example, building a surrogate over active variables, with the state variables held at nominal. It should not be used in more complex nested contexts, where the values of inactive variables are relevant to the function evaluations used to build the surrogate.

orthogonal_least_interpolation
• Keywords Area
• method
• bayes_calibration
• wasabi
• emulator
• pce
• orthogonal_least_interpolation
Build a polynomial chaos expansion from simulation samples using orthogonal least interpolation.
6.2. METHOD

Specification

Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>collocation_points_sequence</td>
<td>posterior_adaptive</td>
<td>Adapt emulator model to increase accuracy in high posterior probability regions</td>
</tr>
<tr>
<td>Optional</td>
<td>import_build-points_file</td>
<td></td>
<td>File containing points you wish to use to build a surrogate</td>
</tr>
</tbody>
</table>

Description

Build a polynomial chaos expansion from simulation samples using orthogonal least interpolation. Unlike the other regression methods expansion_order cannot be set. OLI will produce the lowest degree polynomial that interpolates the data

collocation_points_sequence

- Keywords Area
- method
- bayes_calibration
- wasabi
- emulator
- pce
- orthogonal_least_interpolation
- collocation_points_sequence

Number of collocation points to estimate PCE coefficients

Specification

Alias: none
Argument(s): INTEGRERLIST
CHAPTER 6. KEYWORDS AREA

Description

Specify the number of collocation points used to estimate PCE coefficients using regression or orthogonal-least-interpolation.

Usage Tips

For most use cases, this keyword will specify a single integer number of points. In more advanced UQ studies with hierarchical models, the list of integers can apply to different models and/or model levels

posterior_adaptive

• Keywords Area

• method

• bayes_calibration

• wasabi

• emulator

• pce

• orthogonal_least_interpolation

• posterior_adaptive

Adapt emulator model to increase accuracy in high posterior probability regions

Specification

Alias: none

Argument(s): none

Description

Following an emulator-based MCMC process, this option refines the emulator by selecting points in regions of high posterior probability, performing truth evaluations at these points, updating the emulator, and reperforming the MCMC process. The adaptation is continued until the maximum number of iterations is exceeded or the convergence tolerance is met.

Examples

bayes_calibration queso
chain_samples = 2000 seed = 348
delayed_rejection
emulator
gaussian_process surfpack build_samples = 30
posterior_adaptive max_iterations = 10
proposal_covariance derivatives
6.2. METHOD

import_build_points_file

- Keywords Area
- method
- bayes_calibration
- wasabi
- emulator
- pce
- orthogonal_least_interpolation
- import_build_points_file

File containing points you wish to use to build a surrogate

Specfication

Alias: import_points_file
Argument(s): STRING
Default: no point import from a file

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional/Choose One</td>
<td>Tabular Format (Group 1)</td>
<td>annotated</td>
<td>Selects annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td>custom_annotated</td>
<td>Selects custom-annotated tabular file format</td>
<td></td>
</tr>
<tr>
<td></td>
<td>freeform</td>
<td>Selects freeform file format</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>active_only</td>
<td>Import only active variables from tabular data file</td>
<td></td>
</tr>
</tbody>
</table>

Description

The import_build_points_file allows the user to specify a file that contains a list of points and truth model responses used to construct a surrogate model. These can be used by all methods that (explicitly, e.g. surrogate-based optimization, or implicitly, e.g. efficient global optimization) operate on a surrogate. In particular, these points and responses are used in place of truth model evaluations to construct the initial surrogate. When used to construct surrogate models or emulators these are often called build points or training data.

Default Behavior
By default, methods do not import points from a file.

Usage Tips
Dakota parses input files without regard to whitespace, but the import_build_points_file must be in one of three formats:
• annotated (default)
• custom_annotated
• freeform

Examples

```python
method
    polynomial_chaos
    expansion_order = 4
    import_build_points_file = 'dakota_uq_rosenbrock_pce_import.annot.pts.dat'

annotated
• Keywords Area
• method
• bayes_calibration
• wasabi
• emulator
• pce
• orthogonal_least_interpolation
• import_build_points_file
• annotated

Selects annotated tabular file format
```

Topics

This keyword is related to the topics:
• file_formats

Specification

Alias: none
Argument(s): none
Default: annotated format

Description

An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior
By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips
6.2. **METHOD**

- To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify `custom_annotated header eval_id`
- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to `annotated format`, though `freeform` remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the `freeform` option.

### Examples

Export an annotated top-level tabular data file containing a header row, leading `eval_id` and `interface_id` columns, and data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
annotated
```

Resulting tabular file:

<table>
<thead>
<tr>
<th>eval_id</th>
<th>interface</th>
<th>x1</th>
<th>x2</th>
<th>obj_fn</th>
<th>nln_ineq_con_1</th>
<th>nln_ineq_con_2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>NO_ID</td>
<td>0.9</td>
<td>1.1</td>
<td>0.0002</td>
<td>0.26</td>
<td>0.76</td>
</tr>
<tr>
<td>2</td>
<td>NO_ID</td>
<td>0.90009</td>
<td>1.1</td>
<td>0.0001996404857</td>
<td>0.2601620081</td>
<td>0.759955</td>
</tr>
<tr>
<td>3</td>
<td>NO_ID</td>
<td>0.89991</td>
<td>1.1</td>
<td>0.0002003604863</td>
<td>0.2598380081</td>
<td>0.760045</td>
</tr>
<tr>
<td>...</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- `custom_annotated`
- **Keywords**
  - `Area`
  - `method`
  - `bayes_calibration`
  - `wasabi`
  - `emulator`
  - `pce`
  - `orthogonal_least_interpolation`
  - `import_build_points_file`
  - `custom_annotated`

Selects custom-annotated tabular file format

### Topics

This keyword is related to the topics:

- `file_formats`

### Specification

**Alias:** none

**Argument(s):** none

**Default:** annotated format
### Description

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

**Default Behavior**

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

**Usage Tips**

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

**Examples**

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
custom_annotated header eval_id
```

Resulting tabular file:

```
%eval_id  x1  x2  obj_fn  nln_ineq_con_1  nln_ineq_con_2
1  0.9  1.1  0.0002  0.26  0.76
2  0.90009  1.1  0.0001996404857  0.2601620081  0.759955
3  0.89991  1.1  0.0002003604863  0.2598380081  0.760045
...```
6.2. METHOD

header

- Keywords Area
- method
- bayes_calibration
- wasabi
- emulator
- pce
- orthogonal_least_interpolation
- import_build_points_file
- custom_annotated
- header

Enable header row in custom-annotated tabular file

Specification

Alias: none
  Argument(s): none
  Default: no header

Description

See description of parent custom_annotated

eval_id

- Keywords Area
- method
- bayes_calibration
- wasabi
- emulator
- pce
- orthogonal_least_interpolation
- import_build_points_file
- custom_annotated
- eval_id

Enable evaluation ID column in custom-annotated tabular file
CHAPTER 6. KEYWORDS AREA

**Specification**

*Alias:* none

*Argument(s):* none

*Default:* no eval_id column

**Description**

See description of parent `custom.annotated`

```plaintext
interface_id

- Keywords Area
- method
- bayes_calibration
- wasabi
- emulator
- pce
- orthogonal_least_interpolation
- import_build_points_file
- custom.annotated
- interface_id
```

Enable interface ID column in custom-annotated tabular file

**Specification**

*Alias:* none

*Argument(s):* none

*Default:* no interface_id column

**Description**

See description of parent `custom.annotated`

```plaintext
freeform

- Keywords Area
- method
- bayes_calibration
- wasabi
- emulator
```
6.2. METHOD

- pce
- orthogonal_least_interpolation
- import_build_points_file
- freeform

Selects freeform file format

Topics
This keyword is related to the topics:
- file_formats

Specification

Alias: none  
Argument(s): none  
Default: annotated format

Description
A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior
The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips
- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples
Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```environment
environment
  tabular_data
  tabular_data_file = 'dakota_summary.dat'
  freeform
```

Resulting tabular file:

```
0.9  1.1  0.0002  0.26  0.76
0.90009 1.1  0.0001996404857  0.2601620081  0.759955
0.89991 1.1  0.0002003604863  0.2598380081  0.760045
...```
active_only

- Keywords Area
- method
- bayes_calibration
- wasabi
- emulator
- pce
- orthogonal_least_interpolation
- import_build_points_file
- active_only

Import only active variables from tabular data file

Topics
This keyword is related to the topics:

- file_formats

Specification

Alias: none

Argument(s): none

Description
By default, files for tabular data imports are expected to contain columns for all variables, active and inactive. The keyword active_only indicates that the file to import contains only the active variables.

This option should only be used in contexts where the inactive variables have no influence, for example, building a surrogate over active variables, with the state variables held at nominal. It should not be used in more complex nested contexts, where the values of inactive variables are relevant to the function evaluations used to build the surrogate.

sc

- Keywords Area
- method
- bayes_calibration
- wasabi
- emulator
- sc

Stochastic Collocation polynomial surrogate model
6.2. METHOD

Specification

Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/Optional Required</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>sparse_grid_level_sequence</td>
<td>Level to use in sparse grid integration or interpolation</td>
</tr>
</tbody>
</table>

Description

Selects stochastic collocation (SC) model to use in the Bayesian likelihood calculations. When using SC as a surrogate within the Bayesian framework, the build points (training points) for the stochastic collocation are constructed from a sparse grid.

See Also

These keywords may also be of interest:

- stoch_collocation

sparse_grid_level_sequence

- Keywords Area
- method
- bayes_calibration
- wasabi
- emulator
- sc

Level to use in sparse grid integration or interpolation

Specification

Alias: none
Argument(s): INTEGERLIST
Description

Multi-dimensional integration by the Smolyak sparse grid method (specified with sparse_grid_level and, optionally, dimension_preference). The underlying one-dimensional integration rules are the same as for the tensor-product quadrature case; however, the default rule selection is nested for sparse grids (Genz-Keister for normals/transformed normals and Gauss-Patterson for uniforms/transformed uniforms). This default can be overridden with an explicit non_nested specification (resulting in Gauss-Hermite for normals/transformed normals and Gauss-Legendre for uniforms/transformed uniforms). As for tensor quadrature, the dimension_preference specification enables the use of anisotropic sparse grids (refer to the PCE description in the User’s Manual for the anisotropic index set constraint definition). Similar to anisotropic tensor grids, the dimension with greatest preference will have resolution at the full sparse_grid_level and all other dimension resolutions will be reduced in proportion to their reduced preference. For PCE with either isotropic or anisotropic sparse grids, a summation of tensor-product expansions is used, where each anisotropic tensor-product quadrature rule underlying the sparse grid construction results in its own anisotropic tensor-product expansion as described in case 1. These anisotropic tensor-product expansions are summed into a sparse PCE using the standard Smolyak summation (again, refer to the User’s Manual for additional details). As for quadrature_order, the sparse_grid_level specification admits an array input for enabling specification of multiple grid resolutions used by certain advanced solution methodologies.

Usage Tips

This keyword can be used when using sparse grid integration to calculate PCE coefficients or when generating samples for sparse grid collocation.

For most use cases, this keyword will specify a single integer level. In more advanced UQ studies with hierarchical models, the list of integers can apply to different models and/or model levels

use_derivatives

• Keywords Area

• method

• bayes_calibration

• wasabi

• emulator

• use_derivatives

Use derivative data to construct surrogate models

Specification

Alias: none

Argument(s): none

Default: use function values only

Description

The use_derivatives flag specifies that any available derivative information should be used in global approximation builds, for those global surrogate types that support it (currently, polynomial regression and the Surfpack Gaussian process).

However, its use with Surfpack Gaussian process is not recommended.
standardized_space

- Keywords Area
- method
- bayes_calibration
- wasabi
- standardized_space

Perform Bayesian inference in standardized probability space

**Specification**

Alias: none

Argument(s): none

**Description**

This option transforms the inference process (MCMC sampling and any emulator model management) into a standardized probability space. The variable transformations performed are as described in askey.

**Default Behavior**

The default for the Gaussian process and no emulator options is to perform inference in the original probability space (no transformation). Polynomial chaos and stochastic collocation emulators, on the other hand, are always formed in standardized probability space, such that the inference process is also performed in this standardized space.

**Expected Output**

The user will see the truth model evaluations performed in the original space, whereas any method diagnostics relating to the MCMC samples (e.g., QUESO data in the outputData directory) will report points and response data (response gradients and Hessians, if present, will differ but response values will not) that correspond to the transformed space.

**Usage Tips**

Selecting standardized_space generally has the effect of scaling the random variables to be of comparable magnitude, which can improve the efficiency of the Bayesian inference process.

**Examples**

```
method,
  bayes_calibration queso
  samples = 2000 seed = 348
  dram
  standardized_space
```

**data_distribution**

- Keywords Area
- method
- bayes_calibration
wasabi

data_distribution

(Experimental Capability) Specify the distribution of the experimental data

**Specification**

**Alias:** none

**Argument(s):** none

| Required/- | Description of | Dakota Keyword | Dakota Keyword | Description |
| Optional Required | Group | | | |
| Choose One | Group 1 | gaussian | (Experimental Capability) Gaussian error distribution |
| | | obs_data_filename | (Experimental Capability) Filename from which to read experimental data |

**gaussian**

- Keywords Area
- method
- bayes_calibration
- wasabi
- data_distribution
- gaussian

(Experimental Capability) Gaussian error distribution

**Specification**

**Alias:** none

**Argument(s):** none

| Required/- | Description of | Dakota Keyword | Dakota Keyword | Description |
| Optional Required | Group | | | |
| | | means | (Experimental Capability) Means of Gaussian error distribution |
## 6.2. METHOD

<table>
<thead>
<tr>
<th>Required</th>
<th>covariance</th>
<th>(Experimental Capability) Covariance of a Gaussian error distribution</th>
</tr>
</thead>
</table>

**means**
- Keywords Area
- method
- bayes_calibration
- wasabi
- data_distribution
- gaussian
- means

(Experimental Capability) Means of Gaussian error distribution

### Specification

**Alias:** none

**Argument(s):** REALLIST

**covariance**
- Keywords Area
- method
- bayes_calibration
- wasabi
- data_distribution
- gaussian
- covariance

(Experimental Capability) Covariance of a Gaussian error distribution

### Specification

**Alias:** none

**Argument(s):** REALLIST
### Required-/Optional Required

<table>
<thead>
<tr>
<th>Description of Group 1</th>
<th>Dakota Keyword diagonal</th>
</tr>
</thead>
<tbody>
<tr>
<td>diagonal</td>
<td>matrix</td>
</tr>
</tbody>
</table>

**Keywords Area**

- bayes_calibration
- wasabi
- data_distribution
- gaussian
- covariance
- diagonal

(Experimental Capability) Diagonal error covariance

**Specification**

**Alias:** none

**Argument(s):** none

**matrix**

- Keywords Area
- method
- bayes_calibration
- wasabi
- data_distribution
- gaussian
- covariance
- matrix

(Experimental Capability) Symmetric positive definite error covariance
6.2. METHOD

**Specification**

**Alias:** none  
**Argument(s):** none

- `obs_data_filename`
  - **Keywords Area**
  - `method`
  - `bayes_calibration`
  - `wasabi`
  - `data_distribution`
  - `obs_data_filename`
  
  (Experimental Capability) Filename from which to read experimental data

**Specification**

**Alias:** none  
**Argument(s):** STRING

- `posterior_density_export_filename`
  - **Keywords Area**
  - `method`
  - `bayes_calibration`
  - `wasabi`
  - `posterior_density_export_filename`
  
  (Experimental Capability) Filename for the exported posterior density

**Specification**

**Alias:** none  
**Argument(s):** STRING

- `posterior_samples_export_filename`
  - **Keywords Area**
  - `method`
  - `bayes_calibration`
  - `wasabi`
  - `posterior_samples_export_filename`
  
  (Experimental Capability) Filename for the exported posterior samples
**Specification**

**Alias:** none

**Argument(s):** STRING

**posterior_samples_import_filename**

- **Keywords Area**
- **method**
- **bayes_calibration**
- **wasabi**
- **posterior_samples_import_filename**

(Experimental Capability) Filename for imported posterior samples

**Specification**

**Alias:** none

**Argument(s):** STRING

**generate_posterior_samples**

- **Keywords Area**
- **method**
- **bayes_calibration**
- **wasabi**
- **generate_posterior_samples**

(Experimental Capability) Generate random samples from the posterior density

**Specification**

**Alias:** none

**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/-Optional Required</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td><strong>evaluate_posterior_density</strong></td>
<td></td>
<td>(Experimental Capability) Evaluate the posterior density and output to the specified file</td>
</tr>
</tbody>
</table>
6.2. METHOD

evaluate_posterior_density

- Keywords Area
- method
- bayes_calibration
- wasabi
- generate_posterior_samples
- evaluate_posterior_density

(Experimental Capability) Evaluate the posterior density and output to the specified file

Specification

Alias: none
Argument(s): none

dream

- Keywords Area
- method
- bayes_calibration
- dream

DREAM (DiffeRential Evolution Adaptive Metropolis)

Topics

This keyword is related to the topics:

- bayesian_calibration

Specification

Alias: none
Argument(s): none

| Required/- | Description of | Dakota Keyword | Dakota Keyword     |
| Optional   | Group          | chain_samples  | Description       |
| Required   |               |                | Number of Markov  |
| chain_samples | posterior     | Number of Markov | Chain Monte Carlo  |
| posterior samples |            | Chain Monte Carlo | posterior samples |
### Description

The DiffeRential Evolution Adaptive Metropolis algorithm is described in[86]. For the DREAM method, one can define the number of chains used with `chains` (minimum 3). The total number of generations per chain in DREAM is the number of samples divided by the number of chains. The number of chains randomly selected to be used in the crossover each time a crossover occurs is `crossover_chain_pairs`. There is an extra adaptation during burn-in, in which DREAM estimates a distribution of crossover probabilities that favors large jumps over smaller ones in each of the chains. Normalization is required to ensure that all of the input dimensions contribute equally. In this process, a discrete number of candidate points for each crossover value is generated. This parameter is `num_cr`. The `gr_threshold` is the convergence tolerance for the Gelman-Rubin statistic which will govern the convergence of the multiple chain process. The integer `jump_step` forces a long jump every `jump_step` generations. For more details about these parameters, see[86].

**Attention:** While the `emulator` specification for DREAM includes the keyword posterior_adaptive, it is not yet operational.

---

<table>
<thead>
<tr>
<th>Optional</th>
<th>seed</th>
<th>Seed of the random number generator</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>chains</td>
<td>Number of chains in DREAM</td>
</tr>
<tr>
<td>Optional</td>
<td><code>num_cr</code></td>
<td>Number of candidate points for each crossover.</td>
</tr>
<tr>
<td>Optional</td>
<td><code>crossover_chain_pairs</code></td>
<td>Number of chains used in crossover.</td>
</tr>
<tr>
<td>Optional</td>
<td><code>gr_threshold</code></td>
<td>Convergence tolerance for the Gelman-Rubin statistic</td>
</tr>
<tr>
<td>Optional</td>
<td><code>jump_step</code></td>
<td>Number of generations a long jump step is taken</td>
</tr>
<tr>
<td>Optional</td>
<td><code>emulator</code></td>
<td>Use an emulator or surrogate model to evaluate the likelihood function</td>
</tr>
<tr>
<td>Optional</td>
<td><code>standardized_space</code></td>
<td>Perform Bayesian inference in standardized probability space</td>
</tr>
<tr>
<td>Optional</td>
<td><code>export_chain_points_file</code></td>
<td>Export the MCMC chain to the specified filename</td>
</tr>
</tbody>
</table>

---

**chain_samples**

- Keywords Area
6.2. METHOD

- method
- bayes_calibration
- dream
- chain_samples

Number of Markov Chain Monte Carlo posterior samples

**Specification**

**Alias:** samples

**Argument(s):** INTEGER

**Default:** method-dependent

**Description**

The `chain_samples` keyword indicates the number of draws from the posterior distribution to perform. When an emulator is active, this will be the number of samples on the constructed surrogate model.

**Default Behavior**

The default number of chain samples is method-dependent. QUESO methods use 48576. DREAM uses \((\text{number of generations}) \times (\text{number of chains})\).

**Usage Tips**

MCMC methods typically require a large number of chain samples to converge, often thousands to millions.

**Examples**

```
method
  bayes_calibration queso
  chain_samples = 20000
```

**seed**

- **Keywords Area**
- **method**
- **bayes_calibration**
- **dream**
- **seed**

Seed of the random number generator

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** system-generated (non-repeatable)
CHAPTER 6. KEYWORDS AREA

Description

The random seed control provides a mechanism for making a stochastic method repeatable. That is, the use of the same random seed in identical studies will generate identical results.

Default Behavior
If not specified, the seed is randomly generated.

Expected Output
If seed is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

Usage Tips
If a stochastic study was run without seed specified, and the user later wishes to repeat the study using the same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen. That value can then be added to the Dakota input file.

Examples

```dakota
method
sampling
  sample_type lhs
  samples = 10
  seed = 15347
```

chaints

- Keywords Area
- method
- bayes_calibration
- dream
- chains

Number of chains in DREAM

Topics

This keyword is related to the topics:

- bayesian_calibration

Specification

Alias: none
Argument(s): INTEGER
Default: 3

Description

Number of chains in DREAM
6.2. METHOD

num_cr

- **Keywords Area**
- **method**
- **bayes_calibration**
- **dream**
- **num_cr**

Number of candidate points for each crossover.

**Topics**

This keyword is related to the topics:

- **bayesian_calibration**

**Specification**

**Alias:** none  
**Argument(s):** INTEGER  
**Default:** 1

**Description**

In DREAM, there is an extra adaptation during burn-in, in which DREAM estimates a distribution of crossover probabilities that favors large jumps over smaller ones in each of the chains. Normalization is required to ensure that all of the input dimensions contribute equally. In this process, a discrete number of candidate points for each crossover value is generated. This parameter is `num_cr`.

**crossover_chain_pairs**

- **Keywords Area**
- **method**
- **bayes_calibration**
- **dream**
- **crossover_chain_pairs**

Number of chains used in crossover.

**Topics**

This keyword is related to the topics:

- **bayesian_calibration**
CHAPTER 6. KEYWORDS AREA

Specification
Alias: none
Argument(s): INTEGER
Default: 3

Description
The number of chains randomly selected to be used in the crossover each time a crossover occurs.

gr_threshold
- Keywords Area
- method
- bayes_calibration
- dream
- gr_threshold

Convergence tolerance for the Gelman-Rubin statistic

Topics
This keyword is related to the topics:
- bayesian_calibration

Specification
Alias: none
Argument(s): REAL
Default: 1.2

Description
The gr_threshold is the convergence tolerance for the Gelman-Rubin statistic which will govern the convergence of the multiple chain process.

jump_step
- Keywords Area
- method
- bayes_calibration
- dream
- jump_step

Number of generations a long jump step is taken
6.2. METHOD

**Topics**
This keyword is related to the topics:
- bayesian_calibration

**Specification**

**Alias:** none

**Argument(s):** INTEGER
- **Default:** 5

**Description**
The integer jump_step forces a long jump every jump_step generations in DREAM.

**emulator**
- **Keywords Area**
- method
- bayesian_calibration
- dream
- emulator

Use an emulator or surrogate model to evaluate the likelihood function

**Specification**

**Alias:** none
- **Argument(s):** none

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required (Choose One)</td>
<td>emulator type (Group 1)</td>
<td>gaussian_process</td>
<td>Gaussian Process surrogate model</td>
</tr>
<tr>
<td>pce</td>
<td></td>
<td></td>
<td>Polynomial Chaos Expansion surrogate model</td>
</tr>
<tr>
<td>sc</td>
<td></td>
<td></td>
<td>Stochastic Collocation polynomial surrogate model</td>
</tr>
</tbody>
</table>
## Description

This keyword describes the type of emulator used when calculating the likelihood function for the Bayesian calibration. The emulator can be a Gaussian process, polynomial chaos expansion, or stochastic collocation.

**gaussian_process**
- **Keywords Area**
- **method**
- **bayes_calibration**
- **dream**
- **emulator**
- **gaussian_process**

Gaussian Process surrogate model

## Specification

**Alias:** kriging  
**Argument(s):** none  
**Default:** Surfpack Gaussian process

<table>
<thead>
<tr>
<th>Optional</th>
<th>use_derivatives</th>
<th>Use derivative data to construct surrogate models</th>
</tr>
</thead>
</table>

### Required/Optional

<table>
<thead>
<tr>
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<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
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<tbody>
<tr>
<td>surfpack</td>
<td></td>
<td>surfpack</td>
<td>Use the Surfpack version of Gaussian Process surrogates</td>
</tr>
<tr>
<td>build_samples</td>
<td></td>
<td>dakota</td>
<td>Select the built in Gaussian Process surrogate</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Optional</th>
<th>build_samples</th>
<th>Number of initial model evaluations used in build phase</th>
</tr>
</thead>
</table>

6.2. METHOD

<table>
<thead>
<tr>
<th>Optional</th>
<th>posterior_adaptive</th>
<th>Adapt emulator model to increase accuracy in high posterior probability regions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>import_build-points_file</td>
<td>File containing points you wish to use to build a surrogate</td>
</tr>
</tbody>
</table>

Description

Use the Gaussian process (GP) surrogate from Surfpack, which is specified using the `surfpack` keyword. An alternate version of GP surrogates was available in prior versions of Dakota. **For now, both versions are supported but the dakota version is deprecated and intended to be removed in a future release.**

*Known Issue:* When using discrete variables, there have been sometimes significant differences in surrogate behavior observed across computing platforms in some cases. The cause has not yet been fully diagnosed and is currently under investigation. In addition, guidance on appropriate construction and use of surrogates with discrete variables is under development. In the meantime, users should therefore be aware that there is a risk of inaccurate results when using surrogates with discrete variables.

- `surfpack`
  - Keywords Area
  - method
  - bayes_calibration
  - dream
  - emulator
  - gaussian_process
  - surfpack

Use the Surfpack version of Gaussian Process surrogates

**Specification**

**Alias:** none  
**Argument(s):** none

**Description**

This keyword specifies the use of the Gaussian process that is incorporated in our surface fitting library called Surfpack.

Several user options are available:
1. Optimization methods:
   Maximum Likelihood Estimation (MLE) is used to find the optimal values of the hyper-parameters governing the trend and correlation functions. By default the global optimization method DIRECT is used for MLE, but other options for the optimization method are available. See optimization_method.

   The total number of evaluations of the likelihood function can be controlled using the max_trials keyword followed by a positive integer. Note that the likelihood function does not require running the "truth" model, and is relatively inexpensive to compute.

2. Trend Function:
   The GP models incorporate a parametric trend function whose purpose is to capture large-scale variations. See trend.

3. Correlation Lengths:
   Correlation lengths are usually optimized by Surfpack, however, the user can specify the lengths manually. See correlation_lengths.

4. Ill-conditioning
   One of the major problems in determining the governing values for a Gaussian process or Kriging model is the fact that the correlation matrix can easily become ill-conditioned when there are too many input points close together. Since the predictions from the Gaussian process model involve inverting the correlation matrix, ill-conditioning can lead to poor predictive capability and should be avoided.

   Note that a sufficiently bad sample design could require correlation lengths to be so short that any interpolatory GP model would become inept at extrapolation and interpolation.

   The surfpack model handles ill-conditioning internally by default, but behavior can be modified using surfpack.

5. Gradient Enhanced Kriging (GEK).
   The use_derivatives keyword will cause the Surfpack GP to be constructed from a combination of function value and gradient information (if available).

   See notes in the Theory section.

---

**Theory**

**Gradient Enhanced Kriging**

Incorporating gradient information will only be beneficial if accurate and inexpensive derivative information is available, and the derivatives are not infinite or nearly so. Here "inexpensive" means that the cost of evaluating a function value plus gradient is comparable to the cost of evaluating only the function value, for example gradients computed by analytical, automatic differentiation, or continuous adjoint techniques. It is not cost effective to use derivatives computed by finite differences. In tests, GEK models built from finite difference derivatives were also significantly less accurate than those built from analytical derivatives. Note that GEK’s correlation matrix tends to have a significantly worse condition number than Kriging for the same sample design.

This issue was addressed by using a pivoted Cholesky factorization of Kriging’s correlation matrix (which is a small sub-matrix within GEK’s correlation matrix) to rank points by how much unique information they contain. This reordering is then applied to whole points (the function value at a point immediately followed by gradient information at the same point) in GEK’s correlation matrix. A standard non-pivoted Cholesky is then applied to the reordered GEK correlation matrix and a bisection search is used to find the last equation that meets the constraint on the (estimate of) condition number. The cost of performing pivoted Cholesky on Kriging’s correlation matrix is usually negligible compared to the cost of the non-pivoted Cholesky factorization of GEK’s correlation matrix. In tests, it also resulted in more accurate GEK models than when pivoted Cholesky or whole-point-block pivoted Cholesky was performed on GEK’s correlation matrix.
6.2. METHOD

dakota

- Keywords Area
- method
- bayes_calibration
- dream
- emulator
- gaussian_process
- dakota

Select the built in Gaussian Process surrogate

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

A second version of GP surrogates was available in prior versions of Dakota. **For now, both versions are supported but the dakota version is deprecated and intended to be removed in a future release.**

Historically these models were drastically different, but in Dakota 5.1, they became quite similar. They now differ in that the Surfpack GP has a richer set of features/options and tends to be more accurate than the Dakota version. Due to how the Surfpack GP handles ill-conditioned correlation matrices (which significantly contributes to its greater accuracy), the Surfpack GP can be a factor of two or three slower than Dakota’s. As of Dakota 5.2, the Surfpack implementation is the default in all contexts except Bayesian calibration.

More details on the gaussian_process dakota model can be found in[58].

Dakota’s GP deals with ill-conditioning in two ways. First, when it encounters a non-invertible correlation matrix it iteratively increases the size of a "nugget," but in such cases the resulting approximation smooths rather than interpolates the data. Second, it has a point_selection option (default off) that uses a greedy algorithm to select a well-spaced subset of points prior to the construction of the GP. In this case, the GP will only interpolate the selected subset. Typically, one should not need point selection in trust-region methods because a small number of points are used to develop a surrogate within each trust region. Point selection is most beneficial when constructing with a large number of points, typically more than order one hundred, though this depends on the number of variables and spacing of the sample points.

This differs from the point_selection option of the Dakota GP which initially chooses a well-spaced subset of points and finds the correlation parameters that are most likely for that one subset.
CHAPTER 6. KEYWORDS AREA

- emulator
- gaussian_process
- build_samples

Number of initial model evaluations used in build phase

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Description**

The number of build points or training points used in the initial phase of an algorithm or model construction. Typically these are the initial set of data points used to construct (train) a surrogate model (emulator). If the number of build_samples is less than the minimum number of points required to build the surrogate, Dakota will augment the samples to obtain the minimum required.

**Examples**

Perform GP-based adaptive importance sampling, building the GP with 100 points and then performing 100 approximate evaluations to evaluate the probability.

```plaintext
method
gpais
  build_samples = 100
  samples_on_emulator = 100
  max_iterations = 5
  response_levels = -1.065
```

**posterior_adaptive**

- Keywords Area
- method
- bayes_calibration
- dream
- emulator
- gaussian_process
- posterior_adaptive

Adapt emulator model to increase accuracy in high posterior probability regions

**Specification**

**Alias:** none

**Argument(s):** none
6.2. METHOD

Description
Following an emulator-based MCMC process, this option refines the emulator by selecting points in regions of high posterior probability, performing truth evaluations at these points, updating the emulator, and reperforming the MCMC process. The adaptation is continued until the maximum number of iterations is exceeded or the convergence tolerance is met.

Examples
bayes_calibration queso
   chain_samples = 2000 seed = 348
delayed_rejection
emulator
gaussian_process surfpack build_samples = 30
posterior_adaptive max_iterations = 10
proposal_covariance derivatives

import_build_points_file

- Keywords Area
- method
- bayes_calibration
- dream
- emulator
- gaussian_process
- import_build_points_file

File containing points you wish to use to build a surrogate

Specification
Alias: import_points_file
Argument(s): STRING
Default: no point import from a file

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
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<td>Tabular Format (Group 1)</td>
<td>annotated</td>
<td>Selects annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>custom_annotated</td>
<td>Selects custom-annotated tabular file format</td>
</tr>
</tbody>
</table>
CHAPTER 6. KEYWORDS AREA

<table>
<thead>
<tr>
<th>freeform</th>
<th>Selects freeform file format</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>active_only</td>
</tr>
<tr>
<td></td>
<td>Import only active variables from tabular data file</td>
</tr>
</tbody>
</table>

**Description**

The `import_build_points_file` allows the user to specify a file that contains a list of points and truth model responses used to construct a surrogate model. These can be used by all methods that (explicitly, e.g. surrogate-based optimization, or implicitly, e.g. efficient global optimization) operate on a surrogate. In particular, these points and responses are used in place of truth model evaluations to construct the initial surrogate. When used to construct surrogate models or emulators these are often called build points or training data.

**Default Behavior**

By default, methods do not import points from a file.

**Usage Tips**

Dakota parses input files without regard to whitespace, but the `import_build_points_file` must be in one of three formats:

- annotated (default)
- custom_annotated
- freeform

**Examples**

```plaintext
method
    polynomial_chaos
        expansion_order = 4
        import_build_points_file = 'dakota_uq_rosenbrock_pce_import.annot.pts.dat'
```

- annotated
  - Keywords Area
  - method
  - bayes_calibration
  - dream
  - emulator
  - gaussian_process
  - import_build_points_file
  - annotated

Selects annotated tabular file format
6.2. METHOD

Topics
This keyword is related to the topics:

- file_formats

Specification
Alias: none
Argument(s): none
Default: annotated format

Description
An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior
By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips

- To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify custom_annotated header eval_id

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples
Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```plaintext
environment
    tabular_data
        tabular_data_file = 'dakota_summary.dat'
    annotated
```

Resulting tabular file:

```
%eval_id interface x1  x2  obj_fn nln_ineq_con_1 nln_ineq_con_2
1   NO_ID    0.9  1.1  0.0002  0.26  0.76
2   NO_ID    0.90009 1.1  0.0001996404857  0.2601620081  0.759955
3   NO_ID    0.89991 1.1  0.0002003604863  0.2598380081  0.760045
...```
custom.annotated

- Keywords Area
- method
- bayes_calibration
- dream
- emulator
- gaussian_process
- import_build.points_file
- custom.annotated

Selects custom-annotated tabular file format

**Topics**

This keyword is related to the topics:

- file_formats

**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** annotated format

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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</thead>
<tbody>
<tr>
<td>Optional</td>
<td>header</td>
<td></td>
<td>Enable header row in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td>eval_id</td>
<td></td>
<td>Enable evaluation ID column in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td>interface_id</td>
<td></td>
<td>Enable interface ID column in custom-annotated tabular file</td>
</tr>
</tbody>
</table>
Description

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

Default Behavior

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom.annotated, followed by options, in the relevant export/import context.

Usage Tips

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:

```
environment
tabular_data
  tabular_data_file = 'dakota_summary.dat'
custom.annotated header eval_id
```

Resulting tabular file:

```
%eval_id x1 x2 obj_fn nln_ineq_con_1 nln_ineq_con_2
1 0.9 1.1 0.0002 0.26 0.76
2 0.90009 1.1 0.0001996404857 0.2601620081 0.759955
3 0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...```

header

- Keywords Area
- method
- bayes_calibration
- dream
- emulator
- gaussian_process
- import_build_points_file
- custom.annotated
- header

Enable header row in custom-annotated tabular file

```
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none
Argument(s): none
Default: no header

Description

See description of parent custom_annotated

eval_id

• Keywords Area
• method
• bayes_calibration
• dream
• emulator
• gaussian_process
• import_build_points_file
• custom_annotated
• eval_id

Enable evaluation ID column in custom-annotated tabular file

Specification

Alias: none
Argument(s): none
Default: no eval_id column

Description

See description of parent custom_annotated

interface_id

• Keywords Area
• method
• bayes_calibration
• dream
• emulator
• gaussian_process
6.2. METHOD

- import_build_points_file
- custom_annotated
- interface_id

Enable interface ID column in custom-annotated tabular file

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no interface_id column

**Description**

See description of parent custom_annotated

**freeform**

- Keywords Area
- method
- bayes_calibration
- dream
- emulator
- gaussian_process
- import_build_points_file
- freeform

Selects freeform file format

**Topics**

This keyword is related to the topics:

- file_formats

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** annotated format
Description

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior

The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips

- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```python
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
freeform
```

Resulting tabular file:

```
0.9 1.1 0.0002 0.26 0.76
0.90009 1.1 0.0001996404857 0.2601620081 0.759955
0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...```

```python
active_only
```
6.2. METHOD

Topics
This keyword is related to the topics:

- file_formats

Specification
Alias: none
Argument(s): none

Description
By default, files for tabular data imports are expected to contain columns for all variables, active and inactive. The keyword active_only indicates that the file to import contains only the active variables.
This option should only be used in contexts where the inactive variables have no influence, for example, building a surrogate over active variables, with the state variables held at nominal. It should not be used in more complex nested contexts, where the values of inactive variables are relevant to the function evaluations used to build the surrogate.

pce

- Keywords Area
- method
- bayes_calibration
- dream
- emulator
- pce

Polynomial Chaos Expansion surrogate model

Specification
Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required (Choose One)</td>
<td>Group 1</td>
<td>sparse_grid_level_sequence</td>
<td>Level to use in sparse grid integration or interpolation</td>
</tr>
</tbody>
</table>
### Description

Selects a polynomial chaos expansion (PCE) surrogate model to use in the Bayesian likelihood calculations. When using PCE as a surrogate within the Bayesian framework, the PCE coefficients can be computed either from integration using a sparse grid or from regression using a random/unstructured data set.

### See Also

These keywords may also be of interest:

- polynomial\_chaos
- sparse\_grid\_level\_sequence
- Keywords Area
- method
- bayes\_calibration
- dream
- emulator
- pce
- sparse\_grid\_level\_sequence

Level to use in sparse grid integration or interpolation

### Specification

**Alias:** none

**Argument(s):** INTEGERLIST

### Description

Multi-dimensional integration by the Smolyak sparse grid method (specified with sparse\_grid\_level and, optionally, dimension\_preference). The underlying one-dimensional integration rules are the same as for the tensor-product quadrature case; however, the default rule selection is nested for sparse grids (Genz-Keister for normals/transformed normals and Gauss-Patterson for uniforms/transformed uniforms). This default can be overridden with an explicit non\_nested specification (resulting in Gauss-Hermite for normals/transformed normals.
and Gauss-Legendre for uniforms/transfomed uniforms). As for tensor quadrature, the dimension_preference specification enables the use of anisotropic sparse grids (refer to the PCE description in the User’s Manual for the anisotropic index set constraint definition). Similar to anisotropic tensor grids, the dimension with greatest preference will have resolution at the full sparse_grid_level and all other dimension resolutions will be reduced in proportion to their reduced preference. For PCE with either isotropic or anisotropic sparse grids, a summation of tensor-product expansions is used, where each anisotropic tensor-product quadrature rule underlying the sparse grid construction results in its own anisotropic tensor-product expansion as described in case 1. These anisotropic tensor-product expansions are summed into a sparse PCE using the standard Smolyak summation (again, refer to the User’s Manual for additional details). As for quadrature_order, the sparse_grid_level specification admits an array input for enabling specification of multiple grid resolutions used by certain advanced solution methodologies.

Usage Tips
This keyword can be used when using sparse grid integration to calculate PCE coefficients or when generating samples for sparse grid collocation.

For most use cases, this keyword will specify a single integer level. In more advanced UQ studies with hierarchical models, the list of integers can apply to different models and/or model levels

expansion_order_sequence

- Keywords Area
- method
- bayes_calibration
- dream
- emulator
- pce
- expansion_order_sequence

The (initial) order of a polynomial expansion

Specification

Alias: none

Argument(s): INTEGERLIST

<table>
<thead>
<tr>
<th>Required/-Optional Required/(Choose One)</th>
<th>Description of Group 1</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>collocation_points_sequence</td>
<td>Number of collocation points to estimate PCE coefficients</td>
<td></td>
</tr>
</tbody>
</table>
### Chapter 6. Keywords Area

<table>
<thead>
<tr>
<th><strong>collocation_ratio</strong></th>
<th>Set the number of points used to build a PCE via regression to be proportional to the number of terms in the expansion.</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>cross_validation</strong></td>
<td>Use cross validation to choose the ‘best’ polynomial order of a polynomial chaos expansion. Adapt emulator model to increase accuracy in high posterior probability regions.</td>
</tr>
<tr>
<td><strong>posterior_adaptive</strong></td>
<td>Adapt emulator model to increase accuracy in high posterior probability regions.</td>
</tr>
<tr>
<td><strong>import_build_points_file</strong></td>
<td>File containing points you wish to use to build a surrogate.</td>
</tr>
</tbody>
</table>

### Description

When the expansion_order for a polynomial chaos expansion is specified, the coefficients may be computed by integration based on random samples or by regression using either random or sub-sampled tensor product quadrature points.

Multidimensional integration by Latin hypercube sampling (specified with `expansion_samples`). In this case, the expansion order $p$ cannot be inferred from the numerical integration specification and it is necessary to provide an `expansion_order` to specify $p$ for a total-order expansion.

Linear regression (specified with either `collocation_points` or `collocation_ratio`). A total-order expansion is used and must be specified using `expansion_order` as described in the previous option. To avoid requiring the user to calculate $N$ from $n$ and $p$, the `collocation_ratio` allows for specification of a constant factor applied to $N$ (e.g., `collocation_ratio = 2` produces samples = $2N$). In addition, the default linear relationship with $N$ can be overridden using a real-valued exponent specified using `ratio_order`. In this case, the number of samples becomes $cN^o$ where $c$ is the `collocation_ratio` and $o$ is the `ratio_order`. The `use_derivatives` flag informs the regression approach to include derivative matching equations (limited to gradients at present) in the least squares solutions, enabling the use of fewer collocation points for a given expansion order and dimension (number of points required becomes $\frac{cN^o}{n+p}$). When admissible, a constrained least squares approach is employed in which response values are first reproduced exactly and error in reproducing response derivatives is minimized. Two collocation grid options are supported: the default is Latin hypercube sampling (“point collocation”), and an alternate approach of “probabilistic collocation” is also available through inclusion of the `tensor_grid` keyword. In this alternate case, the collocation grid is defined using a subset of tensor-product quadrature points: the order of the tensor-product grid is selected as one more than the expansion order in each dimension (to avoid sampling at roots of the basis polynomials) and then the tensor multi-index is uniformly sampled to generate a non-repeated subset of tensor quadrature points.
If `collocation_points` or `collocation_ratio` is specified, the PCE coefficients will be determined by regression. If no regression specification is provided, appropriate defaults are defined. Specifically SVD-based least-squares will be used for solving over-determined systems and under-determined systems will be solved using LASSO. For the situation when the number of function values is smaller than the number of terms in a PCE, but the total number of samples including gradient values is greater than the number of terms, the resulting over-determined system will be solved using equality constrained least squares. Technical information on the various methods listed below can be found in the Linear regression section of the Theory Manual. Some of the regression methods (OMP, LASSO, and LARS) are able to produce a set of possible PCE coefficient vectors (see the Linear regression section in the Theory Manual). If cross validation is inactive, then only one solution, consistent with the noise_tolerance, will be returned. If cross validation is active, Dakota will choose between possible coefficient vectors found internally by the regression method across the set of expansion orders (1,....,expansion_order) and the set of specified noise tolerances and return the one with the lowest cross validation error indicator.

**Usage Tips**

For most use cases, this keyword will specify a single integer order. In more advanced UQ studies with hierarchical models, the list of integers can apply to different models and/or model levels.

`collocation_points_sequence`

- **Keywords Area**
- **method**
- **bayes_calibration**
- **dream**
- **emulator**
- **pce**
- **expansion_order_sequence**
- **collocation_points_sequence**

Number of collocation points to estimate PCE coefficients

**Specification**

**Alias:** none

**Argument(s):** INTEGERLIST

**Description**

Specify the number of collocation points used to estimate PCE coefficients using regression or orthogonal-least-interpolation.

**Usage Tips**

For most use cases, this keyword will specify a single integer number of points. In more advanced UQ studies with hierarchical models, the list of integers can apply to different models and/or model levels.
collocation\_ratio

- Keywords Area
- method
- bayes\_calibration
- dream
- emulator
- pce
- expansion\_order\_sequence
- collocation\_ratio

Set the number of points used to build a PCE via regression to be proportional to the number of terms in the expansion.

**Specification**

**Alias:** none  
**Argument(s):** REAL

**Description**

Set the number of points used to build a PCE via regression to be proportional to the number of terms in the expansion. To avoid requiring the user to calculate N from n and p, the collocation\_ratio allows for specification of a constant factor applied to N (e.g., collocation\_ratio = 2, produces samples = 2N). In addition, the default linear relationship with N can be overridden using a real-valued exponent specified using ratio\_order. In this case, the number of samples becomes \(cN^o\) where \(c\) is the collocation\_ratio and \(o\) is the ratio\_order. The use\_derivatives flag informs the regression approach to include derivative matching equations (limited to gradients at present) in the least squares solutions, enabling the use of fewer collocation points for a given expansion order and dimension (number of points required becomes \(\frac{cN^o}{n+1}\)).

cross\_validation

- Keywords Area
- method
- bayes\_calibration
- dream
- emulator
- pce
- expansion\_order\_sequence
- cross\_validation

Use cross validation to choose the ‘best’ polynomial order of a polynomial chaos expansion.
6.2. **METHOD**

Specification

**Alias:** none

**Argument(s):** none

**Description**

Use cross validation to choose the 'best' polynomial degree of a polynomial chaos expansion. 10 fold cross validation is used to estimate the cross validation error of a total-order polynomial expansion for orders 1 through to order. The order chosen is the one that produces the lowest cross validation error. If there are not enough points to perform 10 fold cross validation then one-at-a-time cross validation will be performed.

```
posterior_adaptive
```

- Keywords Area
- method
- bayes_calibration
- dream
- emulator
- pce
- expansion_order_sequence
- posterior_adaptive

Adapt emulator model to increase accuracy in high posterior probability regions

Specification

**Alias:** none

**Argument(s):** none

**Description**

Following an emulator-based MCMC process, this option refines the emulator by selecting points in regions of high posterior probability, performing truth evaluations at these points, updating the emulator, and reperforming the MCMC process. The adaptation is continued until the maximum number of iterations is exceeded or the convergence tolerance is met.

**Examples**

```
bayes_calibration queso
  chain_samples = 2000 seed = 348
delayed_rejection
emulator
  gaussian_process surfpack build_samples = 30
  posterior_adaptive max_iterations = 10
  proposal_covariance derivatives
```
import_build_points_file
• Keywords Area
• method
• bayes_calibration
• dream
• emulator
• pce
• expansion_order_sequence
• import_build_points_file
File containing points you wish to use to build a surrogate

Specification
Alias: import_points_file
Argument(s): STRING
Default: no point import from a file

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group Tabular Format (Group 1)</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional (Choose One)</td>
<td>annotated</td>
<td>custom_annotated</td>
<td>Selects custom-annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td>freeform</td>
<td>freeform</td>
<td>Selects freeform file format</td>
</tr>
<tr>
<td>Optional</td>
<td>active_only</td>
<td>Import only active variables from tabular data file</td>
<td></td>
</tr>
</tbody>
</table>

Description
The import_build_points_file allows the user to specify a file that contains a list of points and truth model responses used to construct a surrogate model. These can be used by all methods that (explicitly, e.g. surrogate-based optimization, or implicitly, e.g. efficient global optimization) operate on a surrogate. In particular, these points and responses are used in place of truth model evaluations to construct the initial surrogate. When used to construct surrogate models or emulators these are often called build points or training data.

Default Behavior
By default, methods do not import points from a file.

Usage Tips
Dakota parses input files without regard to whitespace, but the import_build_points_file must be in one of three formats:
6.2. METHOD

- annotated (default)
- custom_annotated
- freeform

Examples

```python
method
polyomial_chaos
  expansion_order = 4
  import_build_points_file = 'dakota_uq_rosenbrock_pce_import.annot.pts.dat'

annotated
  Keywords Area
  method
  bayes_calibration
  dream
  emulator
  pce
  expansion_order_sequence
  import_build_points_file
  annotated

Selects annotated tabular file format
```

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none
  Argument(s): none
  Default: annotated format

Description

An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior

By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips
To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify custom.annotated header eval_id

Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

**Examples**

Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```python
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
annotated
```

Resulting tabular file:

```
%eval_id interface x1  x2  obj_fn nln_ineq_con_1 nln_ineq_con_2
1  NO_ID  0.9  1.1  0.0002  0.26  0.76
2  NO_ID  0.90009  1.1  0.0001996404857  0.2601620081  0.759955
3  NO_ID  0.89991  1.1  0.0002003604863  0.2598380081  0.760045
...```

custom.annotated

- Keywords Area
- method
- bayes_calibration
- dream
- emulator
- pce
- expansion_order_sequence
- import_build_points_file
- custom.annotated

Selects custom-annotated tabular file format

**Topics**

This keyword is related to the topics:

- file_formats

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** annotated format
### Description

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

#### Default Behavior

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

#### Usage Tips

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

#### Examples

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:

```plaintext
environment
  tabular_data
    tabular_data_file = 'dakota_summary.dat'
custom_annotated header eval_id
```

Resulting tabular file:

```
%eval_id x1 x2 obj_fn nln_ineq_con_1 nln_ineq_con_2
1 0.9 1.1 0.0002 0.26 0.76
2 0.90009 1.1 0.0001996404857 0.2601620081 0.759955
3 0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...```
header
  • Keywords Area
  • method
  • bayes_calibration
  • dream
  • emulator
  • pce
  • expansion_order_sequence
  • import_build_points_file
  • custom_annotated
  • header

Enable header row in custom-annotated tabular file

Specification

Alias: none
  Argument(s): none
  Default: no header

Description

See description of parent custom_annotated

eval_id
  • Keywords Area
  • method
  • bayes_calibration
  • dream
  • emulator
  • pce
  • expansion_order_sequence
  • import_build_points_file
  • custom_annotated
  • eval_id

Enable evaluation ID column in custom-annotated tabular file
6.2. METHOD

Specification

Alias: none
  Argument(s): none
  Default: no eval_id column

Description

See description of parent custom_annotated

  interface_id
  • Keywords Area
  • method
  • bayes_calibration
  • dream
  • emulator
  • pce
  • expansion_order_sequence
  • import_build_points_file
  • custom_annotated
  • interface_id

  Enable interface ID column in custom-annotated tabular file

Specification

Alias: none
  Argument(s): none
  Default: no interface_id column

Description

See description of parent custom_annotated

  freeform
  • Keywords Area
  • method
  • bayes_calibration
  • dream
  • emulator
• pce
• expansion_order_sequence
• import_build_points_file
• freeform

Selects freeform file format

**Topics**

This keyword is related to the topics:

• file_formats

**Specification**

Alias: none
Argument(s): none
Default: annotated format

**Description**

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

**Default Behavior**

The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

**Usage Tips**

• Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.
• When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
• In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).
• Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

**Examples**

Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
freeform
```

Resulting tabular file:

```
0.9  1.1  0.0002  0.26  0.76
0.90009  1.1  0.0001996404857  0.2601620081  0.759955
0.89991  1.1  0.0002003604863  0.2598380081  0.760045
...
```
6.2. METHOD

active_only

- Keywords Area
- method
- bayes_calibration
- dream
- emulator
- pce
- expansion_order_sequence
- import_build_points_file
- active_only

Import only active variables from tabular data file

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none

Argument(s): none

Description

By default, files for tabular data imports are expected to contain columns for all variables, active and inactive. The keyword active_only indicates that the file to import contains only the active variables.

This option should only be used in contexts where the inactive variables have no influence, for example, building a surrogate over active variables, with the state variables held at nominal. It should not be used in more complex nested contexts, where the values of inactive variables are relevant to the function evaluations used to build the surrogate.

orthogonal_least_interpolation

- Keywords Area
- method
- bayes_calibration
- dream
- emulator
- pce
- orthogonal_least_interpolation

Build a polynomial chaos expansion from simulation samples using orthogonal least interpolation.
CHAPTER 6. KEYWORDS AREA

Specification

**Alias:** none

**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required</td>
<td></td>
<td>collocation_points_sequence</td>
<td>Number of collocation points to estimate PCE coefficients</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>posterior_adaptive</td>
<td>Adapt emulator model to increase accuracy in high posterior probability regions</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>import_build_points_file</td>
<td>File containing points you wish to use to build a surrogate</td>
</tr>
</tbody>
</table>

Description

Build a polynomial chaos expansion from simulation samples using orthogonal least interpolation. Unlike the other regression methods `expansion_order` cannot be set. OLI will produce the lowest degree polynomial that interpolates the data

```
collocation_points_sequence
```

- **Keywords Area**
- **method**
- **bayes_calibration**
- **dream**
- **emulator**
- **pce**
- **orthogonal_least_interpolation**
- **collocation_points_sequence**

Number of collocation points to estimate PCE coefficients

**Specification**

**Alias:** none

**Argument(s):** INTEGERLIST
6.2. METHOD

**Description**

Specify the number of collocation points used to estimate PCE coefficients using regression or orthogonal-least-interpolation.

**Usage Tips**

For most use cases, this keyword will specify a single integer number of points. In more advanced UQ studies with hierarchical models, the list of integers can apply to different models and/or model levels.

**posterior_adaptive**

- **Keywords Area**
- **method**
- **bayes_calibration**
- **dream**
- **emulator**
- **pce**
- **orthogonal_least_interpolation**
- **posterior_adaptive**

Adapt emulator model to increase accuracy in high posterior probability regions.

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

Following an emulator-based MCMC process, this option refines the emulator by selecting points in regions of high posterior probability, performing truth evaluations at these points, updating the emulator, and reperforming the MCMC process. The adaptation is continued until the maximum number of iterations is exceeded or the convergence tolerance is met.

**Examples**

```plaintext
bayes_calibration queso
chain_samples = 2000 seed = 348
delayed_rejection
evaluator
gaussian_process surfpack build_samples = 30
posterior_adaptive max_iterations = 10
proposal_covariance derivatives
```
import_build_points_file

- Keywords Area
- method
- bayes_calibration
- dream
- emulator
- pce
- orthogonal_least_interpolation
- import_build_points_file

File containing points you wish to use to build a surrogate

**Specification**

**Alias:** import_points_file  
**Argument(s):** STRING  
**Default:** no point import from a file

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional (Choose One)</td>
<td>Tabular Format (Group 1)</td>
<td>annotated</td>
<td>Selects annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>custom_annotated</td>
<td>Selects custom-annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>freeform</td>
<td>Selects freeform file format</td>
</tr>
</tbody>
</table>

**Description**

The `import_build_points_file` allows the user to specify a file that contains a list of points and truth model responses used to construct a surrogate model. These can be used by all methods that (explicitly, e.g. surrogate-based optimization, or implicitly, e.g. efficient global optimization) operate on a surrogate. In particular, these points and responses are used in place of truth model evaluations to construct the initial surrogate. When used to construct surrogate models or emulators these are often called build points or training data.

**Default Behavior**

By default, methods do not import points from a file.

**Usage Tips**

Dakota parses input files without regard to whitespace, but the `import_build_points_file` must be in one of three formats:
6.2. METHOD

- annotated (default)
- custom_annotated
- freeform

Examples

```
method
    polynomial_choas
        expansion_order = 4
        import_build_points_file = 'dakota_uq_rosenbrock_pce_import.annot.pts.dat'

annotated
- Keywords Area
- method
- bayes_calibration
- dream
- emulator
- pce
- orthogonal_least_interpolation
- import_build_points_file
- annotated
```

Selects annotated tabular file format

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none

Argument(s): none

Default: annotated format

Description

An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior

By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips
To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify custom_annotated header eval_id.

Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
```

Resulting tabular file:

```
%eval_id interface x1 x2 obj_fn nln_ineq_con_1 nln_ineq_con_2
1 NO_ID 0.9 1.1 0.0002 0.26 0.76
2 NO_ID 0.90009 1.1 0.0001996404857 0.2601620081 0.759955
3 NO_ID 0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...```

custom_annotated

- Keywords Area
- method
- bayes_calibration
- dream
- emulator
- pce
- orthogonal_least_interpolation
- import_build_points_file
- custom_annotated

Selects custom-annotated tabular file format

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none
Argument(s): none
Default: annotated format
6.2. METHOD

### Description

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

#### Default Behavior

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

#### Usage Tips

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

#### Examples

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:

```environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
custom_annotated header eval_id
```

Resulting tabular file:

```
%eval_id  x1  x2  obj_fn  nln_ineq_con_1  nln_ineq_con_2
1  0.9  1.1  0.0002  0.26  0.76
2  0.90009  1.1  0.0001996404857  0.2601620081  0.759955
3  0.89991  1.1  0.0002003604863  0.2598380081  0.760045
...
```
header
  • Keywords Area
  • method
  • bayes_calibration
  • dream
  • emulator
  • pce
  • orthogonal_least_interpolation
  • import_build_points_file
  • custom_annotated
  • header

Enable header row in custom-annotated tabular file

**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** no header

**Description**

See description of parent `custom_annotated`

eval_id
  • Keywords Area
  • method
  • bayes_calibration
  • dream
  • emulator
  • pce
  • orthogonal_least_interpolation
  • import_build_points_file
  • custom_annotated
  • eval_id

Enable evaluation ID column in custom-annotated tabular file
6.2. METHOD

Specification

Alias: none
Argument(s): none
Default: no eval_id column

Description

See description of parent custom_annotated

interface_id

• Keywords Area
• method
• bayes_calibration
• dream
• emulator
• pce
• orthogonal_least_interpolation
• import_build_points_file
• custom_annotated
• interface_id

Enable interface ID column in custom-annotated tabular file

Specification

Alias: none
Argument(s): none
Default: no interface_id column

Description

See description of parent custom_annotated

freeform

• Keywords Area
• method
• bayes_calibration
• dream
• emulator
• pce
• orthogonal_least_interpolation
• import_build_points_file
• freeform
  Selects freeform file format

Topics
This keyword is related to the topics:
  • file_formats

Specification
Alias: none
  Argument(s): none
  Default: annotated format

Description
A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior
The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips
• Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.
• When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
• In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).
• Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples
Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
freeform
```

Resulting tabular file:

```
0.9 1.1 0.0002 0.26 0.76
0.90009 1.1 0.0001996404857 0.2601620081 0.759955
0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...
```
active_only

- Keywords Area
- method
- bayes_calibration
- dream
- emulator
- pce
- orthogonal_least_interpolation
- import_build_points_file
- active_only

Import only active variables from tabular data file

**Topics**

This keyword is related to the topics:

- file_formats

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

By default, files for tabular data imports are expected to contain columns for all variables, active and inactive. The keyword `active_only` indicates that the file to import contains only the active variables.

This option should only be used in contexts where the inactive variables have no influence, for example, building a surrogate over active variables, with the state variables held at nominal. It should not be used in more complex nested contexts, where the values of inactive variables are relevant to the function evaluations used to build the surrogate.

**sc**

- Keywords Area
- method
- bayes_calibration
- dream
- emulator
- sc

Stochastic Collocation polynomial surrogate model
### Specification

**Alias:** none  
**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/Optional Required</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>none</td>
<td>sparse grid level-sequence</td>
<td>sparse_grid_level-sequence</td>
<td>Level to use in sparse grid integration or interpolation</td>
</tr>
</tbody>
</table>

### Description

Selects stochastic collocation (SC) model to use in the Bayesian likelihood calculations. When using SC as a surrogate within the Bayesian framework, the build points (training points) for the stochastic collocation are constructed from a sparse grid.

### See Also

These keywords may also be of interest:

- **stoch_collocation**

  **sparse_grid_level_sequence**

  - **Keywords Area**
  - **method**
  - **bayes_calibration**
  - **dream**
  - **emulator**
  - **sc**
  - **sparse_grid_level_sequence**

  Level to use in sparse grid integration or interpolation

### Specification

**Alias:** none  
**Argument(s):** INTEGERLIST
6.2. METHOD

Description

Multi-dimensional integration by the Smolyak sparse grid method (specified with sparse_grid_level and, optionally, dimension_preference). The underlying one-dimensional integration rules are the same as for the tensor-product quadrature case; however, the default rule selection is nested for sparse grids (Genz-Keister for normals/transformed normals and Gauss-Patterson for uniforms/transformed uniforms). This default can be overridden with an explicit non_nested specification (resulting in Gauss-Hermite for normals/transformed normals and Gauss-Legendre for uniforms/transformed uniforms). As for tensor quadrature, the dimension_preference specification enables the use of anisotropic sparse grids (refer to the PCE description in the User’s Manual for the anisotropic index set constraint definition). Similar to anisotropic tensor grids, the dimension with greatest preference will have resolution at the full sparse_grid_level and all other dimension resolutions will be reduced in proportion to their reduced preference. For PCE with either isotropic or anisotropic sparse grids, a summation of tensor-product expansions is used, where each anisotropic tensor-product quadrature rule underlying the sparse grid construction results in its own anisotropic tensor-product expansion as described in case 1. These anisotropic tensor-product expansions are summed into a sparse PCE using the standard Smolyak summation (again, refer to the User’s Manual for additional details). As for quadrature_order, the sparse_grid_level specification admits an array input for enabling specification of multiple grid resolutions used by certain advanced solution methodologies.

Usage Tips

This keyword can be used when using sparse grid integration to calculate PCE coefficients or when generating samples for sparse grid collocation.

For most use cases, this keyword will specify a single integer level. In more advanced UQ studies with hierarchical models, the list of integers can apply to different models and/or model levels.

use_derivatives

- Keywords Area
- method
- bayes_calibration
- dream
- emulator
- use_derivatives

Use derivative data to construct surrogate models

Specification

Alias: none

Argument(s): none

Default: use function values only

Description

The use_derivatives flag specifies that any available derivative information should be used in global approximation builds, for those global surrogate types that support it (currently, polynomial regression and the Surfpack Gaussian process).

However, its use with Surfpack Gaussian process is not recommended.
standardized_space

- Keywords Area
- method
- bayes_calibration
- dream
- standardized_space

Perform Bayesian inference in standardized probability space

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

This option transforms the inference process (MCMC sampling and any emulator model management) into a standardized probability space.

The variable transformations performed are as described in askey.

**Default Behavior**

The default for the Gaussian process and no emulator options is to perform inference in the original probability space (no transformation). Polynomial chaos and stochastic collocation emulators, on the other hand, are always formed in standardized probability space, such that the inference process is also performed in this standardized space.

**Expected Output**

The user will see the truth model evaluations performed in the original space, whereas any method diagnostics relating to the MCMC samples (e.g., QUESO data in the outputData directory) will report points and response data (response gradients and Hessians, if present, will differ but response values will not) that correspond to the transformed space.

**Usage Tips**

Selecting standardized_space generally has the effect of scaling the random variables to be of comparable magnitude, which can improve the efficiency of the Bayesian inference process.

**Examples**

```
method, bayes_calibration queso
  samples = 2000 seed = 348
dram
  standardized_space
```

**export_chain_points_file**

- Keywords Area
- method
- bayes_calibration
6.2. **METHOD**

- dream
- export_chain_points_file

Export the MCMC chain to the specified filename

**Specification**

**Alias:** none  
**Argument(s):** STRING  
**Default:** chain export to default filename

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional*(Choose One)*</td>
<td>Tabular Format (Group 1)</td>
<td>annotated</td>
<td>Selects annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>custom_annotated</td>
<td>Selects custom-annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>freeform</td>
<td>Selects freeform file format</td>
</tr>
</tbody>
</table>

**Description**

The filename to which the final MCMC posterior chain will be exported.  
**Default Behavior** No export to file.  
**Expected Output** A tabular data file will be produced in the specified format (annotated by default) containing samples from the posterior distribution.  
**Usage Tips**  
**Additional Discussion**

- annotated
  - Keywords Area
  - method
  - bayes_calibration
  - dream
  - export_chain_points_file
  - annotated
    Selects annotated tabular file format

**Topics**

This keyword is related to the topics:

- file_formats
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none
  Argument(s): none
  Default: annotated

Description
An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior
By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips
- To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify custom_annotated header eval_id
- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples
Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
annotated
```

Resulting tabular file:

```
%eval_id interface x1 x2 obj fn nln_ineq_con_1 nln_ineq_con_2
1 NO_ID 0.9 1.1 0.0002 0.26 0.76
2 NO_ID 0.90009 1.1 0.0001996404857 0.2601620081 0.759955
3 NO_ID 0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...```

custom_annotated
- Keywords Area
- method
- bayes_calibration
- dream
- export_chain_points_file
- custom_annotated

Selects custom-annotated tabular file format
6.2. METHOD

Topics
This keyword is related to the topics:

- file_formats

Specification
Alias: none  
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>header</td>
<td>Enable header row in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>eval_id</td>
<td>Enable evaluation ID column in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>interface_id</td>
<td>Enable interface ID column in custom-annotated tabular file</td>
</tr>
</tbody>
</table>

Description
A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

Default Behavior
The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom.annotated, followed by options, in the relevant export/import context.

Usage Tips
- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples
Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
custom_annotated header eval_id

Resulting tabular file:

<table>
<thead>
<tr>
<th>eval_id</th>
<th>x1</th>
<th>x2</th>
<th>obj_fn</th>
<th>nln_ineq_con_1</th>
<th>nln_ineq_con_2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.9</td>
<td>1.1</td>
<td>0.0002</td>
<td>0.26</td>
<td>0.76</td>
</tr>
<tr>
<td>2</td>
<td>0.90009</td>
<td>1.1</td>
<td>0.0001996404857</td>
<td>0.2601620081</td>
<td>0.759955</td>
</tr>
<tr>
<td>3</td>
<td>0.89991</td>
<td>1.1</td>
<td>0.0002003604863</td>
<td>0.2598380081</td>
<td>0.760045</td>
</tr>
<tr>
<td>...</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

header

- Keywords Area
- method
- bayes_calibration
- dream
- export_chain_points_file
- custom_annotated
- header

Enable header row in custom-annotated tabular file

Specification

Alias: none
Argument(s): none

Description

See description of parent custom_annotated

eval_id

- Keywords Area
- method
- bayes_calibration
- dream
- export_chain_points_file
- custom_annotated
- eval_id

Enable evaluation ID column in custom-annotated tabular file
6.2. METHOD

Specification

Alias: none
Argument(s): none

Description

See description of parent custom_annotated

interface_id

- Keywords Area
- method
- bayes_calibration
- dream
- export_chain_points_file
- custom_annotated
- interface_id

Enable interface ID column in custom-annotated tabular file

Specification

Alias: none
Argument(s): none

Description

See description of parent custom_annotated

freeform

- Keywords Area
- method
- bayes_calibration
- dream
- export_chain_points_file
- freeform

Selects freeform file format

Topics

This keyword is related to the topics:

- file_formats


**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** annotated

**Description**

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

**Default Behavior**

The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

**Usage Tips**

- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

**Examples**

Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
freeform
```

Resulting tabular file:

```
0.9 1.1 0.0002 0.26 0.76
0.90009 1.1 0.0001996404857 0.2601620081 0.759955
0.89991 1.1 0.0002003604863 0.2598380081 0.760045
... 
```

**experimental_design**

- Keywords Area
- method
- bayes_calibration
- experimental_design

(Experimental) Adaptively select experimental designs for iterative Bayesian updating
6.2. METHOD

Specification

Alias: none
  Argument(s): none
CHAPTER 6. KEYWORDS AREA

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required</td>
<td></td>
<td>initial_samples</td>
<td>Number of data points used during initial Bayesian calibration</td>
</tr>
<tr>
<td>Required</td>
<td>num_candidates</td>
<td></td>
<td>Number of candidate design points considered</td>
</tr>
<tr>
<td>Optional</td>
<td>max_hifi-evaluations</td>
<td></td>
<td>Maximum number of high-fidelity model runs to be used</td>
</tr>
<tr>
<td>Optional</td>
<td>import_candidate-points_file</td>
<td></td>
<td>Specify text file containing candidate design points</td>
</tr>
</tbody>
</table>

**Description**

This "experimental design" algorithm uses responses produced by a high-fidelity model as data to update the parameters of a low-fidelity model using Bayes’ Rule. It is a capability that is under active development and is currently compatible only with *queso*. The user-specified high-fidelity model should depend only on configuration variables (i.e. design conditions), such as temperature or spatial location, while the user-specified low-fidelity model should depend on both configuration variables and its own model parameters to be calibrated.

The algorithm starts with a preliminary Bayesian calibration using the number of data points specified in `initial_samples`. These data points can be read in through the `calibration_data_file` command in the `response` block. If `num_experiments` is less than `initial_samples` or if no such data file is provided, Latin Hypercube Samples of the design space (specified in the `variables` block) will be run through the user-specified high-fidelity code to supplement the initial data. Once this first calibration is complete, a set of possible experimental design conditions, specified using the configuration variables, is proposed. The user specifies the size of this set using `num_candidates`. The set of candidates itself may be explicitly given through the `import_candidate_points_file` command. If the number of candidates in this file is less than `num_candidates`, or if this file is omitted, the set of candidate designs will again be supplemented with a Latin Hypercube Sample of the design space.

For each candidate design $\xi_i$ in the set of possible design conditions, the mutual information (MI) between the low-fidelity model parameters $\theta$ and the high-fidelity model response $y(\xi_i)$,

$$MI = \int \int f(\theta, y(\xi_i)) \log \frac{f(\theta, y(\xi_i))}{f(\theta)f(y(\xi_i))} d\theta dy,$$

is approximated. The high-fidelity model is replaced by the low-fidelity model and a $k$-nearest neighbor approximation is used in the calculation. The design point $\xi^*$ for which MI is the largest is selected and run through the high-fidelity model to yield a new observation $y(\xi^*)$. This new observation is added to the calibration data, and a subsequent Bayesian calibration is performed. A new MI for each remaining candidate design is computed, and the process repeats until one of three stopping criteria are met.
6.2. Method

Of the three stopping criteria, two are automatically checked by Dakota. If the relative change in the MI from one iteration to the next is sufficiently small or if the set of candidate design conditions has been exhausted, the algorithm terminates. The user may specify the third stopping criteria using `max_hifi_evaluations`. This limits the number of high-fidelity model evaluations that will be performed during this algorithm. It therefore limits the number of iterations through the algorithm that will be performed. Any high-fidelity model runs needed to produce the data set for the initial calibration are not included in this allocation.

In the case that the high-fidelity model must be run independently of Dakota, the user may set `max_hifi_evaluations` to zero. The optimal experimental design point will be calculated and reported, but the high-fidelity model will not be run. For more details, see the User’s Manual.

Expected Output

Information regarding the progress and termination condition of the experimental design algorithm is output to the screen with varying levels of verbosity. Further details can be found, regardless of verbosity, in the output file `experimental_design.output.txt`.

Usage Tips

Due to the optional file read-ins and the supplemental sampling, it is important for the user to check consistency within the input file specifications. For example, if `num_experiments` is less than the number of experiments in the `calibration_data_file`, only the first lines of the file will be used and the rest will be discarded. The same holds true for the `import_candidate_points_file` and `num_candidates`.

The incorporation of variance information in `calibration_data_file` is not yet supported. Only configuration variables and the corresponding high-fidelity model information should be included in the file.

Examples

The input file below illustrates the use of `experimental_design` and its options:

```plaintext
bayes_calibration
  queso
dram
  chain_samples = 1000 seed = 348
experimental_design
  initial_samples = 5
  num_candidates = 10
  import_candidate_points_file = "bayes_experimental_design.cand.dat"
  freeform
  max_hifi_evaluations = 3
```

**initial_samples**

- **Keywords Area**
- **method**
- **bayes_calibration**
- **experimental_design**
- **initial_samples**

Number of data points used during initial Bayesian calibration

**Specification**

**Alias:** samples

**Argument(s):** INTEGER

**Default:** method-dependent
CHAPTER 6. KEYWORDS AREA

Description

The experimental design algorithm starts with a preliminary Bayesian calibration. The keyword `initial_samples` specifies the number of data points used during this initial calibration. These data points may come from external data sources through `calibration_data_file`, from an LHS sample of the design space, or both.

`num_candidates`

- Keywords Area
- method
- bayes_calibration
- experimental_design
- `num_candidates`

Number of candidate design points considered

Specification

Alias: none

Argument(s): INTEGER

Default: 1

Description

After the initial Bayesian calibration, a set of candidate design points is created, from which the optimal design(s) will be chosen. This set is of size `num_candidates`. These candidate points may be specified by the user through `import_candidate_points_file`, from an LHS sample of the design space, or both.

`max_hifi_evaluations`

- Keywords Area
- method
- bayes_calibration
- experimental_design
- `max_hifi_evaluations`

Maximum number of high-fidelity model runs to be used

Specification

Alias: none

Argument(s): INTEGER
6.2. METHOD

Description

There are three stopping criteria by which the Bayesian experimental design algorithm will be terminated:

- The high-fidelity model has been run $\text{max\_hifi\_evaluations}$ times
- The set of candidate design points have been exhausted
- The relative change in the mutual information from one iteration to the next is sufficiently small. The first criterion is controlled by this keyword specification.

Default Behavior

If no maximum number of high-fidelity model runs is specified, only the last two stopping criteria listed above will be evaluated.

Usage Tips

Be wary that $\text{max\_hifi\_evaluations}$ does not include any high-fidelity model evaluations that need to be run to produce the data set for the initial Bayesian calibration. This number only includes those evaluations performed on the sequentially chosen optimal design points.

If $\text{max\_hifi\_evaluations}$ is set to zero, the a single optimal experimental design point will be selected, and Dakota will exit without running the high-fidelity model.

**import_candidate_points_file**

- Keywords Area:
  - method
  - bayes_calibration
  - experimental_design
  - import_candidate_points_file

Specify text file containing candidate design points.

**Specification**

Alias: none

Argument(s): STRING

Default: no point import from a file

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Optional/Choose One</th>
<th>Description of Group tabular_format (Group 1)</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>annotated</td>
<td>Selects annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>custom_annotated</td>
<td>Selects custom-annotated tabular file format</td>
</tr>
</tbody>
</table>
CHAPTER 6. KEYWORDS AREA

**Description**

Enables text file import of user-specified design points (i.e. configuration variables). No model responses should be included. Each row should correspond to a single design or configuration.

**Default Behavior**

Be default, methods do not import points from a file.

**Usage Tips**

Dakota parses input files without regard to whitespace, but the import_build_points_file must be in one of three formats:

- annotated (default)
- custom_annotated
- freeform

**Topics**

This keyword is related to the topics:

- file_formats

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** annotated

<table>
<thead>
<tr>
<th>freeform</th>
<th>Selects freeform file format</th>
</tr>
</thead>
</table>
6.2. METHOD

Description
An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior
By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips
- To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify custom_annotated header eval_id
- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples
Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
  tabular_data_file = 'dakota_summary.dat'
annotated

Resulting tabular file:

```eval_id interface  x1  x2  obj_fn  nln_ineq_con_1  nln_ineq_con_2
1  NO_ID  0.9  1.1  0.0002  0.26  0.76
2  NO_ID  0.90009  1.1  0.0001996404857  0.2601620081  0.759955
3  NO_ID  0.89991  1.1  0.0002003604863  0.2598380081  0.760045
...
```

custom_annotated

- Keywords Area
- method
- bayes_calibration
- experimental_design
- import_candidate_points_file
- custom_annotated

Selects custom-annotated tabular file format
Topics
This keyword is related to the topics:

- file_formats

Specification
Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>header</td>
<td></td>
<td>Enable header row in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td>eval_id</td>
<td></td>
<td>Enable evaluation ID column in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td>interface_id</td>
<td></td>
<td>Enable interface ID column in custom-annotated tabular file</td>
</tr>
</tbody>
</table>

Description
A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

Default Behavior
The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

Usage Tips
- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples
Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:
6.2. METHOD

environment
  tabular_data
    tabular_data_file = 'dakota_summary.dat'
    custom_annotated header eval_id

Resulting tabular file:

<table>
<thead>
<tr>
<th>%eval_id</th>
<th>x1</th>
<th>x2</th>
<th>obj_fn</th>
<th>nln_ineq_con_1</th>
<th>nln_ineq_con_2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.9</td>
<td>1.1</td>
<td>0.0002</td>
<td>0.26</td>
<td>0.76</td>
</tr>
<tr>
<td>2</td>
<td>0.90009</td>
<td>1.1</td>
<td>0.0001996404857</td>
<td>0.2601620081</td>
<td>0.759955</td>
</tr>
<tr>
<td>3</td>
<td>0.89991</td>
<td>1.1</td>
<td>0.0002003604863</td>
<td>0.2598380081</td>
<td>0.760045</td>
</tr>
<tr>
<td>...</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

header
- Keywords Area
- method
- bayes_calibration
- experimental_design
- import_candidate_points_file
- custom_annotated
- header

Enable header row in custom-annotated tabular file

Specification

Alias: none
  Argument(s): none

Description

See description of parent custom_annotated

eval_id
- Keywords Area
- method
- bayes_calibration
- experimental_design
- import_candidate_points_file
- custom_annotated
- eval_id

Enable evaluation ID column in custom-annotated tabular file
Specification

Alias: none
Argument(s): none

Description

See description of parent `custom_annotated`

interface_id

- Keywords Area
- method
- bayes_calibration
- experimental_design
- import_candidate_points_file
- custom_annotated
- interface_id

Enable interface ID column in custom-annotated tabular file

Specification

Alias: none
Argument(s): none

Description

See description of parent `custom_annotated`

freeform

- Keywords Area
- method
- bayes_calibration
- experimental_design
- import_candidate_points_file
- freeform

Selects freeform file format

Topics

This keyword is related to the topics:

- file_formats
6.2. *METHOD*

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

**Default Behavior**

The *annotated* format is the default for tabular export/import. To change this behavior, specify *freeform* in the relevant export/import context.

**Usage Tips**

- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to *annotated* format, though *freeform* remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- In *freeform*, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the *freeform* option.

**Examples**

Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
freeform
```

Resulting tabular file:

```
0.9  1.1  0.0002  0.26  0.76
0.90009 1.1  0.0001996404857  0.2601620081  0.759955
0.89991 1.1  0.0002003604863  0.2598380081  0.760045
...
```

calibrate_error_multipliers

- **Keywords Area**

- **method**

- **bayes_calibration**

- **calibrate_error_multipliers**

Calibrate hyper-parameter multipliers on the observation error covariance
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): none

Default: none
### Description

Calibrate one or more multipliers on the user-provided observation error covariance (variance_type). Options include one multiplier on the whole block-diagonal covariance structure, one multiplier per_experiment covariance block, one multiplier per_response covariance block, or separate multipliers for each response/experiment pair (for a total of number experiments X number response groups).

**Default Behavior:** No hyper-parameter calibration. When hyper-parameter calibration is enabled, the default prior on the multiplier is a diffuse inverse gamma, with mean and mode approximately 1.0.

**Expected Output:** Final calibration results will include both inference parameters and one or more calibrated hyper-parameters.

**Usage Tips:** The per_response option can be useful when each response has its own measurement error process, but all experiments were gathered with the same equipment and conditions. The per_experiment option might be used when working with data from multiple independent laboratories.

### Examples

Perform Bayesian calibration with 2 calibration variables and two hyper-parameter multipliers, one per each of two responses. The multipliers are assumed the same across the 10 experiments. The priors on the multipliers are specified using the hyperprior_alphas and hyperprior_betas keywords.

---

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required*(Choose One)*</td>
<td>Group 1</td>
<td>one</td>
<td>Calibrate one hyper-parameter multiplier across all responses/experiments</td>
</tr>
<tr>
<td></td>
<td></td>
<td>per_experiment</td>
<td>Calibrate one hyper-parameter multiplier per experiment</td>
</tr>
<tr>
<td></td>
<td></td>
<td>per_response</td>
<td>Calibrate one hyper-parameter multiplier per response</td>
</tr>
<tr>
<td></td>
<td></td>
<td>both</td>
<td>Calibrate one hyper-parameter multiplier for each response/experiment pair</td>
</tr>
</tbody>
</table>

| Optional | hyperprior_alphas | Shape (alpha) of the inverse gamma hyper-parameter prior |
bayes_calibration queso
samples = 1000 seed = 348
dram
calibrate_error_multipliers per_response
hyperprior_alphas = 27.0
hyperprior_betas = 26.0

variables
uniform_uncertain 2
upper_bounds 1.e8 10.0
lower_bounds 1.e6 0.1
initial_point 2.85e7 2.5
descriptors 'E' 'w'

responses
calibration_terms = 2
calibration_data_file = 'expdata.withsigma.dat'
freeform
num_experiments = 10
variance_type = 'scalar'

one

• Keywords Area
• method
• bayes_calibration
• calibrate_error_multipliers
• one

Calibrate one hyper-parameter multiplier across all responses/experiments

Specification
Alias: none
Argument(s): none

Description
A single hyper-parameter multiplying all response/experiment covariance blocks will be estimated.

per_experiment

• Keywords Area
• method
• bayes_calibration
• calibrate_error_multipliers
• per_experiment

Calibrate one hyper-parameter multiplier per experiment
6.2. METHOD

Specification

Alias: none
  Argument(s): none

Description

One hyper-parameter multiplying each experiment covariance block will be estimated.

per_response

- Keywords Area
- method
- bayes_calibration
- calibrate_error_multipliers
- per_response
  Calibrate one hyper-parameter multiplier per response

Specification

Alias: none
  Argument(s): none

Description

One hyper-parameter multiplying each response covariance block will be estimated.

both

- Keywords Area
- method
- bayes_calibration
- calibrate_error_multipliers
- both
  Calibrate one hyper-parameter multiplier for each response/experiment pair

Specification

Alias: none
  Argument(s): none

Description

One hyper-parameter multiplying each experiment/response covariance block will be estimated.
hyperprior_alphas

- Keywords Area
- method
- bayes_calibration
- calibrate_error_multipliers
- hyperprior_alphas

Shape (alpha) of the inverse gamma hyper-parameter prior

**Specification**

**Alias:** none  
**Argument(s):** REALLIST

<table>
<thead>
<tr>
<th>Required/-Optional Required</th>
<th>Description of Group</th>
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</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>hyperprior_betas</td>
<td>Scale (beta) of the inverse gamma hyper-parameter prior</td>
</tr>
</tbody>
</table>

**Description**

Shape of the prior distribution for calibrated error multipliers. Either a single value or number of hyper-parameters values may be specified. 

**Default:** 102.0 (with beta = 103.0) so mean and mode are approximately 1.0 and standard deviation is about 0.1.

hyperprior_betas

- Keywords Area
- method
- bayes_calibration
- calibrate_error_multipliers
- hyperprior_alphas
- hyperprior_betas

Scale (beta) of the inverse gamma hyper-parameter prior

**Specification**

**Alias:** none  
**Argument(s):** REALLIST
6.2. METHOD

Description

Scale of the prior distribution for calibrated error multipliers. Either a single value or number of hyper-parameters values may be specified.

Defaults to 103.0 (with alpha = 102.0) so mean and mode are approximately 1.0 and standard deviation is about 0.1.

burn_in_samples

- Keywords Area
- method
- bayes_calibration
- burn_in_samples

Manually specify the burn in period for the MCMC chain.

Specification

Alias: none

Argument(s): INTEGER

Default: 0

Description

The burn in period is the number of samples at the beginning of the MCMC chain that are discarded. The resulting chain is less dependent on the starting point of the chain.

Default Behavior
If not specified, no MCMC samples are discarded

Expected Output
If burn_in_samples is specified, an additional tabular output file containing the final MCMC chain is generated.

Examples

An example method block of a Dakota input file is given below

```
method,
  bayes_calibration queso
  chain_samples = 1000 seed = 348
  dram
  proposal_covariance
    diagonal values 1.0e6 1.0e-1
  burn_in_samples 100
```

posterior_stats

- Keywords Area
- method
- bayes_calibration
• **posterior_stats**

  Compute information-theoretic metrics on posterior parameter distribution

### Specification

**Alias:** none  
**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>kl_divergence</td>
<td></td>
<td>kl_divergence</td>
</tr>
<tr>
<td>Optional</td>
<td>mutual_info</td>
<td></td>
<td>mutal_info</td>
</tr>
</tbody>
</table>

**Description**

Information theory allows for the calculation and quantification of the information contained within a distribution. It is particularly useful for distributions which are not Gaussian, such as those which are bimodal or highly skewed. The `posterior_stats` command calculates information metrics relating to the posterior distribution of the model parameters. These metrics are approximated by making use of the MCMC chain produced during the Bayesian update. This capability can be used with any Bayesian method.

**kl_divergence**

- **Keywords Area**
- **method**
- **bayes_calibration**
- **posterior_stats**
- **kl_divergence**

  Calculate the Kullback-Leibler Divergence

### Specification

**Alias:** none  
**Argument(s):** none

### Description

The Kullback-Leibler (KL) Divergence, also called the relative entropy, provides a measure of the difference between two probability distributions. By specifying `kl_divergence`, the KL Divergence between the posterior $f(\theta | y^{Data})$ and the prior $f(\theta)$ parameter distributions is calculated such that

$$D_{KL} = \int f(\theta | y^{Data}) \log \frac{f(\theta | y^{Data})}{f(\theta)} \, d\theta$$
This quantity can be interpreted as the amount of information gained about the parameters during the Bayesian update.

**Expected Output**

If `kl_divergence` is specified, the calculated value will be reported to the screen at the end of the calibration, following the sample statistics of the response functions. Example output is given below.

**Additional Discussion**

The quantity calculated is a $k$-nearest neighbor approximation of the possibly multi-dimensional integral given above. Therefore, some applications whose true KL Divergence is quite close to zero may report a negative KL Divergence.

**Examples**

Below is a method block of a Dakota input file that indicates the calculation of the KL Divergence:

```
method,
  bayes_calibration queso
  dram
  seed = 34785
  chain_samples = 1000
  posterior_stats kl_divergence
```

The calculated KL approximation is indicated in the screen output by "Information gained from prior to posterior" as shown below:

```
Sample moment statistics for each response function:

<table>
<thead>
<tr>
<th>Response Function</th>
<th>Mean</th>
<th>Std Dev</th>
<th>Skewness</th>
<th>Kurtosis</th>
</tr>
</thead>
<tbody>
<tr>
<td>least_sq_term_1</td>
<td>3.9982462078e-01</td>
<td>4.7683816550e-04</td>
<td>-2.3448518080e+00</td>
<td>7.7381497770e+00</td>
</tr>
</tbody>
</table>

Information gained from prior to posterior = 1.0066819600e+01

<<<< Iterator bayes_calibration completed.
<<<< Environment execution completed.
```

**mutual_info**

- **Keywords Area**
- **method**
- **bayes_calibration**
- **posterior_stats**
- **mutual_info**

This capability is currently inactive.

**Specification**

**Alias:** none

**Argument(s):** none
model_discrepancy

- Keywords Area
- method
- bayes_calibration
- model_discrepancy

(Experimental) Post-calibration calculation of model discrepancy correction

**Specification**

**Alias:** none

**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>discrepancy_type</td>
<td>Specify the type of model discrepancy</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>num_prediction_configs</td>
<td>Specify number of prediction locations for model discrepancy</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>prediction_configs</td>
<td>List prediction locations for model discrepancy</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>import_prediction_configs</td>
<td>Specify text file containing prediction configurations for model discrepancy</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>export_-discrepancy_file</td>
<td>Output file for prediction discrepancy calculations</td>
</tr>
</tbody>
</table>
6.2. METHOD

<table>
<thead>
<tr>
<th>Optional</th>
<th>export_corrected_model_file</th>
<th>Output file for corrected model prediction calculations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>export_corrected_variance_file</td>
<td>Output file for prediction variance calculations</td>
</tr>
</tbody>
</table>

Description

The goal of parameter calibration is to minimize the difference between experimental data, \(d(x)\), and model observations, \(M(\theta, x)\), where \(\theta\) are the model parameters and \(x\) is a configuration variable, such as temperature or pressure. However, it is not uncommon that, at the conclusion of parameter calibration, the agreement between experimental data and the calibrated model is not "close enough." This is often due to model form or structural error. In this case, the canonical equation

\[
d(x) = M(\theta, x) + \epsilon
\]

is replaced by one that also includes model discrepancy \(\delta(x)\),

\[
d(x) = M(\theta, x) + \delta(x) + \epsilon.
\]

In the Dakota implementation, the calculation of \(\delta(x)\) is performed after the model parameters \(\theta\) are calibrated. For each observable \(d_i\), the discrepancy

\[
\delta_i(x_j) = d_i(x_j) - M_i(\theta^*, x_j)
\]

is calculated for each value \(x_j\) of the configuration variable, where \(\theta^*\) is the optimal parameter value obtained during the calibration. It should be emphasized that the model discrepancy is only a function of the configuration variables, and there is one discrepancy regression model for each observable \(d_i\). This set of discrepancy models may be specified to be either Gaussian process or polynomial regression models of constant, linear, or quadratic order, and each model is fit to the calculated discrepancy values. See the discrepancy_type command for more details regarding these options.

The user may then specify new or "prediction" configurations at which the corrected model \(M(\theta^*, x_{\text{new}}) + \delta(x_{\text{new}})\) should be calculated, using one of the num_prediction_configs, prediction_configs, or import_prediction_configs keywords. If none of these keywords is specified, the number of prediction configurations is set to 10. The corresponding prediction variances are also calculated, according to

\[
\Sigma_{\text{total}}(x) = \Sigma_\delta(x) + \sigma^2_{\text{exp}} I.
\]

Here, \(\Sigma_\delta(x)\) is the (co)variance calculated from the Gaussian process or polynomial regression model, and \(\sigma^2_{\text{exp}}\) is the maximum variance, taken over all configuration variables for that observation. Further details can be found in the Dakota User’s and Theory Manuals.

Expected Output

The resulting values of \(\delta(x_{\text{new}})\) will be exported to the file specified using export_discrepancy_file or to the default file dakota_discrepancy_tabular.dat. The values of the corrected model at the specified prediction configurations will be exported to the file specified using export_corrected_model_file or to the default file dakota_corrected_model_tabular.dat, and the corresponding prediction variances will be exported to dakota_discrepancy_variance_tabular.dat or the file specified with export_corrected_variance_file.
Examples

The input files below illustrate the options available to `model_discrepancy`.

```plaintext
model_discrepancy
discrepancy_type  gaussian_process
num_prediction_configs  11
export_discrepancy_file  "discrepancy_values.txt"
export_corrected_model_file  "corrected_model.txt"
export_corrected_variance_file  "prediction_variance.txt"

model_discrepancy
discrepancy_type  polynomial
correction_order  constant
prediction_configs  1  1.5  2  2.5  3

model_discrepancy
discrepancy_type  polynomial
correction_order  linear
import_prediction_configs  "prediction_configs.txt"
```

discrepancy_type

- **Keywords Area**
- **method**
- **bayes_calibration**
- **model_discrepancy**
- **discrepancy_type**

Specify the type of model discrepancy.

Specification

**Alias:** none

**Argument(s):** none

**Default:** gaussian process

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>gaussian_process</td>
<td>Use the Surfpack version of Gaussian process as the discrepancy model</td>
</tr>
</tbody>
</table>
6.2. METHOD

<table>
<thead>
<tr>
<th>Optional</th>
<th>polynomial</th>
<th>Use a polynomial surrogate as the discrepancy model</th>
</tr>
</thead>
<tbody>
<tr>
<td>correction_order</td>
<td>Trend function order of the model discrepancy</td>
<td></td>
</tr>
</tbody>
</table>

**Description**

After the model parameters are calibrated, the difference between the data and the calibrated model, i.e. the model discrepancy, is calculated

\[
\delta_i(x_j) = d_i(x_j) - M_i(\theta^*, x_j).
\]

Each \(\delta_i\) corresponds to a different regression model. These regression models must all be either Gaussian process or polynomial models, and they are functions of the configuration variable \(x\). The order of the trend function may be selected using the `correction_order` command by specifying `constant`, `linear`, or `quadratic`.

**gaussian_process**

- Keywords Area
- method
- bayes_calibration
- model_discrepancy
- discrepancy_type
- gaussian_process

Use the Surfpack version of Gaussian process as the discrepancy model

**Specification**

Alias: kriging

Argument(s): none

**Description**

This keyword specifies a generic version of the Gaussian process implemented in the surface-fitting library called Surfpack. With the exception of the `correction_order` specification, all default options are used in the approximation of the model discrepancy function. That is, DIRECT is used as the optimization method for finding the maximum likelihood estimates of the hyper-parameters that govern the trend and correlation functions, the correlation lengths are optimized by Surfpack, and ill-conditioning is handled internally; gradient-enhanced kriging is not provided as an option in this application.

By selecting this option, each discrepancy function will take the form of a Gaussian process
polynomial
• Keywords Area
• method
• bayes_calibration
• model_discrepancy
• discrepancy_type
• polynomial

Use a polynomial surrogate as the discrepancy model

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

For the purposes of model discrepancy, constant, linear, and quadratic polynomial surrogate models are available. These models are less expensive to calculate than Gaussian process models but are consequently less flexible to discrepancy trends that are not constant, linear, or quadratic in nature. For more information, see the Dakota User’s and Theory Manuals.

By specifying this command, each discrepancy function will take the form of a polynomial regression. They will all have the same order.

**correction_order**

• Keywords Area
• method
• bayes_calibration
• model_discrepancy
• discrepancy_type
• correction_order

Trend function order of the model discrepancy

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** 2
6.2. METHOD

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>(Choose One)</em></td>
<td>Correction Order (Group 1)</td>
<td>constant</td>
<td>Use constant trend discrepancy function</td>
</tr>
<tr>
<td></td>
<td></td>
<td>linear</td>
<td>Use linear trend discrepancy function</td>
</tr>
<tr>
<td></td>
<td></td>
<td>quadratic</td>
<td>Use quadratic trend discrepancy function</td>
</tr>
</tbody>
</table>

**Description**

Whether Gaussian process or polynomial regression model is selected as the discrepancy formulation, the order of the trend function may be specified using the `correction_order` command followed by either `constant`, `linear`, or `quadratic`.

- **constant**
  - **Keywords Area**
  - **method**
  - `bayes_calibration`
  - `model_discrepancy`
  - `discrepancy_type`
  - `correction_order`
  - **constant**
    
    Use constant trend discrepancy function

- **linear**
  - **Keywords Area**
  - **method**
  - `bayes_calibration`
  - `model_discrepancy`
  - `discrepancy_type`
  - `correction_order`
  - **linear**
    
    Use linear trend discrepancy function

**Specification**

**Alias:** none

**Argument(s):** none
**Specification**

*Alias:* none

*Argument(s):* none

- **quadratic**
  - **Keywords Area**
  - **method**
  - **bayes_calibration**
  - **model_discrepancy**
  - **discrepancy_type**
  - **correction_order**
  - **quadratic**

Use quadratic trend discrepancy function

---

**Specification**

*Alias:* none

*Argument(s):* none

- **num_prediction_configs**
  - **Keywords Area**
  - **method**
  - **bayes_calibration**
  - **model_discrepancy**
  - **num_prediction_configs**

Specify number of prediction locations for model discrepancy

---

**Specification**

*Alias:* none

*Argument(s):* **INTEGER**

*Default:* 0

**Description**

Following the calculation of the model discrepancy functions, \( \delta_i \), and the corrected model \( M_i + \delta_i \) may be calculated at new or “prediction” configurations. Using the **num_prediction_configs** command, the user may specify the number of prediction configurations they wish to be computed. The new configuration locations will be spread uniformly in the configuration variable domain specified in the **variables** block of the input file.

**Usage Tips**

If none of **num_prediction_configs**, **prediction_configs**, or **import_prediction_configs** is specified, the number of prediction configurations is set to 10.
6.2. METHOD

prediction_configs

- Keywords Area
- method
- bayes_calibration
- model_discrepancy
- prediction_configs

List prediction locations for model discrepancy

Specification

Alias: none
Argument(s): REALLIST

Description

Following the calculation of the model discrepancy functions, \( \delta_i \), and the corrected model \( M_i + \delta_i \) may be calculated at new or "prediction" configurations. Using the `prediction_configs` command, the user may explicitly list the locations of the prediction configurations they wish to be computed. See parent command for an example.

Usage Tips

If none of `num_prediction_configs`, `prediction_configs`, or `import_prediction_configs` is specified, Dakota sets `num_prediction_configs` to 10.

import_prediction_configs

- Keywords Area
- method
- bayes_calibration
- model_discrepancy
- import_prediction_configs

Specify text file containing prediction configurations for model discrepancy

Specification

Alias: none
Argument(s): STRING
Default: no point import from a file

<table>
<thead>
<tr>
<th>Required/- Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### Description

Enables text file import of user-specified prediction configurations at which to calculate the corrected model \( M_i + \delta_i \).

#### Usage Tips

Dakota parses input files without regard to whitespace, but the `import_prediction_configs` file must be in one of three formats:

- `annotated` (default)
- `custom_annotated`
- `freeform`

#### annotated

- **Keywords Area**
- **method**
- **bayes_calibration**
- **model_discrepancy**
- **import_prediction_configs**
- **annotated**

Selects annotated tabular file format

### Topics

This keyword is related to the topics:

- **file Formats**

### Specification

**Alias:** none  
**Argument(s):** none  
**Default:** annotated
6.2. **METHOD**

**Description**

An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

**Default Behavior**

By default, Dakota imports and exports tabular files in annotated format. The `annotated` keyword can be used to explicitly specify this.

**Usage Tips**

- To specify pre-Dakota 6.1 tabular format, which did not include `interface_id`, specify `custom_annotated
header eval_id`

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to `annotated` format, though `freeform` remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the `freeform` option.

**Examples**

Export an annotated top-level tabular data file containing a header row, leading `eval_id` and `interface_id` columns, and data for variables and responses. Input file fragment:

```
environment
  tabular_data
    tabular_data_file = 'dakota_summary.dat'
    annotated
```

Resulting tabular file:

<table>
<thead>
<tr>
<th>eval_id</th>
<th>interface</th>
<th>x1</th>
<th>x2</th>
<th>obj_fn</th>
<th>nln_ineq_con_1</th>
<th>nln_ineq_con_2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>NO_ID</td>
<td>0.9</td>
<td>1.1</td>
<td>0.0002</td>
<td>0.26</td>
<td>0.76</td>
</tr>
<tr>
<td>2</td>
<td>NO_ID</td>
<td>0.90009</td>
<td>1.1</td>
<td>0.0001996404857</td>
<td>0.2601620081</td>
<td>0.7599555</td>
</tr>
<tr>
<td>3</td>
<td>NO_ID</td>
<td>0.89991</td>
<td>1.1</td>
<td>0.0002003604863</td>
<td>0.2598380081</td>
<td>0.760045</td>
</tr>
<tr>
<td>...</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**custom_annotated**

- **Keywords Area**
- **method**
- **bayes_calibration**
- **model_discrepancy**
- **import_prediction_configs**
- **custom_annotated**

Selects custom-annotated tabular file format
Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional/Optional</td>
<td></td>
<td>header</td>
<td>Enable header row in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>eval_id</td>
<td>Enable evaluation ID column in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>interface_id</td>
<td>Enable interface ID column in custom-annotated tabular file</td>
</tr>
</tbody>
</table>

Description

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

Default Behavior

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom.annotated, followed by options, in the relevant export/import context.

Usage Tips

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:
6.2. METHOD

evironment
  tabular_data
  tabular_data_file = 'dakota_summary.dat'
  custom_annotated header eval_id

Resulting tabular file:

<table>
<thead>
<tr>
<th>%eval_id</th>
<th>x1</th>
<th>x2</th>
<th>obj_fn</th>
<th>nln_ineq_con_1</th>
<th>nln_ineq_con_2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.9</td>
<td>1.1</td>
<td>0.0002</td>
<td>0.26</td>
<td>0.76</td>
</tr>
<tr>
<td>2</td>
<td>0.90009</td>
<td>1.1</td>
<td>0.0001996404857</td>
<td>0.2601620081</td>
<td>0.759955</td>
</tr>
<tr>
<td>3</td>
<td>0.89991</td>
<td>1.1</td>
<td>0.0002003604863</td>
<td>0.2598380081</td>
<td>0.760045</td>
</tr>
</tbody>
</table>

header

- Keywords Area
- method
- bayes_calibration
- model_discrepancy
- import_prediction_configs
- custom_annotated
- header

Enable header row in custom-annotated tabular file

Specification

Alias: none
  Argument(s): none

Description

See description of parent custom_annotated

eval_id

- Keywords Area
- method
- bayes_calibration
- model_discrepancy
- import_prediction_configs
- custom_annotated
- eval_id

Enable evaluation ID column in custom-annotated tabular file
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): none

Description

See description of parent custom_annotated

interface_id

- Keywords Area
- method
- bayes_calibration
- model_discrepancy
- import_prediction_configs
- custom_annotated
- interface_id

Enable interface ID column in custom-annotated tabular file

Specification

Alias: none

Argument(s): none

Description

See description of parent custom_annotated

freeform

- Keywords Area
- method
- bayes_calibration
- model_discrepancy
- import_prediction_configs
- freeform

Selects freeform file format

Topics

This keyword is related to the topics:

- file_formats
6.2. **METHOD**

**Specification**

**Alias:** none  
**Argument(s):** none

**Description**

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

**Default Behavior**

The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

**Usage Tips**

- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

**Examples**

Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```plaintext
evironment  
tabular_data  
  tabular_data_file = 'dakota_summary.dat'  
  freeform
```

Resulting tabular file:

```
0.9 1.1 0.0002 0.26 0.76
0.90009 1.1 0.0001996404857 0.2601620081 0.759955
0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...
```

**export_discrepancy_file**

- **Keywords Area**
- **method**
- **bayes_calibration**
- **model_discrepancy**
- **export_discrepancy_file**

Output file for prediction discrepancy calculations
**Specification**

*Alias:* none

*Argument(s):* STRING

*Default:* discrepancy export to default filename

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group Tabular Format (Group 1)</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional (Choose One)</td>
<td></td>
<td>annotated</td>
<td>Selects annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>custom_annotated</td>
<td>Selects custom-annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>freeform</td>
<td>Selects freeform file format</td>
</tr>
</tbody>
</table>

**Description**

Enables the user to specify the name and format of the file to which prediction discrepancy information is output. The file will contain the values of the discrepancy model $\delta_i$ calculated at those points specified with `num_predictions`, `prediction_configs`, or `import_prediction_configs`

**Default Behavior**

If `export_discrepancy_file` is not specified, information will be automatically output to `dakota_discrepancy_tabular.dat`.

**Usage Tips**

Dakota exports tabular data in one of three formats:

- annotated (default)
- custom_annotated
- freeform

**annotated**

- Keywords Area
- method
- bayes_calibration
- model_discrepancy
- export_discrepancy_file
- annotated

Selects annotated tabular file format
6.2. METHOD

Topics
This keyword is related to the topics:

- file_formats

Specification
Alias: none
  Argument(s): none
  Default: annotated

Description
An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior
By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips
- To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify custom annotated header eval_id
- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples
Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```
environment
tabular_data
  tabular_data_file = 'dakota_summary.dat'
annotated
```

Resulting tabular file:

```
%eval_id interface x1 x2 obj_fn nln_ineq_con_1 nln_ineq_con_2
1 NO_ID 0.9 1.1 0.0002 0.26 0.76
2 NO_ID 0.90009 1.1 0.0001996404857 0.2601620081 0.759955
3 NO_ID 0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...```
The **custom.annotated** keyword allows user options for whether the header row, `eval_id` column, and `interface_id` column appear in the tabular file, thus bridging freeform and (fully) annotated.

### Default Behavior
The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify `custom.annotated`, followed by options, in the relevant export/import context.

### Usage Tips

**Description**
A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, `eval_id` column, and `interface_id` column appear in the tabular file, thus bridging freeform and (fully) annotated.

**Topics**
This keyword is related to the topics:

- file.formats
Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

**Examples**

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
    tabular_data_file = 'dakota_summary.dat'
custom_annotated header eval_id
```

Resulting tabular file:

```
%eval_id  x1  x2  obj_fn  nln_ineq_con_1  nln_ineq_con_2
1  0.9  1.1  0.0002  0.26  0.76
2  0.90009  1.1  0.0001996404857  0.2601620081  0.759955
3  0.89991  1.1  0.0002003604863  0.2598380081  0.760045
...```

**header**

- **Keywords Area**
- **method**
- **bayes_calibration**
- **model_discrepancy**
- **export_discrepancy_file**
- **custom_discrepancy_file**
- **custom_annotated**
- **header**

Enable header row in custom-annotated tabular file

**Specification**

**Alias:** none
**Argument(s):** none

**Description**

See description of parent **custom_annotated**
eval_id
- Keywords Area
- method
- bayes_calibration
- model_discrepancy
- export_discrepancy_file
- custom_annotated
- eval_id

Enable evaluation ID column in custom-annotated tabular file

**Specification**

Alias: none
Argument(s): none

**Description**

See description of parent custom_annotated

interface_id
- Keywords Area
- method
- bayes_calibration
- model_discrepancy
- export_discrepancy_file
- custom_annotated
- interface_id

Enable interface ID column in custom-annotated tabular file

**Specification**

Alias: none
Argument(s): none

**Description**

See description of parent custom_annotated
6.2. METHOD

**freeform**

- Keywords Area
- method
- bayes\_calibration
- model\_discrepancy
- export\_discrepancy\_file
- freeform

Selects freeform file format

**Topics**

This keyword is related to the topics:

- file\_formats

**Specification**

**Alias:** none
- **Argument(s):** none
- **Default:** annotated

**Description**

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

**Default Behavior**

The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

**Usage Tips**

- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- In freeform, the num\_rows x num\_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.
Examples
Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```plaintext
environment
  tabular_data
  tabular_data_file = 'dakota_summary.dat'
  freeform
Resulting tabular file:

0.9     1.1     0.0002     0.26     0.76
0.90009 1.1 0.0001996404857 0.2601620081 0.759955
0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...
```

`export_corrected_model_file`
- Keywords Area
- method
- bayes_calibration
- model_discrepancy
- export_corrected_model_file

Output file for corrected model prediction calculations

Specification
Alias: none
Argument(s): STRING
Default: corrected model export to default filename

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional(Choose One)</td>
<td>Tabular Format (Group 1)</td>
<td>annotated</td>
<td>Selects annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>custom_annotated</td>
<td>Selects custom-annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>freeform</td>
<td>Selects freeform file format</td>
</tr>
</tbody>
</table>

Description
Enables the user to specify the name and format of the file to which corrected model $M_i + \delta_i$ information is output. The file will contain the values of the discrepancy model $\delta_i$ calculated at those points specified with `num_predictions`, `prediction_configs`, or `import_prediction_configs`.

Corresponding variance information is also output to file, see `export_corrected_variance_file`
If `export_corrected_model_file` is not specified, information will be automatically output to `dakota-corrected_model_tabular.dat`.

**Usage Tips**

Dakota exports tabular data in one of three formats:

- annotated (default)
- custom_annotated
- freeform

**annotated**

- **Keywords Area**
- method
- bayes_calibration
- model_discrepancy
- export_corrected_model_file
- annotated

Selects annotated tabular file format

**Topics**

This keyword is related to the topics:

- file_formats

**Specification**

**Alias:** none

*Argument(s):* none

**Default:** annotated

**Description**

An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

**Default Behavior**

By default, Dakota imports and exports tabular files in annotated format. The `annotated` keyword can be used to explicitly specify this.

**Usage Tips**

- To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify `custom_annotated header eval_id`
- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to `annotated` format, though `freeform` remains an option.
• When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

• Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples
Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
annotated
```

Resulting tabular file:

```
%eval_id interface x1 x2 obj_fn nln_ineq_con_1 nln_ineq_con_2
1 NO_ID 0.9 1.1 0.0002 0.26 0.76
2 NO_ID 0.90009 1.1 0.0001996404857 0.2601620081 0.759955
3 NO_ID 0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...```

custom_annotated

• Keywords Area

• method

• bayes_calibration

• model_discrepancy

• export_corrected_model_file

• custom_annotated

Selects custom-annotated tabular file format

Topics
This keyword is related to the topics:

• file_formats

Specification
Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
</table>
6.2. METHOD

<table>
<thead>
<tr>
<th>Optional</th>
<th>header</th>
<th>Enable header row in custom-annotated tabular file</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>eval_id</td>
<td>Enable evaluation ID column in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td>interface_id</td>
<td>Enable interface ID column in custom-annotated tabular file</td>
</tr>
</tbody>
</table>

**Description**

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

**Default Behavior**

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

**Usage Tips**

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

**Examples**

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:

```
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
custom_annotated header eval_id
```

Resulting tabular file:

```
%eval_id  x1   x2   obj_fn nln_ineq_con_1 nln_ineq_con_2
1   0.9  1.1    0.0002     0.26     0.76
2  0.90009  1.1  0.0001996404857  0.2601620081  0.759955
3  0.89991  1.1  0.0002003604863  0.2598380081  0.760045
...```
header
- Keywords Area
- method
- bayes_calibration
- model_discrepancy
- export_corrected_model_file
- custom_annotated
- header

Enable header row in custom-annotated tabular file

**Specification**
**Alias:** none  
**Argument(s):** none

**Description**
See description of parent `custom_annotated`

eval_id
- Keywords Area
- method
- bayes_calibration
- model_discrepancy
- export_corrected_model_file
- custom_annotated
- eval_id

Enable evaluation ID column in custom-annotated tabular file

**Specification**
**Alias:** none  
**Argument(s):** none

**Description**
See description of parent `custom_annotated`
6.2. **METHOD**

- **interface_id**
  - **Keywords Area**
  - **method**
  - **bayes_calibration**
  - **model_discrepancy**
  - **export_corrected_model_file**
  - **custom_annotated**
  - **interface_id**

Enable interface ID column in custom-annotated tabular file

**Specification**

**Alias:** none  
**Argument(s):** none

**Description**

See description of parent **custom_annotated**

- **freeform**
  - **Keywords Area**
  - **method**
  - **bayes_calibration**
  - **model_discrepancy**
  - **export_corrected_model_file**
  - **freeform**

Selects freeform file format

**Topics**

This keyword is related to the topics:

- **file_formats**

**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** annotated
CHAPTER 6. KEYWORDS AREA

Description
A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior
The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips
• Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.
• When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
• In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).
• Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples
Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```plaintext
evironment
tabular_data
tabular_data_file = 'dakota_summary.dat'
freeform
```

Resulting tabular file:

```
0.9  1.1  0.0002  0.26  0.76
0.90009 1.1  0.0001996404857  0.2601620081  0.759955
0.89991 1.1  0.0002003604863  0.2598380081  0.760045
...
```

`export_corrected_variance_file`

• Keywords Area
• method
• bayes_calibration
• model_discrepancy
• export_corrected_variance_file

Output file for prediction variance calculations

Specification
Alias: none
Argument(s): STRING
Default: corrected model variance export to default filename
### Description

Enables the user to specify the name and format of the file to which corrected model variance information is output. The file will contain the values of the variances computed at those points specified with `num_predictions`, `prediction_configs`, or `import_prediction_configs`

The prediction variance for each observable $d_i$ is calculated according to

$$\Sigma_{\text{total}}(x) = \Sigma_\delta(x) + \sigma^2_{\text{exp}} I.$$ 

Here, $\Sigma_\delta(x)$ is the (co)variance calculated from the Gaussian process or polynomial regression model, details of which can be found in the Dakota User’s and Theory Manuals. If experimental variance information is provided for the calibration, the maximum variance found for the observable $d_i$ is used as $\sigma^2_{\text{exp}}$. For more details, see the Dakota User’s and Theory Manuals.

#### Default Behavior

If `export_corrected_variance_file` is not specified, information will be automatically output to `dakota_discrepancy_variance_tabular.dat`.

#### Usage Tips

Dakota exports tabular data in one of three formats:

- annotated (default)
- custom_annotated
- freeform

#### annotated

- Keywords Area
- method
- bayes_calibration
- model_discrepancy
- export_corrected_variance_file
- annotated

Selects annotated tabular file format

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group Tabular Format (Group 1)</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<tr>
<td>Optional (Choose One)</td>
<td></td>
<td>annotated</td>
<td>Selects annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>custom_annotated</td>
<td>Selects custom-annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>freeform</td>
<td>Selects freeform file format</td>
</tr>
</tbody>
</table>
CHAPTER 6. KEYWORDS AREA

Topics
This keyword is related to the topics:

- file_formats

Specification
Alias: none
Argument(s): none
Default: annotated

Description
An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior
By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips
- To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify custom.annotated header eval_id
- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples
Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
annotated
```

Resulting tabular file:

```
%eval_id interface  x1  x2  obj_fn  nln_ineq_con_1  nln_ineq_con_2
1  NO_ID  0.9  1.1  0.0002  0.26  0.76
2  NO_ID  0.90009  1.1  0.0001996404857  0.2601620081  0.759955
3  NO_ID  0.89991  1.1  0.0002003604863  0.2598380081  0.760045
...```
6.2. METHOD

custom_annotated

- Keywords Area
- method
- bayes_calibration
- model_discrepancy
- export_corrected_variance_file
- custom_annotated

Selects custom-annotated tabular file format

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none

Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>header</td>
<td>header</td>
<td>Enable header row in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td>eval_id</td>
<td>eval_id</td>
<td>Enable evaluation ID column in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td>interface_id</td>
<td>interface_id</td>
<td>Enable interface ID column in custom-annotated tabular file</td>
</tr>
</tbody>
</table>

Description

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

Default Behavior

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

Usage Tips
Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to **annotated** format, though **freeform** remains an option.

When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the **freeform** option.

**Examples**

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval, id (no interface, id), and data for variables and responses. Input file fragment:

```plaintext
environment
   tabular_data
   tabular_data_file = 'dakota_summary.dat'
   custom_annotated header eval_id
```

Resulting tabular file:

```plaintext
%eval_id  x1  x2  obj_fn  nln_ineq_con_1  nln_ineq_con_2
1  0.9  1.1  0.0002  0.26  0.76
2  0.90009  1.1  0.0001996404857  0.2601620081  0.759955
3  0.89991  1.1  0.0002003604863  0.2598380081  0.760045
...
```

**header**

- **Keywords Area**
  - **method**
  - **bayes_calibration**
  - **model_discrepancy**
  - **export_corrected_variance_file**
  - **custom_annotated**
    - **header**

Enable header row in custom-annotated tabular file

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

See description of parent **custom_annotated**
6.2. METHOD

```eval_id

- **Keywords Area**
- **method**
- **bayes_calibration**
- **model_discrepancy**
- **export_corrected_variance_file**
- **custom_annotated**
- **eval_id**

Enable evaluation ID column in custom-annotated tabular file

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

See description of parent **custom_annotated**

```interface_id

- **Keywords Area**
- **method**
- **bayes_calibration**
- **model_discrepancy**
- **export_corrected_variance_file**
- **custom_annotated**
- **interface_id**

Enable interface ID column in custom-annotated tabular file

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

See description of parent **custom_annotated**
freeform

- Keywords Area
- method
- bayes_calibration
- model_discrepancy
- export_corrected_variance_file
- freeform

Selects freeform file format

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none

Argument(s): none

Default: annotated

Description

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior

The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips

- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.
6.2. METHOD

Examples
Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```
environment
  tabular_data
    tabular_data_file = 'dakota_summary.dat'
  freeform

Resulting tabular file:

0.9 1.1 0.0002 0.26 0.76
0.90009 1.1 0.0001996404857 0.2601620081 0.759955
0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...
```

`sub_sampling_period`

- Keywords Area
- method
- bayes_calibration
- `sub_sampling_period`

Specify a sub-sampling of the MCMC chain

Specification

**Alias:** none
**Argument(s):** INTEGER
**Default:** 0

Description

If a `sub_sampling_period` is specified, the MCMC chain is filtered such that only the sample at the beginning of each period is in the final MCMC chain. The `sub_sampling_period` should therefore be greater than or equal to the correlation length of the samples.

**Default Behavior**
If not specified, all MCMC samples are included in the final chain.

**Expected Output**
If specified, an additional tabular output file containing the final (sub-sampled) MCMC chain is generated.

Examples

An example method block of a Dakota input file is given below

```
method,
  bayes_calibration queso
    chain_samples = 1000 seed = 348
  dram
  proposal_covariance
    diagonal values 1.0e6 1.0e-1
  sub_sampling_period 100
```
probability_levels

- Keywords Area
- method
- bayes_calibration
- probability_levels

Specify probability levels at which to compute credible and prediction intervals

**Specification**

**Alias:** none
**Argument(s):** REALLIST
**Default:** No CDF/CCDF response levels to compute

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>num_probability_levels</td>
<td></td>
<td>This capability is currently inactive</td>
</tr>
</tbody>
</table>

**Description**

Credible and prediction intervals of model responses are computed for specified probabilities. Credible intervals are calculated from the response function values corresponding to the final MCMC chain. Calculation of prediction intervals consider these response values as well as the experimental uncertainty, which is specified by the user via the `variance_type` command.

**Expected Output**

If `probability_levels` is specified, Dakota will create a table containing the credible intervals for each response function. The corresponding table containing the prediction intervals will also be created if a `variance_type` has been specified. This information is output to the screen and to a file. In addition, the output file contains the means and standard deviations of each response function and Gaussian approximations of the 5/95 credible and prediction intervals, in which the lower bound is two standard deviations below the mean and the upper bound is two standard deviations above the mean.

**Usage Tips**

Only one probability level needs to be specified for each desired interval. Both corresponding end points of the intervals are automatically calculated. For example, if 0.05 is specified, both the 0.05 and 0.95 probability levels are output to the screen and output file.

**Additional Discussion**

Credible intervals propagate uncertainties in parameter density information to the quantity of interest and quantify how well the model fits the provided data. Prediction intervals propagate both parameter and experimental measurement uncertainties and contain the next experimental or simulated observation with the specified probability.

**Examples**

Below is a Dakota input file specifying the calculation of credible and prediction intervals

```plaintext
method,
bayes_calibration queso
  chain_samples = 1000 seed = 348
```
6.2. METHOD

dram
proposal_covariance
diagonal values 1.0e6 1.0e-1
probability_levels 0.05 0.1
0.075 0.1

variables,
uniform_uncertain 2
upper_bounds 1.e8 10.0
lower_bounds 1.e6 0.1
initial_point 2.85e7 2.5
descriptors 'E' 'w'
continuous_state 4
initial_state 3 40000 500 1000
descriptors 't' 'R' 'X' 'Y'

interface,
direct
analysis_driver = 'mod_cantilever'

responses,

calibration_terms = 2

calibration_data_file = 'dakota_cantilever_queso.withsigma.dat'

freeform
num_experiments = 10
variance_type = 'scalar'
descriptors = 'stress' 'displacement'
no_gradients
no_hessians

The resulting screen output below shows the table of credible and prediction intervals.

<table>
<thead>
<tr>
<th>Credibility Intervals for stress</th>
<th>Probability Level</th>
</tr>
</thead>
<tbody>
<tr>
<td>Response Level</td>
<td>Probability Level</td>
</tr>
<tr>
<td>----------------------------------</td>
<td>-------------------</td>
</tr>
<tr>
<td>2.4764049695e+03</td>
<td>5.0000000000e-02</td>
</tr>
<tr>
<td>2.8242874802e+03</td>
<td>9.5000000000e-01</td>
</tr>
<tr>
<td>2.4990608791e+03</td>
<td>1.0000000000e-01</td>
</tr>
<tr>
<td>2.7952985803e+03</td>
<td>9.0000000000e-01</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Credibility Intervals for displacement</th>
<th>Probability Level</th>
</tr>
</thead>
<tbody>
<tr>
<td>Response Level</td>
<td>Probability Level</td>
</tr>
<tr>
<td>----------------------------------------</td>
<td>-------------------</td>
</tr>
<tr>
<td>2.7409870925e-01</td>
<td>7.5000000000e-02</td>
</tr>
<tr>
<td>3.0991296255e-01</td>
<td>9.2500000000e-01</td>
</tr>
<tr>
<td>2.7538816802e-01</td>
<td>1.0000000000e-01</td>
</tr>
<tr>
<td>3.0889319332e-01</td>
<td>9.0000000000e-01</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Prediction Intervals for stress</th>
<th>Probability Level</th>
</tr>
</thead>
<tbody>
<tr>
<td>Response Level</td>
<td>Probability Level</td>
</tr>
<tr>
<td>---------------------------------------</td>
<td>-------------------</td>
</tr>
<tr>
<td>2.0964882850e+03</td>
<td>5.0000000000e-02</td>
</tr>
<tr>
<td>3.1993026765e+03</td>
<td>9.5000000000e-01</td>
</tr>
<tr>
<td>2.1822183238e+03</td>
<td>1.0000000000e-01</td>
</tr>
<tr>
<td>3.1099058450e+03</td>
<td>9.0000000000e-01</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Prediction Intervals for displacement</th>
<th>Probability Level</th>
</tr>
</thead>
<tbody>
<tr>
<td>Response Level</td>
<td>Probability Level</td>
</tr>
<tr>
<td>---------------------------------------</td>
<td>-------------------</td>
</tr>
<tr>
<td>2.3559036055e-01</td>
<td>7.5000000000e-02</td>
</tr>
<tr>
<td>3.5097481218e-01</td>
<td>9.2500000000e-01</td>
</tr>
<tr>
<td>2.4016170870e-01</td>
<td>1.0000000000e-01</td>
</tr>
<tr>
<td>3.4701712866e-01</td>
<td>9.0000000000e-01</td>
</tr>
</tbody>
</table>

num_probability_levels
Keywords Area
method
bayes_calibration
probability_levels
num_probability_levels

This capability is currently inactive

**Specification**

Alias: none

**Argument(s):** INTEGERLIST

**Default:** probability_levels evenly distributed among response functions

**convergence_tolerance**

Keywords Area
method
bayes_calibration

convergence_tolerance

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Topics

This keyword is related to the topics:

- method_independent_controls

**Specification**

Alias: none

**Argument(s):** REAL

**Default:** 1.e-4

**Description**

The convergence_tolerance specification provides a real value for controlling the termination of iteration. For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by convergence_tolerance, then this convergence criterion is satisfied on the current iteration. Therefore, permissible values are between 0 and 1, non-inclusive.

**Behavior Varies by Package/Library**

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.
Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- DOT: must be satisfied for two consecutive iterations

- NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of convergence_tolerance approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., convergence_tolerance = 1.e-6 will result in approximately six digits of accuracy in the final objective function).

- NL2SOL: See nl2sol

max_iterations

- Keywords Area
- method
- bayes_calibration
- max_iterations

Number of iterations allowed for optimizers and adaptive UQ methods

Topics

This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none

Argument(s): INTEGER

Default: 100 (exceptions: fsu_cvt, local_reliability: 25; global, {reliability, interval_est, evidence} / efficient-global: 25*n)

Description

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed max_iterations iterations. See also max_function_evaluations.

Default Behavior

Default value is 100.
**model_pointer**

- **Keywords Area**
- **method**
- **bayes_calibration**
- **model_pointer**

Identifier for model block to be used by a method

**Topics**

This keyword is related to the topics:

- **block_pointer**

**Specification**

**Alias:** none

**Argument(s):** STRING

**Default:** method use of last model parsed (or use of default model if none parsed)

**Description**

The **model_pointer** is used to specify which **model** block will be used to perform the function evaluations needed by the Dakota method.

**Default Behavior**

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a **model** block in the Dakota input file that has a corresponding **id_model** with the same name.

**Usage Tips**

When doing advanced analyses that involve using multiple methods and multiple models, defining a **model_pointer** for each method is imperative.

See **block_pointer** for details about pointers.

**Examples**

```
environment
  tabular_graphics_data
  method_pointer = 'UQ'

method
  id_method = 'UQ'
  model_pointer = 'Surr'
  sampling,
    samples = 10
    seed = 98765 rng rnum2
    response_levels = 0.1 0.2 0.6
    0.1 0.2 0.6
    0.1 0.2 0.6
  sample_type lhs
  distribution cumulative

model
  id_model = 'Surr'
```
6.2. METHOD

surrogate global,
dace_method_pointer = 'DACE'  
polynomial quadratic

method
id_method = 'DACE'
model_pointer = 'DACE_M'
sampling sample_type lhs
  samples = 121 seed = 5034 rng rnum2

model
id_model = 'DACE_M'
single
  interface_pointer = 'I1'

variables
uniform_uncertain = 2
  lower_bounds = 0. 0.
  upper_bounds = 1. 1.
  descriptors = 'x1' 'x2'

interface
id_interface = 'I1'
  system asynch evaluation_concurrency = 5
  analysis_driver = 'text_book'

responses
response_functions = 3
  no_gradients
  no_hessians

6.2.60 dace

  • Keywords Area
  • method
  • dace

Design and Analysis of Computer Experiments

Topics
This keyword is related to the topics:

  • package_ddace
  • design_and_analysis_of_computer_experiments

Specification
Alias: none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required (Choose One)</td>
<td>DACE type (Group 1)</td>
<td>grid</td>
<td>Options</td>
</tr>
<tr>
<td>----------------------</td>
<td>---------------------</td>
<td>--------------</td>
<td>--------------------------------------------</td>
</tr>
<tr>
<td></td>
<td>grid</td>
<td>random</td>
<td>Uses purely random Monte Carlo sampling to sample variables</td>
</tr>
<tr>
<td></td>
<td></td>
<td>oas</td>
<td>Orthogonal Array Sampling</td>
</tr>
<tr>
<td></td>
<td></td>
<td>lhs</td>
<td>Uses Latin Hypercube Sampling (LHS) to sample variables</td>
</tr>
<tr>
<td></td>
<td></td>
<td>oa_lhs</td>
<td>Orthogonal Array Latin Hypercube Sampling</td>
</tr>
<tr>
<td></td>
<td></td>
<td>box_behnken</td>
<td>Box-Behnken Design</td>
</tr>
<tr>
<td>Optional</td>
<td>samples</td>
<td></td>
<td>Number of samples for sampling-based methods</td>
</tr>
<tr>
<td>Optional</td>
<td>seed</td>
<td></td>
<td>Seed of the random number generator</td>
</tr>
<tr>
<td>Optional</td>
<td>main_effects</td>
<td></td>
<td>ANOVA</td>
</tr>
<tr>
<td>Optional</td>
<td>quality_metrics</td>
<td></td>
<td>Calculate metrics to assess the quality of quasi-Monte Carlo samples</td>
</tr>
<tr>
<td>Optional</td>
<td>variance_based_decomp</td>
<td></td>
<td>Activates global sensitivity analysis based on decomposition of response variance into contributions from variables</td>
</tr>
</tbody>
</table>
### Description

The Distributed Design and Analysis of Computer Experiments (DDACE) library provides the following DACE techniques:

1. grid sampling (*grid*)
2. pure random sampling (*random*)
3. orthogonal array sampling (*oas*)
4. latin hypercube sampling (*lhs*)
5. orthogonal array latin hypercube sampling (*oa_lhs*)
6. Box-Behnken (*box_behnken*)
7. central composite design (*central_composite*)

These methods all generate point sets that may be used to drive a set of computer experiments. Note that all of the DACE methods generated randomized designs, except for Box-Behnken and Central composite which are classical designs. That is, the grid sampling will generate a randomized grid, not what one typically thinks of as a grid of uniformly spaced points over a rectangular grid. Similarly, the orthogonal array is a randomized version of an orthogonal array: it does not generate discrete, fixed levels.

In addition to the selection of the method, there are keywords that affect the method outputs:

1. *main_effects*
2. *quality_metrics*
3. *variance_based_decomp*

And keywords that affect the sampling:

1. *fixed_seed*
2. *symbols*
3. *samples*
4. *seed*
See Also

These keywords may also be of interest:

- `fsu_cvt`
- `fsu_quasi_mc`
- `psuade_moat`

**grid**

- `Keywords Area`
- `method`
- `dace`
- `grid`

Grid Sampling

**Specification**

**Alias**: none
**Argument(s)**: none

**Description**

The grid option in DACE will produce a randomized grid of points. If you are interested in a regular grid of points, use the multidimensional parameter study (under Parameter Studies) instead. Grid Sampling

**random**

- `Keywords Area`
- `method`
- `dace`
- `random`

Uses purely random Monte Carlo sampling to sample variables

**Specification**

**Alias**: none
**Argument(s)**: none
6.2. METHOD

Description

The random keyword invokes Monte Carlo sampling as the means of drawing samples of uncertain variables according to their probability distributions.

Default Behavior

In most contexts, Monte Carlo sampling is not the default sampling mode (exception: multilevel_sampling). To change this behavior, the random keyword must be specified in conjunction with the sample_type keyword.

Usage Tips

Monte Carlo sampling is more computationally expensive than Latin Hypercube Sampling as it requires a larger number of samples to accurately estimate statistics.

Examples

```plaintext
method
  sampling
    sample_type random
    samples = 200

oas
  • Keywords Area
  • method
  • dace
  • oas

Orthogonal Array Sampling
```

Specification

Alias: none

Argument(s): none

Description

Orthogonal array sampling (OAS) is a widely used technique for running experiments and systematically testing factor effects. An orthogonal array sample can be described as a 4-tuple \((m; n; s; r)\), where \(m\) is the number of sample points, \(n\) is the number of input variables, \(s\) is the number of symbols, and \(r\) is the strength of the orthogonal array. The number of sample points, \(m\), must be a multiple of the number of symbols, \(s\). The number of symbols refers to the number of levels per input variable. The strength refers to the number of columns where we are guaranteed to see all the possibilities an equal number of times. Note that the DACE OAS capability produces a randomized orthogonal array: the samples for a particular level are randomized within that level.

If one examines the sample sets in an orthogonal array by looking at the rows as individual samples and columns as the variables sampled, one sees that the columns are orthogonal to each other in an orthogonal array. This feature is important in main effects analysis, which is a sensitivity analysis technique that identifies which variables have the most influence on the output.
 lhs
    • Keywords Area
    • method
    • dace
    • lhs

Uses Latin Hypercube Sampling (LHS) to sample variables

**Specification**

Alias: none

Argument(s): none

**Description**

The `lhs` keyword invokes Latin Hypercube Sampling as the means of drawing samples of uncertain variables according to their probability distributions. This is a stratified, space-filling approach that selects variable values from a set of equi-probable bins.

**Default Behavior**

Latin Hypercube Sampling is the default sampling mode in most contexts (exception: multilevel_sampling).

To explicitly specify LHS in the Dakota input file, the `lhs` keyword must appear in conjunction with the `sample_type` keyword.

**Usage Tips**

Latin Hypercube Sampling is very robust and can be applied to any problem. It is fairly effective at estimating the mean of model responses and linear correlations with a reasonably small number of samples relative to the number of variables.

**Examples**

```
method
   sampling
      sample_type lhs
      samples = 20
```

**oa_lhs**

- Keywords Area
- method
- dace
- oa_lhs

Orthogonal Array Latin Hypercube Sampling

**Specification**

Alias: none

Argument(s): none
6.2. METHOD

Description
The Orthogonal Array Latin Hypercube Sampling option in DACE produces a “latinized” version of an orthogonal array. That is, after the orthogonal array is generated, the samples go through a stratification process to produce samples that have been both orthogonalized and stratified.

See Also
These keywords may also be of interest:

- oas

box_benhken

- Keywords Area
- method
- dace
- box_benhken

Box-Behnken Design

Specification
Alias: none

Argument(s): none

Description
The Box-Behnken design is similar to a Central Composite design, with some differences. The Box-Behnken design is a quadratic design in that it does not contain an embedded factorial or fractional factorial design. In this design the treatment combinations are at the midpoints of edges of the process space and at the center, as compared with CCD designs where the extra points are placed at star points on a circle outside of the process space. Box-Behnken designs are rotatable (or near rotatable) and require 3 levels of each factor.

central_composite

- Keywords Area
- method
- dace
- central_composite

Central Composite Design

Specification
Alias: none

Argument(s): none
CHAPTER 6. KEYWORDS AREA

Description

A central composite design (CCD), contains an embedded factorial or fractional factorial design with a center points that is augmented with a group of "star points" that allow estimation of curvature.

Examples

See the User’s Manual for an example.

samples

- Keywords Area
- method
- dace
- samples

Number of samples for sampling-based methods

Specification

Alias: none

Argument(s): INTEGER

Default: 0

Description

The samples keyword is used to define the number of samples (i.e., randomly chosen sets of variable values) at which to execute a model.

Default Behavior

By default, Dakota will use the minimum number of samples required by the chosen method.

Usage Tips

To obtain linear sensitivities or to construct a linear response surface, at least dim+1 samples should be used, where "dim" is the number of variables. For sensitivities to quadratic terms or quadratic response surfaces, at least (dim+1)(dim+2)/2 samples are needed. For uncertainty quantification, we recommend at least 10*dim samples. For variance_based_decomp, we recommend hundreds to thousands of samples. Note that for variance_based_decomp, the number of simulations performed will be N*(dim+2).

Examples

method
sampling
  sampling_type lhs
  samples = 20
6.2. METHOD

seed

- Keywords Area
- method
- dace
- seed

Seed of the random number generator

Specification

Alias: none

Argument(s): INTEGER

Default: system-generated (non-repeatable)

Description

The random seed control provides a mechanism for making a stochastic method repeatable. That is, the use of the same random seed in identical studies will generate identical results.

Default Behavior
If not specified, the seed is randomly generated.

Expected Output
If seed is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

Usage Tips
If a stochastic study was run without seed specified, and the user later wishes to repeat the study using the same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen. That value can then be added to the Dakota input file.

Examples

```
method
  sampling
    sample_type lhs
    samples = 10
    seed = 15347
```

main_effects

- Keywords Area
- method
- dace
- main_effects

ANOVA
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none
               Argument(s): none
               Default: No main_effects

Description

The main_effects control prints Analysis-of-Variance main effects results (e.g. ANOVA tables with p-values per variable). The main_effects control is only operational with the orthogonal arrays or Latin Hypercube designs, not for Box Behnken or Central Composite designs.

Main effects is a sensitivity analysis method which identifies the input variables that have the most influence on the output. In main effects, the idea is to look at the mean of the response function when variable A (for example) is at level 1 vs. when variable A is at level 2 or level 3. If these mean responses of the output are statistically significantly different at different levels of variable A, this is an indication that variable A has a significant effect on the response. The orthogonality of the columns is critical in performing main effects analysis, since the column orthogonality means that the effects of the other variables "cancel out" when looking at the overall effect from one variable at its different levels.

quality_metrics

- Keywords Area
- method
- dace
- quality_metrics

Calculate metrics to assess the quality of quasi-Monte Carlo samples

Topics

This keyword is related to the topics:

- package_fsudace

Specification

Alias: none
               Argument(s): none
               Default: No quality_metrics

Description

quality_metrics calculates four quality metrics relating to the volumetric spacing of the samples. The four quality metrics measure different aspects relating to the uniformity of point samples in hypercubes. Desirable properties of such point samples are:

- are the points equally spaced
- do the points cover the region
and are they isotropically distributed
with no directional bias in the spacing

The four quality metrics we report are:

• h: the point distribution norm, which is a measure of uniformity of the point distribution
• chi: a regularity measure, and provides a measure of local uniformity of a set of points
• tau: the second moment trace measure
• d: the second moment determinant measure

All of these values are scaled so that smaller is better (the smaller the metric, the better the uniformity of the point distribution).

Examples
Complete explanation of these measures can be found in [38].

\texttt{variance\_based\_decomp}

• Keywords Area
• method
• dace
• \texttt{variance\_based\_decomp}

Activates global sensitivity analysis based on decomposition of response variance into contributions from variables.

Specification
\textbf{Alias}: none
\textbf{Argument(s)}: none
\textbf{Default}: no variance-based decomposition

| Required/-| Description of | Dakota Keyword | Dakota Keyword |
| Required/| Optional Group | drop\_tolerance | Description |
| Optional | | | Suppresses output of sensitivity indices with values lower than this tolerance |
Description

Dakota can calculate sensitivity indices through variance based decomposition using the keyword `variance_based_decomp`. These indicate how important the uncertainty in each input variable is in contributing to the output variance.

**Default Behavior**

Because of the computational cost, `variance_based_decomp` is turned off as a default.

If the user specified a number of samples, N, and a number of nondeterministic variables, M, variance-based decomposition requires the evaluation of \( N \times (M+2) \) samples. **Note that specifying this keyword will increase the number of function evaluations above the number requested with the `samples` keyword since replicated sets of sample values are evaluated.**

**Expected Outputs**

When `variance_based_decomp` is specified, sensitivity indices for main effects and total effects will be reported. Main effects (roughly) represent the percent contribution of each individual variable to the variance in the model response. Total effects represent the percent contribution of each individual variable in combination with all other variables to the variance in the model response.

**Usage Tips**

To obtain sensitivity indices that are reasonably accurate, we recommend that N, the number of samples, be at least one hundred and preferably several hundred or thousands.

**Examples**

```plaintext
method,
  sampling
    sample_type lhs
    samples = 100
    variance_based_decomp
```

**Theory**

In this context, we take sensitivity analysis to be global, not local as when calculating derivatives of output variables with respect to input variables. Our definition is similar to that of[73]: “The study of how uncertainty in the output of a model can be apportioned to different sources of uncertainty in the model input.”

Variance based decomposition is a way of using sets of samples to understand how the variance of the output behaves, with respect to each input variable. A larger value of the sensitivity index, \( S_i \), means that the uncertainty in the input variable \( i \) has a larger effect on the variance of the output. More details on the calculations and interpretation of the sensitivity indices can be found in[73] and[87].

**drop_tolerance**

- `Keywords Area`
- `method`
- `dace`
- `variance_based_decomp`
- `drop_tolerance`

Suppresses output of sensitivity indices with values lower than this tolerance.
6.2. METHOD

Specification

Alias: none

Argument(s): REAL
Default: All VBD indices displayed

Description

The drop_tolerance keyword allows the user to specify a value below which sensitivity indices generated by variance_based_decomp are not displayed.

Default Behavior
By default, all sensitivity indices generated by variance_based_decomp are displayed.

Usage Tips
For polynomial_choas, which outputs main, interaction, and total effects by default, the univariate-effects may be a more appropriate option. It allows suppression of the interaction effects since the output volume of these results can be prohibitive for high dimensional problems. Similar to suppression of these interactions is the covariance control, which can be selected to be diagonal_c covariance or full_c covariance, with the former supporting suppression of the off-diagonal covariance terms (to save compute and memory resources and reduce output volume).

Examples

method,
sampling
  sample_type lhs
  samples = 100
  variance_based_decomp
drop_tolerance = 0.001

fixed_seed

- Keywords Area
- method
- dace
- fixed_seed

Reuses the same seed value for multiple random sampling sets

Specification

Alias: none

Argument(s): none
Default: not fixed; pattern varies run-to-run

Description

The fixed_seed flag is relevant if multiple sampling sets will be generated over the coarse of a Dakota analysis. This occurs when using advance methods (e.g., surrogate-based optimization, optimization under uncertainty). The same seed value is reused for each of these multiple sampling sets, which can be important for reducing variability in the sampling results.
Default Behavior
The default behavior is to not use a fixed seed, as the repetition of the same sampling pattern can result in a modeling weakness that an optimizer could potentially exploit (resulting in actual reliabilities that are lower than the estimated reliabilities). For repeatable studies, the seed must also be specified.

Examples

```plaintext
method
sampling
  sample_type lhs
  samples = 10
  fixed_seed
```

symbols
- Keywords Area
- method
- dace
- symbols

Number of replications in the sample set

Specification
Alias: none
Argument(s): INTEGER
Default: default for sampling algorithm

Description
symbols is related to the number of levels per variable in the sample set (a larger number of symbols equates to more stratification and fewer replications). For example, if symbols = 7, each variable would be divided into seven levels.

model_pointer
- Keywords Area
- method
- dace
- model_pointer

Identifier for model block to be used by a method

Topics
This keyword is related to the topics:
- block_pointer
6.2. METHOD

Specification

Alias: none

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)

Description

The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.

Usage Tips

When doing advanced analyses that involve using multiple methods and multiple models, defining a model_pointer for each method is imperative.

See block_pointer for details about pointers.

Examples

```plaintext
environment
   tabular_graphics_data
   method_pointer = 'UQ'

method
   id_method = 'UQ'
   model_pointer = 'SURR'
   sampling,
   samples = 10
   seed = 98765 rng rnum2
   response_levels = 0.1 0.2 0.6
   0.1 0.2 0.6
   0.1 0.2 0.6
   sample_type lhs
   distribution cumulative

model
   id_model = 'SURR'
   surrogate global,
   dace_method_pointer = 'DACE'
   polynomial quadratic

method
   id_method = 'DACE'
   model_pointer = 'DACE_M'
   sampling sample_type lhs
   samples = 121 seed = 5034 rng rnum2

model
   id_model = 'DACE_M'
   single
   interface_pointer = 'I1'

variables
   uniform_uncertain = 2
   lower_bounds = 0. 0.
   upper_bounds = 1. 1.
   descriptors = 'x1' 'x2'
```
CHAPTER 6. KEYWORDS AREA

interface
  id_interface = 'I1'
  system.asynch.evaluation_concurrency = 5
  analysis_driver = 'text_book'

responses
  response_functions = 3
  no_gradients
  no_hessians

6.2.61 fsu_cvt

- Keywords Area
- method
- fsu_cvt

Design of Computer Experiments - Centroidal Voronoi Tessellation

Topics
This keyword is related to the topics:
- package_fsudace
- design_and_analysis_of_computer_experiments

Specification
Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>samples</td>
<td></td>
<td>Number of samples for sampling-based methods</td>
</tr>
<tr>
<td>Optional</td>
<td>seed</td>
<td></td>
<td>Seed of the random number generator</td>
</tr>
<tr>
<td>Optional</td>
<td>latinize</td>
<td></td>
<td>Adjust samples to improve the discrepancy of the marginal distributions</td>
</tr>
</tbody>
</table>
The FSU Centroidal Voronoi Tessellation method (*fsu_cvt*) produces a set of sample points that are (approximately) a Centroidal Voronoi Tessellation. The primary feature of such a set of points is that they have good volumetric spacing; the points tend to arrange themselves in a pattern of cells that are roughly the same shape.

To produce this set of points, an almost arbitrary set of initial points is chosen, and then an internal set of iterations is carried out. These iterations repeatedly replace the current set of sample points by an estimate of the centroids of the corresponding Voronoi subregions. [18].

The user may generally ignore the details of this internal iteration. If control is desired, however, there are a few variables with which the user can influence the iteration. The user may specify:

- `max_iterations`, the number of iterations carried out

<table>
<thead>
<tr>
<th>Optional</th>
<th>quality_metrics</th>
<th>Calculate metrics to assess the quality of quasi-Monte Carlo samples</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>variance_based_decomp</td>
<td>Activates global sensitivity analysis based on decomposition of response variance into contributions from variables</td>
</tr>
<tr>
<td>Optional</td>
<td>fixed_seed</td>
<td>Reuses the same seed value for multiple random sampling sets</td>
</tr>
<tr>
<td>Optional</td>
<td>trial_type</td>
<td>Specify how the trial samples are generated</td>
</tr>
<tr>
<td>Optional</td>
<td>num_trials</td>
<td>The number of secondary sample points generated to adjust the location of the primary sample points</td>
</tr>
<tr>
<td>Optional</td>
<td>max_iterations</td>
<td>Number of iterations allowed for optimizers and adaptive UQ methods</td>
</tr>
<tr>
<td>Optional</td>
<td>model_pointer</td>
<td>Identifier for model block to be used by a method</td>
</tr>
</tbody>
</table>

### Description

The FSU Centroidal Voronoi Tessellation method (*fsu_cvt*) produces a set of sample points that are (approximately) a Centroidal Voronoi Tessellation. The primary feature of such a set of points is that they have good volumetric spacing; the points tend to arrange themselves in a pattern of cells that are roughly the same shape.

To produce this set of points, an almost arbitrary set of initial points is chosen, and then an internal set of iterations is carried out. These iterations repeatedly replace the current set of sample points by an estimate of the centroids of the corresponding Voronoi subregions. [18].

The user may generally ignore the details of this internal iteration. If control is desired, however, there are a few variables with which the user can influence the iteration. The user may specify:

- `max_iterations`, the number of iterations carried out
• **num_trials**, the number of secondary sample points generated to adjust the location of the primary sample points

• **trial_type**, which controls how these secondary sample points are generated

This method generates sets of uniform random variables on the interval [0,1]. If the user specifies lower and upper bounds for a variable, the [0,1] samples are mapped to the [lower, upper] interval.

**Theory**

This method is designed to generate samples with the goal of low discrepancy. Discrepancy refers to the nonuniformity of the sample points within the hypercube.

Discrepancy is defined as the difference between the actual number and the expected number of points one would expect in a particular set B (such as a hyper-rectangle within the unit hypercube), maximized over all such sets. Low discrepancy sequences tend to cover the unit hypercube reasonably uniformly.

Centroidal Voronoi Tessellation does very well volumetrically: it spaces the points fairly equally throughout the space, so that the points cover the region and are isotropically distributed with no directional bias in the point placement. There are various measures of volumetric uniformity which take into account the distances between pairs of points, regularity measures, etc. Note that Centroidal Voronoi Tessellation does not produce low-discrepancy sequences in lower dimensions. The lower-dimension (such as 1-D) projections of Centroidal Voronoi Tessellation can have high discrepancy.

**See Also**

These keywords may also be of interest:

• **dace**

• **fsu_quasi_mc**

• **psuade_moat**

**samples**

• **Keywords Area**

• **method**

• **fsu_cvt**

• **samples**

Number of samples for sampling-based methods

**Specification**

**Alias**: none

**Argument(s)**: INTEGER

**Default**: 0
6.2. METHOD

Description
The samples keyword is used to define the number of samples (i.e., randomly chosen sets of variable values) at which to execute a model.

Default Behavior
By default, Dakota will use the minimum number of samples required by the chosen method.

Usage Tips
To obtain linear sensitivities or to construct a linear response surface, at least dim+1 samples should be used, where "dim" is the number of variables. For sensitivities to quadratic terms or quadratic response surfaces, at least (dim+1)(dim+2)/2 samples are needed. For uncertainty quantification, we recommend at least 10*dim samples. For variance_based_decomp, we recommend hundreds to thousands of samples. Note that for variance_based_decomp, the number of simulations performed will be N*(dim+2).

Examples
method sampling
  sample_type lhs
  samples = 20

seed

• Keywords Area

• method

• fsu_cv

• seed

Seed of the random number generator

Specification
Alias: none
Argument(s): INTEGER
Default: system-generated (non-repeatable)

Description
The random seed control provides a mechanism for making a stochastic method repeatable. That is, the use of the same random seed in identical studies will generate identical results.

Default Behavior
If not specified, the seed is randomly generated.

Expected Output
If seed is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

Usage Tips
If a stochastic study was run without seed specified, and the user later wishes to repeat the study using the same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen. That value can then be added to the Dakota input file.
Examples

```python
method	sampling
    sample_type lhs
    samples = 10
    seed = 15347
```

latinize

- **Keywords Area**
- **method**
- **fsu_cvt**
- **latinize**

Adjust samples to improve the discrepancy of the marginal distributions

Specification

Alias: none

Argument(s): none

Default: No latinization

Description

The `latinize` control takes the samples and "latinizes" them, meaning that each original sample is moved so that it falls into one strata or bin in each dimension as in Latin Hypercube sampling. The default setting is NOT to latinize. However, one may be interested in doing this in situations where one wants better discrepancy of the 1-dimensional projections (the marginal distributions).

quality_metrics

- **Keywords Area**
- **method**
- **fsu_cvt**
- **quality_metrics**

Calculate metrics to assess the quality of quasi-Monte Carlo samples

Topics

This keyword is related to the topics:

- **package_fsudace**

Specification

Alias: none

Argument(s): none

Default: No quality_metrics
Description

The quality_metrics calculates four quality metrics relating to the volumetric spacing of the samples. The four quality metrics measure different aspects relating to the uniformity of point samples in hypercubes. Desirable properties of such point samples are:

- are the points equally spaced
- do the points cover the region
- and are they isotropically distributed
- with no directional bias in the spacing

The four quality metrics we report are:

- $h$: the point distribution norm, which is a measure of uniformity of the point distribution
- $\chi$: a regularity measure, and provides a measure of local uniformity of a set of points
- $\tau$: the second moment trace measure
- $d$: the second moment determinant measure

All of these values are scaled so that smaller is better (the smaller the metric, the better the uniformity of the point distribution).

Examples

Complete explanation of these measures can be found in [38].

variance_based_decomp

- **Keywords Area**
- method
- fsu_cvt
- variance_based_decomp

Activates global sensitivity analysis based on decomposition of response variance into contributions from variables.

Specification

**Alias:** none

**Argument(s):** none

**Default:** no variance-based decomposition
Description
Dakota can calculate sensitivity indices through variance based decomposition using the keyword `variance_based_decomp`. These indicate how important the uncertainty in each input variable is in contributing to the output variance.

**Default Behavior**
Because of the computational cost, `variance_based_decomp` is turned off as a default.
If the user specified a number of samples, N, and a number of nondeterministic variables, M, variance-based decomposition requires the evaluation of N*(M+2) samples. **Note that specifying this keyword will increase the number of function evaluations above the number requested with the `samples` keyword since replicated sets of sample values are evaluated.**

**Expected Outputs**
When `variance_based_decomp` is specified, sensitivity indices for main effects and total effects will be reported. Main effects (roughly) represent the percent contribution of each individual variable to the variance in the model response. Total effects represent the percent contribution of each individual variable in combination with all other variables to the variance in the model response.

**Usage Tips**
To obtain sensitivity indices that are reasonably accurate, we recommend that N, the number of samples, be at least one hundred and preferably several hundred or thousands.

**Examples**
```plaintext
method,
sampling
    sample_type lhs
    samples = 100
    variance_based_decomp
```

**Theory**
In this context, we take sensitivity analysis to be global, not local as when calculating derivatives of output variables with respect to input variables. Our definition is similar to that of [73]: “The study of how uncertainty in the output of a model can be apportioned to different sources of uncertainty in the model input.”

Variance based decomposition is a way of using sets of samples to understand how the variance of the output behaves, with respect to each input variable. A larger value of the sensitivity index, $S_i$, means that the uncertainty in the input variable $i$ has a larger effect on the variance of the output. More details on the calculations and interpretation of the sensitivity indices can be found in [73] and [87].

**drop_tolerance**
- Keywords Area
- method
- fsu_cvt
6.2. METHOD

- **variance_based_decomp**
- **drop_tolerance**

Suppresses output of sensitivity indices with values lower than this tolerance

**Specification**

Alias: none

**Argument(s):** REAL

**Default:** All VBD indices displayed

**Description**

The **drop_tolerance** keyword allows the user to specify a value below which sensitivity indices generated by **variance_based_decomp** are not displayed.

**Default Behavior**

By default, all sensitivity indices generated by **variance_based_decomp** are displayed.

**Usage Tips**

For **polynomial_chaos**, which outputs main, interaction, and total effects by default, the **univariate_effects** may be a more appropriate option. It allows suppression of the interaction effects since the output volume of these results can be prohibitive for high dimensional problems. Similar to suppression of these interactions is the covariance control, which can be selected to be diagonal_covariance or full_covariance, with the former supporting suppression of the off-diagonal covariance terms (to save compute and memory resources and reduce output volume).

**Examples**

```
method,
sampling
  sample_type lhs
  samples = 100
  variance_based_decomp
  drop_tolerance = 0.001
```

**fixed_seed**

- **Keywords Area**
- **method**
- **fsu_cvt**
- **fixed_seed**

Reuses the same seed value for multiple random sampling sets

**Specification**

Alias: none

**Argument(s):** none

**Default:** not fixed; pattern varies run-to-run
Description

The fixed_seed flag is relevant if multiple sampling sets will be generated over the course of a Dakota analysis. This occurs when using advance methods (e.g., surrogate-based optimization, optimization under uncertainty). The same seed value is reused for each of these multiple sampling sets, which can be important for reducing variability in the sampling results.

Default Behavior

The default behavior is to not use a fixed seed, as the repetition of the same sampling pattern can result in a modeling weakness that an optimizer could potentially exploit (resulting in actual reliabilities that are lower than the estimated reliabilities). For repeatable studies, the seed must also be specified.

Examples

```text
method
  sampling
    sample_type lhs
    samples = 10
    fixed_seed
```

trial_type

- Keywords Area
- method
- fsu_cvt
- trial_type

Specify how the trial samples are generated

Specification

Alias: none

<table>
<thead>
<tr>
<th>Argument(s): none</th>
</tr>
</thead>
<tbody>
<tr>
<td>Default: random</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required (Choose One)</td>
<td>trial type (Group 1)</td>
<td>grid</td>
<td>Description</td>
</tr>
<tr>
<td>--------------------</td>
<td>-----------------------</td>
<td>----------------</td>
<td>----------------</td>
</tr>
<tr>
<td></td>
<td>halton</td>
<td>Generate samples from a Halton sequence</td>
<td></td>
</tr>
<tr>
<td></td>
<td>random</td>
<td>Uses purely random Monte Carlo sampling to sample variables</td>
<td></td>
</tr>
</tbody>
</table>

Description

The user has the option to specify the method by which the trials are created to adjust the centroids. The trial_type can be one of three types:
• random, where points are generated randomly
• halton, where points are generated according to the Halton sequence
• grid, where points are placed on a regular grid over the hyperspace.

grid

Keywords Area
• method
• fsu_cvt
• trial_type
• grid

Samples on a regular grid

Specification

Alias: none
Argument(s): none

Description

Points are placed on a regular grid over the hyperspace.

See Also

These keywords may also be of interest:

• trial_type

halton

Keywords Area
• method
• fsu_cvt
• trial_type
• halton

Generate samples from a Halton sequence

Topics

This keyword is related to the topics:

• package_fsubace
CHAPTER 6. KEYWORDS AREA

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

The quasi-Monte Carlo sequences of Halton are deterministic sequences determined by a set of prime bases. These sequences generate random numbers with the goal of filling a unit hypercube uniformly. Generally, we recommend that the user leave the default setting for the bases, which are the lowest primes. Thus, if one wants to generate a sample set for 3 random variables, the default bases used are 2, 3, and 5 in the Halton sequence. To give an example of how these sequences look, the Halton sequence in base 2 starts with points 0.5, 0.25, 0.75, 0.125, 0.625, etc. The first few points in a Halton base 3 sequence are 0.33333, 0.66667, 0.11111, 0.44444, 0.77777, etc. Notice that the Halton sequence tends to alternate back and forth, generating a point closer to zero then a point closer to one. An individual sequence is based on a radix inverse function defined on a prime base. The prime base determines how quickly the [0,1] interval is filled in.

**Theory**

For more information about these sequences, see [43], [44], and [1].

**random**

- **Keywords Area**
- **method**
- **fsu_cvt**
- **trial_type**
- **random**

Uses purely random Monte Carlo sampling to sample variables

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

The random keyword invokes Monte Carlo sampling as the means of drawing samples of uncertain variables according to their probability distributions.

**Default Behavior**

In most contexts, Monte Carlo sampling is not the default sampling mode (exception: multilevel_sampling). To change this behavior, the random keyword must be specified in conjunction with the sample_type keyword.

**Usage Tips**

Monte Carlo sampling is more computationally expensive than Latin Hypercube Sampling as it requires a larger number of samples to accurately estimate statistics.
Examples

```plaintext
method
  sampling
    sample_type random
    samples = 200
```

**num_trials**

- Keywords Area
- method
- fsu_cvt
- num_trials

The number of secondary sample points generated to adjust the location of the primary sample points

**Specification**

Alias: none

Argument(s): INTEGER
Default: 10000

**Description**

In general, the variable with the most influence on the quality of the final sample set is `num_trials`, which determines how well the Voronoi subregions are sampled.

Generally, `num_trials` should be "large", certainly much bigger than the number of sample points being requested; a reasonable value might be 10,000, but values of 100,000 or 1 million are not unusual.

**max_iterations**

- Keywords Area
- method
- fsu_cvt
- max_iterations

Number of iterations allowed for optimizers and adaptive UQ methods

**Topics**

This keyword is related to the topics:

- method_independent_controls

**Specification**

Alias: none

Argument(s): INTEGER
Default: 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence} / efficient_global: 25*n)
CHAPTER 6. KEYWORDS AREA

Description
The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed \texttt{max_iterations} iterations. See also \texttt{max_function_evaluations}.

Default Behavior
Default value is 100.

\texttt{model_pointer}
- \texttt{Keywords Area}
- \texttt{method}
- \texttt{fsu_cvt}
- \texttt{model_pointer}

Identifier for model block to be used by a method

Topics
This keyword is related to the topics:
- \texttt{block_pointer}

Specification
Alias: none
- \texttt{Argument(s): STRING}
- \texttt{Default: method use of last model parsed (or use of default model if none parsed)}

Description
The \texttt{model_pointer} is used to specify which \texttt{model} block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior
If not specified, a Dakota method will use the last model block parsed. If specified, there must be a \texttt{model} block in the Dakota input file that has a corresponding \texttt{id_model} with the same name.

Usage Tips
When doing advanced analyses that involve using multiple methods and multiple models, defining a \texttt{model_pointer} for each method is imperative.
See \texttt{block_pointer} for details about pointers.

Examples
\begin{verbatim}
environment
  tabular_graphics_data
  method_pointer = 'UQ'

method
  id_method = 'UQ'
  model_pointer = 'SURR'
  sampling,
\end{verbatim}
6.2. METHOD

samples = 10
seed = 98765 rng rnum2
response_levels = 0.1 0.2 0.6
sample_type lhs
distribution cumulative

model
id_model = 'Surr'
surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
id_method = 'DACE'
model_pointer = 'DACE_M'
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = 'DACE_M'
single
interface_pointer = 'I1'

variables
uniform_uncertain = 2
lower_bounds = 0. 0.
upper_bounds = 1. 1.
descriptors = 'x1' 'x2'

interface
id_interface = 'I1'
system asynch evaluation_concurrency = 5
analysis_driver = 'text_book'

responses
response_functions = 3
no_gradients
no_hessians

6.2.62 psuade_moat

- Keywords Area
- method
- psuade_moat

Morris One-at-a-Time

Topics

This keyword is related to the topics:

- package_psuade
- design_and_analysis_of_computer_experiments
### Specification

**Alias:** none  
**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>partitions</td>
<td>partitions</td>
<td>Number of partitions of each variable</td>
</tr>
<tr>
<td>Optional</td>
<td>samples</td>
<td>samples</td>
<td>Number of samples for sampling-based methods</td>
</tr>
<tr>
<td>Optional</td>
<td>seed</td>
<td>seed</td>
<td>Seed of the random number generator</td>
</tr>
<tr>
<td>Optional</td>
<td>model_pointer</td>
<td>model_pointer</td>
<td>Identifier for model block to be used by a method</td>
</tr>
</tbody>
</table>

### Description

The Morris One-At-A-Time (MOAT) method, originally proposed by Morris [62], is a screening method, designed to explore a computational model to distinguish between input variables that have negligible, linear and additive, or nonlinear or interaction effects on the output. The computer experiments performed consist of individually randomized designs which vary one input factor at a time to create a sample of its elementary effects.

The number of samples (samples) must be a positive integer multiple of (number of continuous design variable + 1) and will be automatically adjusted if misspecified.

The number of partitions (partitions) applies to each variable being studied and must be odd (the number of MOAT levels per variable is partitions + 1). This will also be adjusted at runtime as necessary.

For information on practical use of this method, see [73].

### Theory

With MOAT, each dimension of a $k$-dimensional input space is uniformly partitioned into $p$ levels, creating a grid of $p^k$ points $x \in \mathbb{R}^k$ at which evaluations of the model $y(x)$ might take place. An elementary effect corresponding to input $i$ is computed by a forward difference

$$d_i(x) = \frac{g(x + \Delta e_i) - g(x)}{\Delta},$$

where $e_i$ is the $i^{th}$ coordinate vector, and the step $\Delta$ is typically taken to be large (this is not intended to be a local derivative approximation). In the present implementation of MOAT, for an input variable scaled to $[0, 1]$, $\Delta = \frac{p}{2(p-1)}$, so the step used to find elementary effects is slightly larger than half the input range.

The distribution of elementary effects $d_i$ over the input space characterizes the effect of input $i$ on the output of interest. After generating $r$ samples from this distribution, their mean,

$$\mu_i = \frac{1}{r} \sum_{j=1}^{r} d_i^{(j)}$$
6.2. METHOD

modified mean

\[ \mu^*_i = \frac{1}{r} \sum_{j=1}^{r} |d^{(j)}_i|, \]

(using absolute value) and standard deviation

\[ \sigma_i = \sqrt{\frac{1}{r} \sum_{j=1}^{r} \left( d^{(j)}_i - \mu_i \right)^2} \]

are computed for each input \( i \). The mean and modified mean give an indication of the overall effect of an input on the output. Standard deviation indicates nonlinear effects or interactions, since it is an indicator of elementary effects varying throughout the input space.

partitions

- Keywords Area
- method
- psuade_moat
- partitions

Number of partitions of each variable

Specification

Alias: none
Argument(s): INTEGERLIST
Default: 3

Description

Described on the parent page, psuade_moat

samples

- Keywords Area
- method
- psuade_moat
- samples

Number of samples for sampling-based methods

Specification

Alias: none
Argument(s): INTEGER
Default: 0
Description

The samples keyword is used to define the number of samples (i.e., randomly chosen sets of variable values) at which to execute a model.

**Default Behavior**
By default, Dakota will use the minimum number of samples required by the chosen method.

**Usage Tips**
To obtain linear sensitivities or to construct a linear response surface, at least \( \text{dim}+1 \) samples should be used, where “\( \text{dim} \)” is the number of variables. For sensitivities to quadratic terms or quadratic response surfaces, at least \( \frac{(\text{dim}+1)(\text{dim}+2)}{2} \) samples are needed. For uncertainty quantification, we recommend at least \( 10^* \text{dim} \) samples. For variance_based_decomp, we recommend hundreds to thousands of samples. Note that for variance_based_decomp, the number of simulations performed will be \( N^*(\text{dim}+2) \).

Examples

```dakota
method
  sampling
    sample_type lhs
    samples = 20

seed
  • Keywords Area
  • method
  • psuade_moat
  • seed

Seed of the random number generator
```

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** system-generated (non-repeatable)

Description

The random seed control provides a mechanism for making a stochastic method repeatable. That is, the use of the same random seed in identical studies will generate identical results.

**Default Behavior**
If not specified, the seed is randomly generated.

**Expected Output**
If seed is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

**Usage Tips**
If a stochastic study was run without seed specified, and the user later wishes to repeat the study using the same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen. That value can then be added to the Dakota input file.
6.2. METHOD

Examples

```plaintext
method
  sampling
    sample_type lhs
    samples = 10
    seed = 15347
```

**model_pointer**

- **Keywords Area**
- **method**
- **psuade_moat**
- **model_pointer**

Identifier for model block to be used by a method

**Topics**

This keyword is related to the topics:

- **block_pointer**

**Specification**

**Alias:** none  
**Argument(s):** STRING  
**Default:** method use of last model parsed (or use of default model if none parsed)

**Description**

The **model_pointer** is used to specify which **model** block will be used to perform the function evaluations needed by the Dakota method.

**Default Behavior**

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a **model** block in the Dakota input file that has a corresponding **id_model** with the same name.

**Usage Tips**

When doing advanced analyses that involve using multiple methods and multiple models, defining a **model_pointer** for each method is imperative.  
See **block_pointer** for details about pointers.

**Examples**

```plaintext
environment
  tabular_graphics_data
  method_pointer = 'UQ'

method
  id_method = 'UQ'
  model_pointer = 'SURR'
  sampling,
    samples = 10
```
6.2.63  local_evidence

- Keywords Area
- method
- local_evidence

Evidence theory with evidence measures computed with local optimization methods

Topics

This keyword is related to the topics:

- epistemic_uncertainty_quantification_methods
- evidence_theory
6.2. METHOD

Specification

**Alias:** nond_local_evidence

**Argument(s):** none

| Required/- | Description of | Dakota Keyword | Dakota Keyword Description |
|-----------| Group 1       | sqp            | Uses a sequential quadratic programming method for underlying optimization |
| Optional  | nip           | response_levels | Values at which to estimate desired statistics for each response |
| Optional  | probability_levels | gen_reliability_levels | Specify probability levels at which to estimate the corresponding response value |
| Optional  | distribution  |                | Selection of cumulative or complementary cumulative functions |
### Description

Two local optimization methods are available: `sqp` (sequential quadratic programming) or `nlp` (nonlinear interior point method).

#### Additional Resources

See the topic page `evidence_theory` for important background information and usage notes. Refer to `variable_support` for information on supported variable types.

#### See Also

These keywords may also be of interest:

- `global_evidence`
- `global_interval_est`
- `local_interval_est`

#### sqp

Uses a sequential quadratic programming method for underlying optimization

#### Specification

**Alias**: none

**Argument(s)**: none

#### Description

Many uncertainty quantification methods solve a constrained optimization problem under the hood. The `sqp` keyword directs Dakota to use a sequential quadratic programming method to solve that problem. A sequential quadratic programming solves a sequence of linearly constrained quadratic optimization problems to arrive at the solution to the optimization problem.
6.2. METHOD

nip

- Keywords Area
- method
- local_evidence
- nip

Uses a nonlinear interior point method for underlying optimization

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

Many uncertainty quantification methods solve a constrained optimization problem under the hood. The *nip* keyword directs Dakota to use a nonlinear interior point to solve that problem. A nonlinear interior point method traverses the interior of the feasible region to arrive at the solution to the optimization problem.

**response_levels**

- Keywords Area
- method
- local_evidence
- response_levels

Values at which to estimate desired statistics for each response

**Specification**

**Alias:** none

**Argument(s):** REALLIST

**Default:** No CDF/CCDF probabilities/reliabilities to compute

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>num_response_levels</td>
<td>Number of values at which to estimate desired statistics for each response</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### Description

The `response_levels` specification provides the target response values for which to compute probabilities, reliabilities, or generalized reliabilities (forward mapping).

**Default Behavior**

If `response_levels` are not specified, no statistics will be computed. If they are, probabilities will be computed by default.

**Expected Outputs**

If `response_levels` are specified, Dakota will create two tables in the standard output: a Probability Density function (PDF) histogram and a Cumulative Distribution Function (CDF) table. The PDF histogram has the lower and upper endpoints of each bin and the corresponding density of that bin. Note that the PDF histogram has bins defined by the `probability_levels` and/or `response_levels` in the Dakota input file. If there are not very many levels, the histogram will be coarse. Dakota does not do anything to optimize the bin size or spacing. The CDF table has the list of response levels and the corresponding probability that the response value is less than or equal to each response level threshold.

**Usage Tips**

The `num_response_levels` is used to specify which arguments of the `response_level` correspond to which response.

**Examples**

For example, specifying a `response_level` of 52.3 followed with `compute probabilities` will result in the calculation of the probability that the response value is less than or equal to 52.3, given the uncertain distributions on the inputs.

For an example with multiple responses, the following specification

```plaintext
response_levels = 1. 2. .1 .2 .3 .4 10. 20. 30.
num_response_levels = 2 4 3
```

would assign the first two response levels (1., 2.) to response function 1, the next four response levels (.1, .2, .3, .4) to response function 2, and the final three response levels (10., 20., 30.) to response function 3. If the `num_response_levels` key were omitted from this example, then the response levels would be evenly distributed among the response functions (three levels each in this case).

The Dakota input file below specifies a sampling method with response levels of interest.

```plaintext
method,
sampling,
samples = 100 seed = 1
complementary distribution
response_levels = 3.6e+11 4.0e+11 4.4e+11
6.0e+04 6.5e+04 7.0e+04
3.5e+05 4.0e+05 4.5e+05

variables,
normal_uncertain = 2
means = 248.89, 593.33
std_deviations = 12.4, 29.7
descriptors = 'TF1n' 'TF2n'
```
uniform_uncertain = 2
lower_bounds = 199.3, 474.63
upper_bounds = 298.5, 712.
descriptors = 'TF1u' 'TF2u'

weibull_uncertain = 2
alphas = 12., 30.
betas = 250., 590.
descriptors = 'TF1w' 'TF2w'

histogram_bin_uncertain = 2
num_pairs = 3 4
abscissas = 5 8 10 .1 .2 .3 .4
counts = 17 21 0 12 24 12 0
descriptors = 'TF1h' 'TF2h'

histogram_point_uncertain
real = 1
num_pairs = 2
abscissas = 3 4
counts = 1 1
descriptors = 'TF3h'

Given the above Dakota input file, the following excerpt from the output shows the PDF and CCDF generated. Note that the bounds on the bins of the PDF are the response values specified in the input file. The probability levels corresponding to those response values are shown in the CCDF.

Probability Density Function (PDF) histograms for each response function:
PDF for response_fn_1:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.7604749078e+11</td>
<td>3.6000000000e+11</td>
<td>5.3601733194e-12</td>
</tr>
<tr>
<td>3.6000000000e+11</td>
<td>4.0000000000e+11</td>
<td>4.2500000000e-12</td>
</tr>
<tr>
<td>4.0000000000e+11</td>
<td>4.4000000000e+11</td>
<td>3.7500000000e-12</td>
</tr>
<tr>
<td>4.4000000000e+11</td>
<td>5.4196114379e+11</td>
<td>2.2557612778e-12</td>
</tr>
</tbody>
</table>

PDF for response_fn_2:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.6431154744e+04</td>
<td>6.0000000000e+04</td>
<td>2.8742313192e-05</td>
</tr>
<tr>
<td>6.0000000000e+04</td>
<td>6.5000000000e+04</td>
<td>6.4000000000e-05</td>
</tr>
<tr>
<td>6.5000000000e+04</td>
<td>7.0000000000e+04</td>
<td>4.0000000000e-05</td>
</tr>
<tr>
<td>7.0000000000e+04</td>
<td>7.8702465755e+04</td>
<td>1.0341896485e-05</td>
</tr>
</tbody>
</table>

PDF for response_fn_3:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.3796737090e+05</td>
<td>3.5000000000e+05</td>
<td>4.2844660868e-06</td>
</tr>
<tr>
<td>3.5000000000e+05</td>
<td>4.0000000000e+05</td>
<td>8.6000000000e-06</td>
</tr>
<tr>
<td>4.0000000000e+05</td>
<td>4.5000000000e+05</td>
<td>1.8000000000e-06</td>
</tr>
</tbody>
</table>

Level mappings for each response function:
Complementary Cumulative Distribution Function (CCDF) for response_fn_1:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.6000000000e+11</td>
<td>5.5000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.0000000000e+11</td>
<td>3.8000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.4000000000e+11</td>
<td>2.3000000000e-01</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
**CHAPTER 6. KEYWORDS AREA**

Complementary Cumulative Distribution Function (CCDF) for response_fn_2:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.0000000000e+04</td>
<td>6.1000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6.5000000000e+04</td>
<td>2.9000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7.0000000000e+04</td>
<td>9.0000000000e-02</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Complementary Cumulative Distribution Function (CCDF) for response_fn_3:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.5000000000e+05</td>
<td>5.2000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.0000000000e+05</td>
<td>9.0000000000e-02</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.5000000000e+05</td>
<td>0.0000000000e+00</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Theory**

Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.

In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

A forward mapping involves computing the belief and plausibility probability level for a specified response level.

**num_response_levels**

- Keywords Area
- method
- local_evidence
- response_levels
- num_response_levels

Number of values at which to estimate desired statistics for each response

**Specification**

**Alias:** none

**Argument(s):** INTEGERLIST

**Default:** response_levels evenly distributed among response functions

**Description**

The num_response_levels keyword allows the user to specify the number of response values, for each response, at which estimated statistics are of interest. Statistics that can be computed are probabilities and reliabilities, both according to either a cumulative distribution function or a complementary cumulative distribution function.

**Default Behavior**

If num_response_levels is not specified, the response_levels will be evenly distributed among the responses.

**Expected Outputs**
6.2. METHOD

The specific output will be determined by the type of statistics that are specified. In a general sense, the output will be a list of response level-statistic pairs that show the estimated value of the desired statistic for each response level specified.

Examples

```
method
  sampling
    samples = 100
    seed = 34785
    num_response_levels = 1 1 1
    response_levels = 0.5 0.5 0.5

compute

  - Keywords Area
  - method
  - local_evidence
  - response_levels
  - compute

Selection of statistics to compute at each response level
```

Specification

Alias: none
Argument(s): none
Default: probabilities

<table>
<thead>
<tr>
<th>Required/- Optional Required(Choose One)</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>probabilities</strong></td>
<td></td>
<td>gen_reliabilities</td>
<td>Computes generalized reliabilities associated with response levels</td>
</tr>
<tr>
<td><strong>system</strong></td>
<td></td>
<td>system</td>
<td>Compute system reliability (series or parallel)</td>
</tr>
</tbody>
</table>
Description

The `compute` keyword is used to select which forward stastical mapping is calculated at each response level.

Default Behavior

If `response_levels` is not specified, no statistics are computed. If `response_levels` is specified but `compute` is not, probabilities will be computed by default. If both `response_levels` and `compute` are specified, then one of the following must be specified: `probabilities`, `reliabilities`, or `gen_reliabilities`.

Expected Output

The type of statistics specified by `compute` will be reported for each response level.

Usage Tips

CDF/CCDF probabilities are calculated for specified response levels using a simple binning approach.

CDF/CCDF reliabilities are calculated for specified response levels by computing the number of sample standard deviations separating the sample mean from the response level.

Examples

```
method sampling
  sampling_type random
  samples = 100 seed = 1
  complementary_distribution
  response_levels = 3.6e+11 4.0e+11 4.4e+11
                   6.0e+04 6.5e+04 7.0e+04
                   3.5e+05 4.0e+05 4.5e+05
  compute reliabilities
probabilities
```

Computes probabilities associated with response levels

Specification

Alias: none

Argument(s): none

Description

The `probabilities` keyword directs Dakota to compute the probability that the model response will be below (cumulative) or above (complementary cumulative) a specified response value. This is done for every response level designated for each response.

Default Behavior
6.2. METHOD

If \texttt{response\_levels} is specified, the probabilities are computed by default. To explicitly specify it in the Dakota input file, though, the \texttt{probabilities} keyword should be specified in conjunction with the \texttt{compute} keyword.

**Expected Outputs**
The Dakota output is a set of response level-probability pairs that give the probability that the model response will be below or above the corresponding response level, depending on the distribution defined.

**Examples**

```plaintext
method sampling
  sample_type random
  samples = 100 seed = 1
  complementary distribution
  response\_levels = 3.6e+11 4.0e+11 4.4e+11
                   6.0e+04 6.5e+04 7.0e+04
                   3.5e+05 4.0e+05 4.5e+05
  compute probabilities
```

**\texttt{gen\_reliabilities}**

- **Keywords Area**
- **method**
- **local\_evidence**
- **response\_levels**
- **compute**
- **gen\_reliabilities**

Computes generalized reliabilities associated with response levels

**Specification**

- **Alias:** none
  - **Argument(s):** none

**Description**
The \texttt{gen\_reliabilities} keyword directs Dakota to compute generalized reliabilities according to the specified distribution for a specified response value. This is done for every response level designated for each response.

**Default Behavior**
If \texttt{response\_levels} is specified, the generalized reliabilities are not computed by default. To change this behavior, the \texttt{gen\_reliabilities} keyword should be specified in conjunction with the \texttt{compute} keyword.

**Expected Outputs**
The Dakota output is a set of response level-generalized reliability pairs according to the distribution defined.
Examples

method
  sampling
    sample_type random
    samples = 100 seed = 1
    complementary distribution
    response_levels = 3.6e+11 4.0e+11 4.4e+11
                  6.0e+04 6.5e+04 7.0e+04
                  3.5e+05 4.0e+05 4.5e+05
    compute gen_reliabilities

system

  • Keywords Area
  • method
  • local_evidence
  • response_levels
  • compute
  • system

  Compute system reliability (series or parallel)

Specification

Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional Required (Choose One)</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>series</td>
<td>Aggregate response statistics assuming a series system</td>
</tr>
<tr>
<td></td>
<td></td>
<td>parallel</td>
<td>Aggregate response statistics assuming a parallel system</td>
</tr>
</tbody>
</table>

Description

With the system probability/reliability option, statistics for specified response_levels are calculated and reported assuming the response functions combine either in series or parallel to produce a total system response.

For a series system, the system fails when any one component (response) fails. The probability of failure is the complement of the product of the individual response success probabilities.

For a parallel system, the system fails only when all components (responses) fail. The probability of failure is the product of the individual response failure probabilities.
6.2. METHOD

series

• Keywords Area
• method
• local_evidence
• response_levels
• compute
• system
• series

Aggregate response statistics assuming a series system

Specification

Alias: none
Argument(s): none

Description

See parent keyword system for description.

parallel

• Keywords Area
• method
• local_evidence
• response_levels
• compute
• system
• parallel

Aggregate response statistics assuming a parallel system

Specification

Alias: none
Argument(s): none

Description

See parent keyword system for description.
probability_levels
  • Keywords Area
  • method
  • local_evidence
  • probability_levels

Specify probability levels at which to estimate the corresponding response value

### Specification

**Alias:** none  
**Argument(s):** REALLIST  
**Default:** No CDF/CCDF response levels to compute

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>num_probability_levels</td>
<td></td>
<td>Specify which probability_levels correspond to which response levels</td>
</tr>
</tbody>
</table>

### Description

Response levels are calculated for specified CDF/CCDF probabilities by indexing into a sorted samples array (the response levels computed are not interpolated and will correspond to one of the sampled values).

**Expected Output**

If `probability_levels` are specified, Dakota will create two tables in the standard output: a Probability Density function (PDF) histogram and a Cumulative Distribution Function (CDF) table. The PDF histogram has the lower and upper endpoints of each bin and the corresponding density of that bin. Note that the PDF histogram has bins defined by the `probability_levels` and/or `response_levels` in the Dakota input file. If there are not very many levels, the histogram will be coarse. Dakota does not do anything to optimize the bin size or spacing. The CDF table has the list of response levels and the corresponding probability that the response value is less than or equal to each response level threshold.

### Examples

The Dakota input file below specifies a sampling method with probability levels of interest.

```plaintext
method,
  sampling,
    samples = 100 seed = 1
    complementary_distribution
    probability_levels = 1. .66 .33 0.
      1. .8 .5 0.
      1. .3 .2 0.
variables,
  normal_uncertain = 2
  means = 248.89, 593.33
  std_deviations = 12.4, 29.7
```
6.2. METHOD

```
descriptors = 'TF1n' 'TF2n'
uniform_uncertain = 2
lower_bounds = 199.3, 474.63
upper_bounds = 298.5, 712.
descriptors = 'TF1u' 'TF2u'
weibull_uncertain = 2
alphas = 12., 30.
betas = 250., 590.
descriptors = 'TF1w' 'TF2w'
histogram_bin_uncertain = 2
num_pairs = 3 4
abscissas = 5 8 10 .1 .2 .3 .4
counts = 17 21 0 12 24 12 0
descriptors = 'TF1h' 'TF2h'
histogram_point_uncertain
real = 1
num_pairs = 2
abscissas = 3 4
counts = 1 1
descriptors = 'TF3h'

interface,
system asynch evaluation_concurrency = 5
analysis_driver = 'text_book'
responses,
response_functions = 3
no_gradients
no_hessians
```

Given the above Dakota input file, the following excerpt from the output shows the PDF and CCDF generated. Note that the bounds on the bins of the PDF are the response values that correspond the probability levels specified in the input file. Those response values are also shown in the CCDF.

```
Probability Density Function (PDF) histograms for each response function:
PDF for response_fn_1:
     Bin Lower     Bin Upper     Density Value
           --------     --------     ------------
 2.7604749078e+11 3.4221494996e+11 5.1384774972e-12
 3.4221494996e+11 4.0634975300e+11 5.1454122311e-12
 4.0634975300e+11 5.4196114379e+11 2.4334239039e-12

PDF for response_fn_2:
     Bin Lower     Bin Upper     Density Value
           --------     --------     ------------
 4.6431154744e+04 5.6511827775e+04 1.9839945149e-05
 5.6511827775e+04 6.1603813790e+04 5.8916108390e-05
 6.1603813790e+04 7.8702465755e+04 2.9242071306e-05

PDF for response_fn_3:
     Bin Lower     Bin Upper     Density Value
           --------     --------     ------------
 2.3796737090e+05 3.6997214153e+05 5.3028386523e-06
 3.6997214153e+05 3.8100966235e+05 9.0600055634e-06
 3.8100966235e+05 4.4111498127e+05 3.3274925348e-06

Level mappings for each response function:
Complementary Cumulative Distribution Function (CCDF) for response_fn_1:
     Response Level     Probability Level     Reliability Index     General Rel Index
          --------     ------------     ------------     ------------
 2.7604749078e+11 1.0000000000e+00     0.0000000000e+00
 3.4221494996e+11 6.6000000000e-01     0.9000000000e-01
 4.0634975300e+11 3.3000000000e-01     0.6000000000e-01
 5.4196114379e+11 8.8000000000e-02     0.2000000000e+00
```
CHAPTER 6. KEYWORDS AREA

Complementary Cumulative Distribution Function (CCDF) for response_fn_2:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.6431154744e+04</td>
<td>1.0000000000e+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5.6511827775e+04</td>
<td>8.0000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6.1603813790e+04</td>
<td>5.0000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7.8702465755e+04</td>
<td>0.0000000000e+00</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Complementary Cumulative Distribution Function (CCDF) for response_fn_3:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.3796737090e+05</td>
<td>1.0000000000e+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.6997214153e+05</td>
<td>3.0000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.8100966235e+05</td>
<td>2.0000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.4111498127e+05</td>
<td>0.0000000000e+00</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Theory

Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.

In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

An inverse mapping involves computing the belief and plausibility response level for either a specified probability level or a specified generalized reliability level (two results for each level mapping in the evidence-based epistemic case, instead of the one result for each level mapping in the aleatory case).

**num_probability_levels**

- Keywords Area
- method
- local_evidence
- probability_levels
- num_probability_levels

Specify which probability_levels correspond to which response

Specification

**Alias:** none

**Argument(s):** INTEGERLIST

**Default:** probability_levels evenly distributed among response functions

**Description**

See parent page
6.2. METHOD

**Method**

Specifies generalized reliability levels at which to estimate the corresponding response value.

**Specification**

**Alias:** none

**Argument(s):** REALLIST

**Default:** No CDF/CCDF response levels to compute

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>num_gen_reliability_levels</td>
<td>Specify which gen_reliability_levels correspond to which response</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Description**

Response levels are calculated for specified generalized reliabilities by indexing into a sorted samples array (the response levels computed are not interpolated and will correspond to one of the sampled values).

**Theory**

Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.

In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

An inverse mapping involves computing the belief and plausibility response level for either a specified probability level or a specified generalized reliability level (two results for each level mapping in the evidence-based epistemic case, instead of the one result for each level mapping in the aleatory case).

**num_gen_reliability_levels**

- **Keywords Area**
- **method**
- **local_evidence**
- **gen_reliability_levels**
- **num_gen_reliability_levels**

Specify which gen_reliability_levels correspond to which response
**Specification**

Alias: none

- **Argument(s):** INTEGERLIST
- **Default:** gen_reliability.levels evenly distributed among response functions

**Description**

See parent page

**distribution**

- Keywords Area
- method
- local_evidence
- distribution

Selection of cumulative or complementary cumulative functions

**Specification**

Alias: none

- **Argument(s):** none
- **Default:** cumulative (CDF)

<table>
<thead>
<tr>
<th>Required/-Optional Required (Choose One)</th>
<th>Description of Group Group 1</th>
<th>Dakota Keyword cumulative</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
</table>

| | | | Computes statistics according to cumulative functions |

| | | complementary | Computes statistics according to complementary cumulative functions |

**Description**

The `distribution` keyword allows the user to select between a cumulative distribution/belief/plausibility function and a complementary cumulative distribution/belief/plausibility function. This choice affects how probabilities and reliability indices are reported.

**Default Behavior**

- If the `distribution` keyword is present, it must be accompanied by either `cumulative` or `complementary`.
- Otherwise, a cumulative distribution will be used by default.

**Expected Outputs**

Output will be a set of model response-probability pairs determined according to the choice of distribution. The choice of distribution also defines the sign of the reliability or generalized reliability indices.
6.2. METHOD

Examples

```
method
  sampling
    sample_type lhs
    samples = 10
    distribution cumulative
```

cumulative

- Keywords Area
- method
- local_evidence
- distribution
- cumulative

Computes statistics according to cumulative functions

Specification

Alias: none
Argument(s): none

Description

Statistics on model responses will be computed according to a cumulative distribution/belief/plausibility function.

Default Behavior

By default, a cumulative distribution/belief/plausibility function will be used. To explicitly specify it in the Dakota input file, however, the `cumulative` keyword must appear in conjunction with the `distribution` keyword.

Expected Outputs

Output will be a set of model response-probability pairs determined according to a cumulative distribution/belief/plausibility function. The probabilities reported are the probabilities that the model response falls below given response thresholds.

Examples

```
method
  sampling
    sample_type lhs
    samples = 10
    distribution cumulative
```

complementary

- Keywords Area
- method
- local_evidence
- distribution
• complementary

Computes statistics according to complementary cumulative functions

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

Statistics on model responses will be computed according to a complementary cumulative distribution/belief/plausibility function.

**Default Behavior**

By default, a complementary cumulative distribution/belief/plausibility function will not be used. To change that behavior, the `complementary` keyword must be appear in conjunction with the `distribution` keyword.

**Expected Outputs**

Output will be a set of model response-probability pairs determined according to a complementary cumulative distribution/belief/plausibility function. The probabilities reported are the probabilities that the model response falls above given response thresholds.

**Examples**

```
method
  sampling
    sample_type lhs
    samples = 10
    distribution complementary

model_pointer

• Keywords Area

• method

• local_evidence

• model_pointer

Identifier for model block to be used by a method

**Topics**

This keyword is related to the topics:

• block_pointer

**Specification**

**Alias:** none

**Argument(s):** STRING

**Default:** method use of last model parsed (or use of default model if none parsed)
Description

The `model_pointer` is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

**Default Behavior**

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding `id_model` with the same name.

**Usage Tips**

When doing advanced analyses that involve using multiple methods and multiple models, defining a `model_pointer` for each method is imperative.

See `block_pointer` for details about pointers.

**Examples**

```plaintext
environment
tabular_graphics_data
method_pointer = 'UQ'

method
id_method = 'UQ'
model_pointer = 'Surr'
sampling,
samples = 10
seed = 98765 rng rnum2
response_levels = 0.1 0.2 0.6
               0.1 0.2 0.6
               0.1 0.2 0.6
sample_type lhs
distribution cumulative

model
id_model = 'Surr'
surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
id_method = 'DACE'
model_pointer = 'DACE_M'
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = 'DACE_M'
single
interface_pointer = 'I1'

variables
uniform_uncertain = 2
lower_bounds = 0. 0.
upper_bounds = 1. 1.
descriptors = 'x1' 'x2'

interface
id_interface = 'I1'
system asynch evaluation_concurrency = 5
analysis_driver = 'text_book'

responses
```
response_functions = 3
no_gradients
no_hessians

6.2.64 local_interval_est

- Keywords Area
- method
- local_interval_est

Interval analysis using local optimization

Topics

This keyword is related to the topics:

- uncertainty_quantification
- epistemic_uncertainty_quantification_methods
- interval_estimation

Specification

Alias: nond_local_interval_est
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional (Choose One)</td>
<td>sqp</td>
<td>Uses a sequential quadratic programming method for underlying optimization</td>
<td></td>
</tr>
<tr>
<td>nip</td>
<td>Uses a nonlinear interior point method for underlying optimization</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional (Choose One)</td>
<td>sqp</td>
<td>Uses a sequential quadratic programming method for underlying optimization</td>
<td></td>
</tr>
<tr>
<td>nip</td>
<td>Uses a nonlinear interior point method for underlying optimization</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### Description

Interval analysis using local methods ($local\_interval\_est$). If the problem is amenable to local optimization methods (e.g., can provide derivatives or use finite difference method to calculate derivatives), then one can use one of two local methods to calculate these bounds.

- `sqp`
- `nip`

### Additional Resources

Refer to `variable_support` for information on supported variable types.

### Theory

In interval analysis, one assumes that nothing is known about an epistemic uncertain variable except that its value lies somewhere within an interval. In this situation, it is NOT assumed that the value has a uniform probability of occurring within the interval. Instead, the interpretation is that any value within the interval is a possible value or a potential realization of that variable. In interval analysis, the uncertainty quantification problem is one of determining the resulting bounds on the output (defining the output interval) given interval bounds on the inputs. Again, any output response that falls within the output interval is a possible output with no frequency information assigned to it.

### See Also

These keywords may also be of interest:

- `global\_evidence`
- `global\_interval\_est`
- `local\_evidence`

### sqp

- **Keywords Area**
- `method`
- `local\_interval\_est`
- `sqp`

Uses a sequential quadratic programming method for underlying optimization.
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Description

Many uncertainty quantification methods solve a constrained optimization problem under the hood. The sqp keyword directs Dakota to use a sequential quadratic programming method to solve that problem. A sequential quadratic programming solves a sequence of linearly constrained quadratic optimization problems to arrive at the solution to the optimization problem.

nip

• Keywords Area

• method

• local_interval_est

• nip

Uses a nonlinear interior point method for underlying optimization

Specification

Alias: none

Description

Many uncertainty quantification methods solve a constrained optimization problem under the hood. The nip keyword directs Dakota to use a nonlinear interior point to solve that problem. A nonlinear interior point method traverses the interior of the feasible region to arrive at the solution to the optimization problem.

convergence_tolerance

• Keywords Area

• method

• local_interval_est

• convergence_tolerance

Stopping criterion based on convergence of the objective function or statistics

Topics

This keyword is related to the topics:

• method_independent_controls
6.2. METHOD

Specification

Alias: none

Argument(s): REAL

Default: 1.e-4

Description

The convergence_tolerance specification provides a real value for controlling the termination of iteration. For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by convergence_tolerance, then this convergence criterion is satisfied on the current iteration.

Therefore, permissible values are between 0 and 1, non-inclusive.

Behavior Varies by Package/Library

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- DOT: must be satisfied for two consecutive iterations
- NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of convergence_tolerance approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., convergence_tolerance = 1.e-6 will result in approximately six digits of accuracy in the final objective function).
- NL2SOL: See nl2sol

model_pointer

- Keywords Area
- method
- local_interval_est
- model_pointer

Identifier for model block to be used by a method

Topics

This keyword is related to the topics:

- block_pointer
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)

Description

The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.

Usage Tips

When doing advanced analyses that involve using multiple methods and multiple models, defining a model-pointer for each method is imperative.

See block_pointer for details about pointers.

Examples

```dakota
environment
tabular_graphics_data
method_pointer = 'UQ'

method
id_method = 'UQ'
model_pointer = 'SURR'
sampling,
samples = 10
seed = 98765 rng rnum2
response_levels = 0.1 0.2 0.6
0.1 0.2 0.6
0.1 0.2 0.6
sample_type lhs
distribution cumulative

model
id_model = 'SURR'
surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
id_method = 'DACE'
model_pointer = 'DACE_M'
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = 'DACE_M'
single
interface_pointer = 'I1'

variables
uniform_uncertain = 2
lower_bounds = 0. 0.
upper_bounds = 1. 1.
descriptors = 'x1' 'x2'
```
6.2. METHOD

interface
  id_interface = 'I1'
system async evaluation_concurrency = 5
  analysis_driver = 'text_book'

responses
  response_functions = 3
  no_gradients
  no_hessians

6.2.65 local_reliability

- Keywords Area
- method
- local_reliability

Local reliability method

Topics

This keyword is related to the topics:

- uncertainty_quantification
- reliability_methods

Specification

Alias: nond_local_reliability

Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>mpp_search</td>
<td></td>
<td>Specify which MPP search option to use</td>
</tr>
<tr>
<td></td>
<td>response_levels</td>
<td></td>
<td>Values at which to estimate desired statistics for each response</td>
</tr>
<tr>
<td></td>
<td>reliability_levels</td>
<td></td>
<td>Specify reliability levels at which the response values will be estimated</td>
</tr>
</tbody>
</table>
### Description

Local reliability methods compute approximate response function distribution statistics based on specified uncertain variable probability distributions. Each of the local reliability methods can compute forward and inverse mappings involving response, probability, reliability, and generalized reliability levels.

The forward reliability analysis algorithm of computing reliabilities/probabilities for specified response levels is called the Reliability Index Approach (RIA), and the inverse reliability analysis algorithm of computing response levels for specified probability levels is called the Performance Measure Approach (PMA).

The different RIA/PMA algorithm options are specified using the `mpp_search` specification which selects among different limit state approximations that can be used to reduce computational expense during the MPP.

<table>
<thead>
<tr>
<th>Optional</th>
<th>max_iterations</th>
<th>Number of iterations allowed for optimizers and adaptive UQ methods</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>convergence_tolerance</td>
<td>Stopping criterion based on convergence of the objective function or statistics</td>
</tr>
<tr>
<td>Optional</td>
<td>final_moments</td>
<td>Output moments of the specified type and include them within the set of final statistics.</td>
</tr>
<tr>
<td>Optional</td>
<td>distribution</td>
<td>Selection of cumulative or complementary cumulative functions</td>
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<tr>
<td>Optional</td>
<td>probability_levels</td>
<td>Specify probability levels at which to estimate the corresponding response value</td>
</tr>
<tr>
<td>Optional</td>
<td>gen_reliability_levels</td>
<td>Specify generalized reliability levels at which to estimate the corresponding response value</td>
</tr>
<tr>
<td>Optional</td>
<td>model_pointer</td>
<td>Identifier for model block to be used by a method</td>
</tr>
</tbody>
</table>
searches.

**Theory**

The Mean Value method (MV, also known as MVFOSM in [42]) is the simplest, least-expensive method in that it estimates the response means, response standard deviations, and all CDF/CCDF forward/inverse mappings from a single evaluation of response functions and gradients at the uncertain variable means. This approximation can have acceptable accuracy when the response functions are nearly linear and their distributions are approximately Gaussian, but can have poor accuracy in other situations.

All other reliability methods perform an internal nonlinear optimization to compute a most probable point (M-PP) of failure. A sign convention and the distance of the MPP from the origin in the transformed standard normal space ("u-space") define the reliability index, as explained in the section on Reliability Methods in the Uncertainty Quantification chapter of the Users Manual [4]. Also refer to variable support for additional information on supported variable types for transformations to standard normal space. The reliability can then be converted to a probability using either first- or second-order integration, may then be refined using importance sampling, and finally may be converted to a generalized reliability index.

**See Also**

These keywords may also be of interest:

- adaptive_sampling
- gpais
- global_reliability
- sampling
- importance_sampling
- polynomial_chaos
- stoch_collocation

**mpp_search**

- Keywords Area
- method
- local_reliability
- mpp_search

Specify which MPP search option to use

**Topics**

This keyword is related to the topics:

- uncertainty_quantification
- reliability_methods
### Specification

**Alias:** none  
**Argument(s):** none  
**Default:** No MPP search (MV method)

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Group</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<tr>
<td><strong>Required</strong> (Choose One)</td>
<td>Group 1</td>
<td></td>
<td>x_taylor_mean</td>
<td>Form Taylor series approximation in “x-space” at variable means</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>u_taylor_mean</td>
<td>Form Taylor series approximation in “u-space” at variable means</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>x_taylor_mpp</td>
<td>X-space Taylor series approximation with iterative updates</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>u_taylor_mpp</td>
<td>U-space Taylor series approximation with iterative updates</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>x_two_point</td>
<td>Predict MPP using Two-point Adaptive Nonlinear Approximation in “x-space”</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>u_two_point</td>
<td>Predict MPP using Two-point Adaptive Nonlinear Approximation in “u-space”</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>no_approx</td>
<td>Perform MPP search on original response functions (use no approximation)</td>
</tr>
</tbody>
</table>
6.2. METHOD

<table>
<thead>
<tr>
<th>Optional (Choose One)</th>
<th>Group 2</th>
<th>sqp</th>
<th>Uses a sequential quadratic programming method for underlying optimization</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>integration</td>
<td>nip</td>
<td>Uses a nonlinear interior point method for underlying optimization</td>
</tr>
</tbody>
</table>

**Description**

The `x_taylor_mean` MPP search option performs a single Taylor series approximation in the space of the original uncertain variables ("x-space") centered at the uncertain variable means, searches for the MPP for each response/probability level using this approximation, and performs a validation response evaluation at each predicted MPP. This option is commonly known as the Advanced Mean Value (AMV) method. The `u_taylor_mean` option is identical to the `x_taylor_mean` option, except that the approximation is performed in u-space. The `x_taylor_mpp` approach starts with an x-space Taylor series at the uncertain variable means, but iteratively updates the Taylor series approximation at each MPP prediction until the MPP converges. This option is commonly known as the AMV+ method. The `u_taylor_mpp` option is identical to the `x_taylor_mpp` option, except that all approximations are performed in u-space. The order of the Taylor-series approximation is determined by the corresponding responses specification and may be first or second-order. If second-order (methods named AMV² and AMV²+ in [22]), the series may employ analytic, finite difference, or quasi Hessians (BFGS or SR1). The `x_two_point` MPP search option uses an x-space Taylor series approximation at the uncertain variable means for the initial MPP prediction, then utilizes the Two-point Adaptive Nonlinear Approximation (TANA) outlined in [92] for all subsequent MPP predictions. The `u_two_point` approach is identical to `x_two_point`, but all the approximations are performed in u-space. The `x_taylor_mpp` and `u_taylor_mpp`, `x_two_point` and `u_two_point` approaches utilize the `max_iterations` and `convergence_tolerance` method independent controls to control the convergence of the MPP iterations (the maximum number of MPP iterations per level is limited by `max_iterations`, and the MPP iterations are considered converged when \( \| u^{(k+1)} - u^{(k)} \|_2 < \text{convergence_tolerance} \)). And, finally, the `no_approx` option performs the MPP search on the original response functions without the use of any approximations. The optimization algorithm used to perform these MPP searches can be selected to be either sequential quadratic programming (uses the `npsol_sqp` optimizer) or nonlinear interior point (uses the `optpp_q_newton` optimizer) algorithms using the `sqp` or `nip` keywords.

In addition to the MPP search specifications, one may select among different integration approaches for computing probabilities at the MPP by using the `integration` keyword followed by either `first_order` or `second_order`. Second-order integration employs the formulation of [50] (the approach of [13] and the correction of [51] are also implemented, but are not active). Combining the `no_approx` option of the MPP search with first- and second-order integrations results in the traditional first- and second-order reliability methods (FORM and SORM). These integration approximations may be subsequently refined using importance sampling. The refinement specification allows the selection of basic importance sampling (import), adaptive importance sampling (adapt_import), or multimodal adaptive importance sampling (mm_adapt_import), along with the specification of number of samples (samples) and random seed (seed). Additional details on these methods are available in [24] and [22] and in the Uncertainty Quantification Capabilities chapter of the Users Manual.
CHAPTER 6. KEYWORDS AREA

x_taylor_mean

- Keywords Area
- method
- local_reliability
- mpp_search
- x_taylor_mean

Form Taylor series approximation in ”x-space” at variable means

Topics
This keyword is related to the topics:
- reliability_methods

Specification
Alias: none
Argument(s): none

Description
This mpp_search option performs a single Taylor series approximation in the space of the original uncertain variables (”x-space”) centered at the uncertain variable means, searches for the MPP for each response/probability level using this approximation, and performs a validation response evaluation at each predicted MPP. This option is commonly known as the Advanced Mean Value (AMV) method.

u_taylor_mean

- Keywords Area
- method
- local_reliability
- mpp_search
- u_taylor_mean

Form Taylor series approximation in ”u-space” at variable means

Topics
This keyword is related to the topics:
- reliability_methods
6.2. METHOD

Specification
Alias: none
Argument(s): none

Description
This mpp_search option performs a single Taylor series approximation in the transformed space of the uncertain variables ("u-space") centered at the uncertain variable means. This option is commonly known as the Advanced Mean Value (AMV) method, but is performed in u-space instead of x-space.

x_taylor_mpp
- Keywords Area
- method
- local_reliability
- mpp_search
- x_taylor_mpp
  X-space Taylor series approximation with iterative updates

Topics
This keyword is related to the topics:
- reliability_methods

Specification
Alias: none
Argument(s): none

Description
This mpp_search option starts with an x-space Taylor series at the uncertain variable means, but iteratively updates the Taylor series approximation at each MPP prediction until the MPP converges. This option is commonly known as the AMV+ method.

u_taylor_mpp
- Keywords Area
- method
- local_reliability
- mpp_search
- u_taylor_mpp
  U-space Taylor series approximation with iterative updates
Topics
This keyword is related to the topics:

- reliability_methods

Specification
Alias: none
Argument(s): none

Description
This mpp_search option starts with a u-space Taylor series at the uncertain variable means, and iteratively updates the Taylor series approximation at each MPP prediction until the MPP converges. This option is commonly known as the AMV+ method and is identify to x_taylor_mpp except that it is performed in u-space.

x_two_point

- Keywords Area
- method
- local_reliability
- mpp_search
- x_two_point

Predict MPP using Two-point Adaptive Nonlinear Approximation in "x-space"

Topics
This keyword is related to the topics:

- reliability_methods

Specification
Alias: none
Argument(s): none

Description
This mpp_search option uses an x-space Taylor series approximation at the uncertain variable means for the initial MPP prediction, then utilizes the Two-point Adaptive Nonlinear Approximation (TANA) outlined in [Xu98 "Xu and Grandhi, 1998"] for all subsequent MPP predictions.
6.2. METHOD

u_two_point

- Keywords Area
- method
- local_reliability
- mpp_search
- u_two_point

Predict MPP using Two-point Adaptive Nonlinear Approximation in “u-space”

Topics

This keyword is related to the topics:

- reliability_methods

Specification

Alias: none
Argument(s): none

Description

This mpp_search option is identical to x_two_point, but it performs the Two-point Adaptive Nonlinear Approximation (TANA) in u-space instead of x-space.

no_approx

- Keywords Area
- method
- local_reliability
- mpp_search
- no_approx

Perform MPP search on original response functions (use no approximation)

Topics

This keyword is related to the topics:

- reliability_methods

Specification

Alias: none
Argument(s): none
Description

This mpp_search option performs the MPP search on the original response functions without the use of any approximations. Note that the use of the no_approx MPP search with first-order probability integration results in the traditional reliability method called FORM (First-Order Reliability Method). Similarly, the use of no_approx with second-order probability integration results in SORM (Second-Order Reliability Method).

\textbf{sqp}

- Keywords Area
- method
- local_reliability
- mpp_search
- sqp

Uses a sequential quadratic programming method for underlying optimization

Specification

\textbf{Alias:} none
\textbf{Argument(s):} none
\textbf{Default:} sqp

Description

Many uncertainty quantification methods solve a constrained optimization problem under the hood. The \texttt{sqp} keyword directs Dakota to use a sequential quadratic programming method to solve that problem. A sequential quadratic programming solves a sequence of linearly constrained quadratic optimization problems to arrive at the solution to the optimization problem.

\textbf{nip}

- Keywords Area
- method
- local_reliability
- mpp_search
- nip

Uses a nonlinear interior point method for underlying optimization

Specification

\textbf{Alias:} none
\textbf{Argument(s):} none
\textbf{Default:} sqp
6.2. METHOD

Description

Many uncertainty quantification methods solve a constrained optimization problem under the hood. The nip keyword directs Dakota to use a nonlinear interior point to solve that problem. A nonlinear interior point method traverses the interior of the feasible region to arrive at the solution to the optimization problem.

integration

- Keywords Area
- method
- local_reliability
- mpp_search
- integration

Integration approach

Topics

This keyword is related to the topics:

- reliability_methods

Specification

Alias: none

Argument(s): none

Default: First-order integration

<table>
<thead>
<tr>
<th>Required/-Optional Required (Choose One)</th>
<th>Description of Group 1</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>first_order</strong></td>
<td></td>
<td>First-order integration scheme</td>
</tr>
<tr>
<td><strong>second_order</strong></td>
<td></td>
<td>Second-order integration scheme</td>
</tr>
<tr>
<td><strong>probability_refinement</strong></td>
<td></td>
<td>Allow refinement of probability and generalized reliability results using importance sampling</td>
</tr>
</tbody>
</table>

Description

This keyword controls how the probabilities at the MPP are computed: integration is followed by either first_order or second_order, indicating the order of the probability integration.
first_order

- Keywords Area
- method
- local_reliability
- mpp_search
- integration
- first_order

First-order integration scheme

Topics

This keyword is related to the topics:

- reliability_methods

Specification

Alias: none
Argument(s): none

Description

First-order integration in local reliability methods uses the minimum Euclidean distance from the origin to the most probable point (MPP) in transformed space to compute the probability of failure. This distance, commonly called the reliability index Beta, is used to calculate the probability of failure by calculating the standard normal cumulative distribution function at -Beta.

second_order

- Keywords Area
- method
- local_reliability
- mpp_search
- integration
- second_order

Second-order integration scheme

Topics

This keyword is related to the topics:

- reliability_methods
6.2. METHOD

Specification

Alias: none
Argument(s): none

Description

Second-order integration in local reliability methods modifies the first-order integration approach to apply a curvature correction. This correction is based on the formulation of [Hoh88 "Hohenbichler and Rackwitz, 1988"].

**probability_refinement**

- **Keywords Area**
- **method**
- **local_reliability**
- **mpp_search**
- **integration**
- **probability_refinement**

Allow refinement of probability and generalized reliability results using importance sampling.

Topics

This keyword is related to the topics:

- **reliability_methods**

Specification

Alias: sample_refinement
Argument(s): none

| Required/- | Description of Group | Dakota Keyword | Dakota Keyword Description |
| Optional | | import | Description |
| **Required(Choose One)** | Group 1 | adapt_import | Importance sampling option |
| | | mm_adapt_import | Sampling option |
| **Optional** | | refinement_-samples | Number of samples used to refine a probability estimate or sampling design. |
CHAPTER 6. KEYWORDS AREA

<table>
<thead>
<tr>
<th>Optional</th>
<th>seed</th>
<th>Seed of the random number generator</th>
</tr>
</thead>
</table>

**Description**

The `probability_refinement` allows refinement of probability and generalized reliability results using importance sampling. If one specifies `probability_refinement`, there are some additional options. One can specify which type of importance sampling to use (`import`, `adapt_import`, or `mm_adapt_import`). Additionally, one can specify the number of refinement samples to use with `refinement_samples` and the seed to use with `seed`.

The `probability_refinement` density reweighting accounts originally was developed based on Gaussian distributions. It now accounts for additional non-Gaussian cases.

**import**

- Keywords Area
- method
- local_reliability
- mpp_search
- integration
- probability_refinement
- import

Sampling option

**Specification**

Alias: none

Argument(s): none

**Description**

`import` centers a sampling density at one of the initial LHS samples identified in the failure region. It then generates the importance samples, weights them by their probability of occurrence given the original density, and calculates the required probability (CDF or CCDF level).

**adapt_import**

- Keywords Area
- method
- local_reliability
- mpp_search
- integration
6.2. METHOD

- probability_refinement
- adapt_import

Importance sampling option

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

adapt_import centers a sampling density at one of the initial LHS samples identified in the failure region. It then generates the importance samples, weights them by their probability of occurrence given the original density, and calculates the required probability (CDF or CCDF level). This continues iteratively until the failure probability estimate converges.

**mm_adapt_import**

- **Keywords Area**
- method
- local_reliability
- mpp_search
- integration
- probability_refinement
- mm_adapt_import

Sampling option

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

mm_adapt_import starts with all of the samples located in the failure region to build a multimodal sampling density. First, it uses a small number of samples around each of the initial samples in the failure region. Note that these samples are allocated to the different points based on their relative probabilities of occurrence: more probable points get more samples. This early part of the approach is done to search for “representative” points. Once these are located, the multimodal sampling density is set and then mm_adapt_import proceeds similarly to adapt_import (sample until convergence).
refinement_samples

- Keywords Area
- method
- local_reliability
- mpp_search
- integration
- probability_refinement
- refinement_samples

Number of samples used to refine a probability estimate or sampling design.

**Specification**

**Alias:** none

**Argument(s):** INTEGERLIST

**Description**

Probability estimate: Specify the (scalar) number of samples used to improve a probability estimate. If using uni-modal sampling all samples are assigned to the sampling center. If using multi-modal sampling the samples are split between multiple samples according to some internally computed weights.

Sampling design: Specify one or a sequence of refinement samples to augment the initial_samples in a sampling design.

seed

- Keywords Area
- method
- local_reliability
- mpp_search
- integration
- probability_refinement
- seed

Seed of the random number generator

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** system-generated (non-repeatable)
6.2. METHOD

Description

The random seed control provides a mechanism for making a stochastic method repeatable. That is, the use of the same random seed in identical studies will generate identical results.

Default Behavior
If not specified, the seed is randomly generated.

Expected Output
If seed is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

Usage Tips
If a stochastic study was run without seed specified, and the user later wishes to repeat the study using the same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen. That value can then be added to the Dakota input file.

Examples

method
  sampling
    sample_type lhs
    samples = 10
    seed = 15347

response_levels

  • Keywords Area
  • method
  • local_reliability
  • response_levels

Values at which to estimate desired statistics for each response

Specification

Alias: none

Argument(s): REALLIST

Default: No CDF/CCDF probabilities/reliabilities to compute

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword</th>
</tr>
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<tbody>
<tr>
<td>Optional</td>
<td>Group</td>
<td>num_response_</td>
<td>Description</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>_levels</td>
<td>Number of values at which to estimate desired statistics for each response</td>
</tr>
</tbody>
</table>
### Description
The `response_levels` specification provides the target response values for which to compute probabilities, reliabilities, or generalized reliabilities (forward mapping).

**Default Behavior**
If `response_levels` are not specified, no statistics will be computed. If they are, probabilities will be computed by default.

**Expected Outputs**
If `response_levels` are specified, Dakota will create two tables in the standard output: a Probability Density function (PDF) histogram and a Cumulative Distribution Function (CDF) table. The PDF histogram has the lower and upper endpoints of each bin and the corresponding density of that bin. Note that the PDF histogram has bins defined by the `probability_levels` and/or `response_levels` in the Dakota input file. If there are not very many levels, the histogram will be coarse. Dakota does not do anything to optimize the bin size or spacing. The CDF table has the list of response levels and the corresponding probability that the response value is less than or equal to each response level threshold.

**Usage Tips**
The `num_response_levels` is used to specify which arguments of the `response_level` correspond to which response.

### Examples
For example, specifying a `response_level` of 52.3 followed with `compute probabilities` will result in the calculation of the probability that the response value is less than or equal to 52.3, given the uncertain distributions on the inputs.

For an example with multiple responses, the following specification

```plaintext
response_levels = 1. 2 .1 .2 .3 .4 10. 20. 30.
num_response_levels = 2 4 3
```

would assign the first two response levels (1., 2.) to response function 1, the next four response levels (.1, .2, .3, .4) to response function 2, and the final three response levels (10., 20., 30.) to response function 3. If the `num_response_levels` key were omitted from this example, then the response levels would be evenly distributed among the response functions (three levels each in this case).

The Dakota input file below specifies a sampling method with response levels of interest.

```plaintext
method,
  sampling,
  samples = 100 seed = 1
  complementary distribution
  response_levels = 3.6e+11 4.0e+11 4.4e+11
                   6.0e+04 6.5e+04 7.0e+04
                   3.5e+05 4.0e+05 4.5e+05
variables,
  normal_uncertain = 2
  means = 248.89, 593.33
  std_deviations = 12.4, 29.7
  descriptors = 'TF1n' 'TF2n'
```
uniform_uncertain = 2
  lower_bounds = 199.3, 474.63
  upper_bounds = 298.5, 712.
  descriptors = 'TF1u' 'TF2u'
weibull_uncertain = 2
  alphas = 12., 30.
  betas = 250., 590.
  descriptors = 'TF1w' 'TF2w'
histogram_bin_uncertain = 2
  num_pairs = 3 4
  abscissas = 5 8 10 .1 .2 .3 .4
  counts = 17 21 0 12 24 12 0
  descriptors = 'TF1h' 'TF2h'
interface,
system asynch evaluation_concurrency = 5
  analysis_driver = 'text_book'
responses,
  response_functions = 3
  no_gradients
  no_hessians

Given the above Dakota input file, the following excerpt from the output shows the PDF and CCDF generated. Note that the bounds on the bins of the PDF are the response values specified in the input file. The probability levels corresponding to those response values are shown in the CCDF.

Probability Density Function (PDF) histograms for each response function:
PDF for response_fn_1:
<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.7604749078e+11</td>
<td>3.6000000000e+11</td>
<td>5.3601733194e-12</td>
</tr>
<tr>
<td>3.6000000000e+11</td>
<td>4.0000000000e+11</td>
<td>4.2500000000e-12</td>
</tr>
<tr>
<td>4.0000000000e+11</td>
<td>4.4000000000e+11</td>
<td>3.7500000000e-12</td>
</tr>
<tr>
<td>4.4000000000e+11</td>
<td>5.4196114379e+11</td>
<td>2.2557612778e-12</td>
</tr>
</tbody>
</table>
PDF for response_fn_2:
<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.6431154744e+04</td>
<td>6.0000000000e+04</td>
<td>2.8742313192e-05</td>
</tr>
<tr>
<td>6.0000000000e+04</td>
<td>6.5000000000e+04</td>
<td>6.4000000000e-05</td>
</tr>
<tr>
<td>6.5000000000e+04</td>
<td>7.0000000000e+04</td>
<td>4.0000000000e-05</td>
</tr>
<tr>
<td>7.0000000000e+04</td>
<td>7.8702465755e+04</td>
<td>1.0341896485e-05</td>
</tr>
</tbody>
</table>
PDF for response_fn_3:
<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.3796737090e+05</td>
<td>3.5000000000e+05</td>
<td>4.2844660868e-06</td>
</tr>
<tr>
<td>3.5000000000e+05</td>
<td>4.0000000000e+05</td>
<td>8.6000000000e-06</td>
</tr>
<tr>
<td>4.0000000000e+05</td>
<td>4.5000000000e+05</td>
<td>1.8000000000e-06</td>
</tr>
</tbody>
</table>

Complementary Cumulative Distribution Function (CCDF) for response_fn_1:
<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.6000000000e+11</td>
<td>5.5000000000e-01</td>
<td>2.3000000000e-01</td>
<td></td>
</tr>
<tr>
<td>4.0000000000e+11</td>
<td>3.8000000000e-01</td>
<td>3.8000000000e-01</td>
<td></td>
</tr>
</tbody>
</table>
Complementary Cumulative Distribution Function (CCDF) for response_fn_2:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.0000000000e+04</td>
<td>6.1000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6.5000000000e+04</td>
<td>2.9000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7.0000000000e+04</td>
<td>9.0000000000e-02</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Complementary Cumulative Distribution Function (CCDF) for response_fn_3:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.5000000000e+05</td>
<td>5.2000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.0000000000e+05</td>
<td>9.0000000000e-02</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.5000000000e+05</td>
<td>0.0000000000e+00</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Theory

Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.

In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

A forward mapping involves computing the belief and plausibility probability level for a specified response level.

num_response_levels

- Keywords Area
- method
- local_reliability
- response_levels
- num_response_levels

Number of values at which to estimate desired statistics for each response

Specification

Alias: none

Argument(s): INTEGERLIST

Default: response_levels evenly distributed among response functions

Description

The num_response_levels keyword allows the user to specify the number of response values, for each response, at which estimated statistics are of interest. Statistics that can be computed are probabilities and reliabilities, both according to either a cumulative distribution function or a complementary cumulative distribution function.

Default Behavior

If num_response_levels is not specified, the response_levels will be evenly distributed among the responses.

Expected Outputs
6.2. METHOD

The specific output will be determined by the type of statistics that are specified. In a general sense, the output will be a list of response level-statistic pairs that show the estimated value of the desired statistic for each response level specified.

Examples

```plaintext
method
  sampling
    samples = 100
    seed = 34785
    num_response_levels = 1 1 1
    response_levels = 0.5 0.5 0.5

compute

  - Keywords Area
  - method
  - local_reliability
  - response_levels
  - compute

Selection of statistics to compute at each response level

Specification

Alias: none
Argument(s): none
Default: probabilities

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Optional</th>
<th>Required/(Choose One)</th>
<th>Description of Group</th>
<th>Dakota Keyword Description</th>
</tr>
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<tbody>
<tr>
<td></td>
<td></td>
<td>Group 1</td>
<td>probabilities</td>
<td>Reliability probabilities</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>reliabilities</td>
<td>Computes reliabilities associated with response levels</td>
</tr>
</tbody>
</table>
CHAPTER 6. KEYWORDS AREA

<table>
<thead>
<tr>
<th>Optional</th>
<th>system</th>
<th>gen_reliabilities</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Computes generalized reliabilities associated with response levels</td>
</tr>
</tbody>
</table>

**Description**

The `compute` keyword is used to select which forward statistical mapping is calculated at each response level.

**Default Behavior**

If `response_levels` is not specified, no statistics are computed. If `response_levels` is specified but `compute` is not, probabilities will be computed by default. If both `response_levels` and `compute` are specified, then one of the following must be specified: `probabilities`, `reliabilities`, or `gen_reliabilities`.

**Expected Output**

The type of statistics specified by `compute` will be reported for each response level.

**Usage Tips**

CDF/CCDF probabilities are calculated for specified response levels using a simple binning approach.

CDF/CCDF reliabilities are calculated for specified response levels by computing the number of sample standard deviations separating the sample mean from the response level.

**Examples**

```method
sampling
  sample_type random
  samples = 100 seed = 1
  complementary distribution
  response_levels = 3.6e+11 4.0e+11 4.4e+11
                  6.0e+04 6.5e+04 7.0e+04
                  3.5e+05 4.0e+05 4.5e+05
  compute reliabilities

probabilities
```

- **Keywords Area**
- **method**
- **local_reliability**
- **response_levels**
- **compute**
- **probabilities**

Computes probabilities associated with response levels
6.2. METHOD

Specification

Alias: none
  Argument(s): none

Description

The probabilities keyword directs Dakota to compute the probability that the model response will be below (cumulative) or above (complementary cumulative) a specified response value. This is done for every response level designated for each response.

Default Behavior

If response_levels is specified, the probabilities are computed by default. To explicitly specify it in the Dakota input file, though, the probabilities keyword should be specified in conjunction with the compute keyword.

Expected Outputs

The Dakota output is a set of response level-probability pairs that give the probability that the model response will be below or above the corresponding response level, depending on the distribution defined.

Examples

```
method
  sampling
    sample_type random
    samples = 100 seed = 1
  complementary distribution
    response_levels = 3.6e+11 4.0e+11 4.4e+11
                   6.0e+04 6.5e+04 7.0e+04
                   3.5e+05 4.0e+05 4.5e+05
    compute probabilities
```

reliabilities

- Keywords Area
- method
- local_reliability
- response_levels
- compute
- reliabilities

Computes reliabilities associated with response levels

Specification

Alias: none
  Argument(s): none
Description

The **reliabilities** keyword directs Dakota to compute reliabilities according to the specified distribution for a specified response value. This is done for every response level designated for each response.

**Default Behavior**

If **response_levels** is specified, the reliabilities are not computed by default. To change this behavior, the **reliabilities** keyword should be specified in conjunction with the **compute** keyword.

**Expected Outputs**

The Dakota output is a set of response level-reliability pairs according to the distribution defined.

Examples

```plaintext
method sampling
  sample_type random
  samples = 100 seed = 1
  complementary distribution
  response_levels = 3.6e+11 4.0e+11 4.4e+11
                   6.0e+04 6.5e+04 7.0e+04
                   3.5e+05 4.0e+05 4.5e+05
  compute reliabilities

gen_reliabilities

  Keywords Area
  method
  local_reliability
  response_levels
  compute
  gen_reliabilities
```

Computes generalized reliabilities associated with response levels.

Specification

**Alias:** none

**Argument(s):** none

Description

The **gen_reliabilities** keyword directs Dakota to compute generalized reliabilities according to the specified distribution for a specified response value. This is done for every response level designated for each response.

**Default Behavior**

If **response_levels** is specified, the generalized reliabilities are not computed by default. To change this behavior, the **gen_reliabilities** keyword should be specified in conjunction with the **compute** keyword.

**Expected Outputs**

The Dakota output is a set of response level-generalized reliability pairs according to the distribution defined.
6.2. **METHOD**

Examples

```plaintext
method
  sampling
    sample_type random
    samples = 100 seed = 1
    complementary distribution
    response_levels = 3.6e+11 4.0e+11 4.4e+11
                     6.0e+04 6.5e+04 7.0e+04
                     3.5e+05 4.0e+05 4.5e+05
    compute gen_reliabilities
```

**system**

- **Keywords Area**
- **method**
- **local_reliability**
- **response_levels**
- **compute**
- **system**

Compute system reliability (series or parallel)

**Specification**

**Alias:** none

**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Optional</th>
<th>Description of</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Choose One</td>
<td></td>
<td>Group 1</td>
<td>series</td>
<td>Aggregate response statistics assuming a series system</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>parallel</td>
<td>Aggregate response statistics assuming a parallel system</td>
</tr>
</tbody>
</table>

**Description**

With the system probability/reliability option, statistics for specified `response_levels` are calculated and reported assuming the response functions combine either in series or parallel to produce a total system response.

For a series system, the system fails when any one component (response) fails. The probability of failure is the complement of the product of the individual response success probabilities.

For a parallel system, the system fails only when all components (responses) fail. The probability of failure is the product of the individual response failure probabilities.
series

- Keywords Area
- method
- local_reliability
- response_levels
- compute
- system
- series

Aggregate response statistics assuming a series system

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

See parent keyword `system` for description.

parallel

- Keywords Area
- method
- local_reliability
- response_levels
- compute
- system
- parallel

Aggregate response statistics assuming a parallel system

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

See parent keyword `system` for description.
6.2. METHOD

reliability_levels

- Keywords Area
- method
- local_reliability
- reliability_levels

Specify reliability levels at which the response values will be estimated

**Specification**

**Alias:** none

**Argument(s):** REALLIST

**Default:** No CDF/CCDF response levels to compute

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>num_reliability_levels</td>
<td></td>
<td></td>
<td>Specify which reliability_levels correspond to which response</td>
</tr>
</tbody>
</table>

**Description**

Response levels are calculated for specified CDF/CCDF reliabilities by projecting out the prescribed number of sample standard deviations from the sample mean.

**Theory**

Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.

In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

An inverse mapping involves computing the belief and plausibility response level for either a specified probability level or a specified generalized reliability level (two results for each level mapping in the evidence-based epistemic case, instead of the one result for each level mapping in the aleatory case).

num_reliability_levels

- Keywords Area
- method
- local_reliability
- reliability_levels
- num_reliability_levels

Specify which reliability_levels correspond to which response
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none
Argument(s): INTEGERLIST
Default: reliability_levels evenly distributed among response functions

Description

See parent page

max_iterations

- Keywords Area
- method
- local_reliability
- max_iterations

Number of iterations allowed for optimizers and adaptive UQ methods

Topics

This keyword is related to the topics:

- methodIndependent_controls

Specification

Alias: none
Argument(s): INTEGER
Default: 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence} / efficient\_global: 25*n)

Description

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed max_iterations iterations. See also max_function_evaluations.

Default Behavior

Default value is 100.

convergence_tolerance

- Keywords Area
- method
- local_reliability
- convergence_tolerance

Stopping criterion based on convergence of the objective function or statistics
6.2. METHOD

Topics
This keyword is related to the topics:

- method
- independent_controls

Specification
Alias: none
Argument(s): REAL
Default: 1.e-4

Description
The `convergence_tolerance` specification provides a real value for controlling the termination of iteration. For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by convergence_tolerance, then this convergence criterion is satisfied on the current iteration.

Therefore, permissible values are between 0 and 1, non-inclusive.

Behavior Varies by Package/Library
This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- DOT: must be satisfied for two consecutive iterations
- NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of convergence_tolerance approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., convergence_tolerance = 1.e-6 will result in approximately six digits of accuracy in the final objective function).
- NL2SOL: See nl2sol

final_moments

- Keywords Area
- method
- local_reliability
- final_moments

Output moments of the specified type and include them within the set of final statistics.
**Specification**

*Alias*: none

*Argument(s)*: none

*Default*: standard
### 6.2. METHOD

<table>
<thead>
<tr>
<th>Required/-Optional Required (Choose One)</th>
<th>Description of Group objective formulation (Group 1)</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>none</td>
<td>Omit moments from the set of final statistics.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>standard</td>
<td>Output standardized moments and include them within the set of final statistics.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>central</td>
<td>Output central moments and include them within the set of final statistics.</td>
</tr>
</tbody>
</table>

**Description**

When performing a nested study that may employ moment statistics on the inner loop, it can be desirable to control the type of these moments. The `final_moments` specification supports options of `none`, `standard` (default), or `central`, corresponding to omission of moments, standardized moments (mean, standard deviation, skewness, and excess kurtosis), or central moments (mean, variance, 3rd central, and 4th central).

The presence or omission of moment results in the final statistics influences the outer level mappings in the case of a nested study. For example, `final_moments none` can allow for a more compact specification of primary and/or secondary response mappings.

**Examples**

The following method specification overrides the default to print `central` moments and include them in the set of final statistics.

```plaintext
method,
sampling
  samples = 50 seed = 1234
  response_levels = 3.6e+11 1.2e+05 3.5e+05
  final_moments central

Overriding the default to `none` as follows:

```plaintext
method,
sampling
  samples = 50 seed = 1234
  response_levels = 3.6e+11 1.2e+05 3.5e+05
  final_moments none

allows associated nested model mappings to be simplified from:

```plaintext
model
  nested
    sub_method_pointer = 'UQ'
    primary_response_mapping = 0. 0. 1. 0. 0. 1. 0. 0. 0.
    secondary_response_mapping = 0. 0. 0. 0. 0. 0. 0. 0. 1.
```
to a more compact version focused only on the response level mappings (two leading zeros per response function for moment mappings have been removed):

```plaintext
model
  nested
    sub_method_pointer = 'UQ'
    primary_response_mapping = 1. 1. 0.
    secondary_response_mapping = 0. 0. 1.

none

• Keywords Area
• method
• local_reliability
• final_moments
• none

Omit moments from the set of final statistics.

Specification

Alias: none
  Argument(s): none

Description

The omission of moment results from the final statistics can allow for a more compact definition of primary and/or secondary response mappings within a nested model specification.

Examples

method,
  sampling
    samples = 50 seed = 1234
    response_levels = 3.6e+11 1.2e+05 3.5e+05
    final_moments none

standard

• Keywords Area
• method
• local_reliability
• final_moments
• standard

Output standardized moments and include them within the set of final statistics.
6.2. **METHOD**

**Specification**

*Alias:* none

*Argument(s):* none

**Description**

Output standardized moments (mean, standard deviation, skewness, and excess kurtosis) and include the first two within the set of final statistics to be used at a higher level (e.g., optimization under uncertainty, mixed aleatory-epistemic UQ). This inclusion of moment results affects the primary and/or secondary response mappings in a nested model specification.

**Examples**

The following method specification overrides the default to print central moments and include them in the set of final statistics.

```plaintext
method, sampling
  samples = 50 seed = 1234
  response_levels = 3.6e+11 1.2e+05 3.5e+05
  final_moments standard
```

**central**

- **Keywords Area**
- **method**
- **local_reliability**
- **final_moments**
- **central**

Output central moments and include them within the set of final statistics.

**Specification**

*Alias:* none

*Argument(s):* none

**Description**

Output central moments (mean, variance, 3rd central, and 4th central) and include the first two within the set of final statistics to be used at a higher level (e.g., optimization under uncertainty, mixed aleatory-epistemic UQ). This inclusion of moment results affects the primary and/or secondary response mappings in a nested model specification.
Examples
The following method specification overrides the default to print central moments and include them in the set of final statistics.

```plaintext
method,
  sampling
    samples = 50 seed = 1234
    response_levels = 3.6e+11 1.2e+05 3.5e+05
    final_moments central
```

distribution
- Keywords Area
- method
- local_reliability
- distribution

Selection of cumulative or complementary cumulative functions

Specification
Alias: none
Argument(s): none
Default: cumulative (CDF)

<table>
<thead>
<tr>
<th>Required/-Optional Required</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(Choose One)</td>
<td></td>
<td>complementary</td>
<td>Computes statistics according to complementary cumulative functions</td>
</tr>
</tbody>
</table>

Description
The `distribution` keyword allows the user to select between a cumulative distribution/belief/plausibility function and a complementary cumulative distribution/belief/plausibility function. This choice affects how probabilities and reliability indices are reported.

**Default Behavior**
If the `distribution` keyword is present, it must be accompanied by either `cumulative` or `complementary`. Otherwise, a cumulative distribution will be used by default.

**Expected Outputs**
Output will be a set of model response-probability pairs determined according to the choice of distribution. The choice of distribution also defines the sign of the reliability or generalized reliability indices.
6.2. METHOD

Examples

```plaintext
method sampling
  sample_type lhs
  samples = 10
  distribution cumulative
```

cumulative

- **Keywords Area**
- **method**
- **local_reliability**
- **distribution**
- **cumulative**

Computes statistics according to cumulative functions

Specification

**Alias:** none

**Argument(s):** none

Description

Statistics on model responses will be computed according to a cumulative distribution/belief/plausibility function.

**Default Behavior**

By default, a cumulative distribution/belief/plausibility function will be used. To explicitly specify it in the Dakota input file, however, the `cumulative` keyword must be appear in conjunction with the `distribution` keyword.

**Expected Outputs**

Output will be a set of model response-probability pairs determined according to a cumulative distribution/belief/plausibility function. The probabilities reported are the probabilities that the model response falls below given response thresholds.

Examples

```plaintext
method sampling
  sample_type lhs
  samples = 10
  distribution cumulative
```

complementary

- **Keywords Area**
- **method**
- **local_reliability**
- **distribution**
• complementary

Computes statistics according to complementary cumulative functions

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

Statistics on model responses will be computed according to a complementary cumulative distribution/belief/plausibility function.

**Default Behavior**

By default, a complementary cumulative distribution/belief/plausibility function will not be used. To change that behavior, the complementary keyword must be appear in conjunction with the distribution keyword.

**Expected Outputs**

Output will be a set of model response-probability pairs determined according to a complementary cumulative distribution/belief/plausibility function. The probabilities reported are the probabilities that the model response falls above given response thresholds.

**Examples**

```dakota
method
  sampling
    sample_type lhs
    samples = 10
    distribution complementary
```

**probability_levels**

• Keywords Area

• method

• local_reliability

• probability_levels

Specify probability levels at which to estimate the corresponding response value

**Specification**

**Alias:** none

**Argument(s):** REALLIST

**Default:** No CDF/CCDF response levels to compute
6.2. METHOD

<table>
<thead>
<tr>
<th>Optional</th>
<th>num_probability_levels</th>
<th>Specify which probability_levels correspond to which response</th>
</tr>
</thead>
</table>

**Description**

Response levels are calculated for specified CDF/CCDF probabilities by indexing into a sorted samples array (the response levels computed are not interpolated and will correspond to one of the sampled values).

**Expected Output**

If `probability_levels` are specified, Dakota will create two tables in the standard output: a Probability Density function (PDF) histogram and a Cumulative Distribution Function (CDF) table. The PDF histogram has the lower and upper endpoints of each bin and the corresponding density of that bin. Note that the PDF histogram has bins defined by the `probability_levels` and/or `response_levels` in the Dakota input file. If there are not very many levels, the histogram will be coarse. Dakota does not do anything to optimize the bin size or spacing. The CDF table has the list of response levels and the corresponding probability that the response value is less than or equal to each response level threshold.

**Examples**

The Dakota input file below specifies a sampling method with probability levels of interest.

```plaintext
method, sampling,
  samples = 100 seed = 1
complementary distribution
  probability_levels = 1. .66 .33 0.
    1. .8 .5 0.
    1. ..3 .2 0.
variables,
  normal_uncertain = 2
    means = 248.89, 593.33
    std_deviations = 12.4, 29.7
    descriptors = 'TF1n' 'TF2n'
  uniform_uncertain = 2
    lower_bounds = 199.3, 474.63
    upper_bounds = 298.5, 712.
    descriptors = 'TF1u' 'TF2u'
  weibull_uncertain = 2
    alphas = 12., 30.
    betas = 250., 590.
    descriptors = 'TF1w' 'TF2w'
histogram_bin_uncertain = 2
  num_pairs = 3 4
  abscissas = 5 8 10 .1 .2 .3 .4
  counts = 17 21 0 12 24 12 0
  descriptors = 'TF1h' 'TF2h'
histogram_point_uncertain
  real = 1
  num_pairs = 2
  abscissas = 3 4
  counts = 1 1
  descriptors = 'TF3h'
interface,
```
system asynch evaluation_concurrency = 5
analysis_driver = 'text_book'

responses,
response_functions = 3
no_gradients
no_hessians

Given the above Dakota input file, the following excerpt from the output shows the PDF and CCDF generated. Note that the bounds on the bins of the PDF are the response values that correspond the probability levels specified in the input file. Those response values are also shown in the CCDF.

Probability Density Function (PDF) histograms for each response function:
PDF for response_fn_1:
Bin Lower | Bin Upper | Density Value
--------- | --------- | ------------
2.7604749078e+11 | 3.4221494996e+11 | 5.1384774972e-12
3.4221494996e+11 | 4.0634975300e+11 | 5.1454122311e-12
4.0634975300e+11 | 5.419614379e+11 | 2.4334239039e-12
PDF for response_fn_2:
Bin Lower | Bin Upper | Density Value
--------- | --------- | ------------
4.6431154744e+04 | 5.651827725e+04 | 1.9839945149e-05
5.651827725e+04 | 6.1603813790e+04 | 5.8916108390e-05
6.1603813790e+04 | 7.870265755e+04 | 2.9242071306e-05
PDF for response_fn_3:
Bin Lower | Bin Upper | Density Value
--------- | --------- | ------------
2.3796737090e+05 | 3.6997214153e+05 | 5.3028386523e-06
3.6997214153e+05 | 3.810966235e+05 | 9.0600055634e-06
3.810966235e+05 | 4.411498127e+05 | 3.3274925348e-06

Level mappings for each response function:
Complementary Cumulative Distribution Function (CCDF) for response_fn_1:
Response Level | Probability Level | Reliability Index | General Rel Index
--------------- | ----------------- | ----------------- | ------------------
2.7604749078e+11 | 1.0000000000e+00 |                   |                    
3.4221494996e+11 | 6.0000000000e-01 |                   |                    
4.0634975300e+11 | 3.0000000000e-01 |                   |                    
5.419614379e+11 | 0.0000000000e+00 |                   |                    
Complementary Cumulative Distribution Function (CCDF) for response_fn_2:
Response Level | Probability Level | Reliability Index | General Rel Index
--------------- | ----------------- | ----------------- | ------------------
4.6431154744e+04 | 1.0000000000e+00 |                   |                    
5.651827725e+04 | 8.0000000000e-01 |                   |                    
6.1603813790e+04 | 5.0000000000e-01 |                   |                    
7.870265755e+04 | 0.0000000000e+00 |                   |                    
Complementary Cumulative Distribution Function (CCDF) for response_fn_3:
Response Level | Probability Level | Reliability Index | General Rel Index
--------------- | ----------------- | ----------------- | ------------------
2.3796737090e+05 | 1.0000000000e+00 |                   |                    
3.6997214153e+05 | 3.0000000000e-01 |                   |                    
3.810966235e+05 | 2.0000000000e-01 |                   |                    
4.411498127e+05 | 0.0000000000e+00 |                   |                    

Theory

Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.
In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

An inverse mapping involves computing the belief and plausibility response level for either a specified probability level or a specified generalized reliability level (two results for each level mapping in the evidence-based epistemic case, instead of the one result for each level mapping in the aleatory case).

**num_probability_levels**

- **Keywords Area**
- **method**
- **local_reliability**
- **probability_levels**
- **num_probability_levels**

Specify which probability levels correspond to which response

**Specification**

**Alias:** none

**Argument(s):** INTEGERLIST

**Default:** probability_levels evenly distributed among response functions

**Description**

See parent page

**gen_reliability_levels**

- **Keywords Area**
- **method**
- **local_reliability**
- **gen_reliability_levels**

Specify generalized reliability levels at which to estimate the corresponding response value

**Specification**

**Alias:** none

**Argument(s):** REALLIST

**Default:** No CDF/CCDF response levels to compute

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Optional

<table>
<thead>
<tr>
<th>num_gen_reliability_levels</th>
</tr>
</thead>
<tbody>
<tr>
<td>Specify which gen_reliability_levels correspond to which response</td>
</tr>
</tbody>
</table>

**Description**

Response levels are calculated for specified generalized reliabilities by indexing into a sorted samples array (the response levels computed are not interpolated and will correspond to one of the sampled values).

**Theory**

Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.

In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

An inverse mapping involves computing the belief and plausibility response level for either a specified probability level or a specified generalized reliability level (two results for each level mapping in the evidence-based epistemic case, instead of the one result for each level mapping in the aleatory case).

**num_gen_reliability_levels**

- Keywords Area
- method
- local_reliability
- gen_reliability_levels
- num_gen_reliability_levels

Specify which gen_reliability_levels correspond to which response

**Specification**

Alias: none

Argument(s): INTEGERLIST

Default: gen_reliability_levels evenly distributed among response functions

**Description**

See parent page
6.2. METHOD

model_pointer

- Keywords Area
- method
- local_reliability
- model_pointer

Identifier for model block to be used by a method

Topics

This keyword is related to the topics:

- block_pointer

Specification

Alias: none

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)

Description

The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.

Usage Tips

When doing advanced analyses that involve using multiple methods and multiple models, defining a model-pointer for each method is imperative.

See block_pointer for details about pointers.

Examples

environment
  tabular_graphics_data
  method_pointer = 'UQ'

method
  id_method = 'UQ'
  model_pointer = 'SURR'
  sampling,
    samples = 10
  seed = 98765 rng rnum2
  response_levels = 0.1 0.2 0.6
    0.1 0.2 0.6
    0.1 0.2 0.6
  sample_type lhs
distribution cumulative

model
  id_model = 'SURR'
surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
id_method = 'DACE'
model_pointer = 'DACE_M'
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = 'DACE_M'
single
interface_pointer = 'I1'

variables
uniform_uncertain = 2
lower_bounds = 0. 0.
upper_bounds = 1. 1.
descriptors = 'x1' 'x2'

interface
id_interface = 'I1'
system asynch evaluation_concurrency = 5
analysis_driver = 'text_book'

responses
response_functions = 3
no_gradients
no_hessians

6.2.66  global_reliability

- Keywords Area
- method
- global_reliability

Global reliability methods

Topics

This keyword is related to the topics:

- uncertainty_quantification
- reliability_methods

Specification

Alias: nond_global_reliability

Argument(s): none
## 6.2. METHOD

<table>
<thead>
<tr>
<th>Optional</th>
<th>initial_samples</th>
<th>Initial number of samples for sampling-based methods</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required (Choose One)</td>
<td>x_gaussian_process</td>
<td>Create GP surrogate in x-space</td>
</tr>
<tr>
<td>Optional (Choose One)</td>
<td>u_gaussian_process</td>
<td>Create GP surrogate in u-space</td>
</tr>
<tr>
<td>Optional (Choose One)</td>
<td>surfpack</td>
<td>Use the Surfpack version of Gaussian Process surrogates</td>
</tr>
<tr>
<td>Optional</td>
<td>dakota</td>
<td>Select the built in Gaussian Process surrogate</td>
</tr>
<tr>
<td>Optional</td>
<td>import_build-points_file</td>
<td>File containing points you wish to use to build a surrogate</td>
</tr>
<tr>
<td>Optional</td>
<td>export_approx-points_file</td>
<td>Output file for evaluations of a surrogate model</td>
</tr>
<tr>
<td>Optional</td>
<td>use_derivatives</td>
<td>Use derivative data to construct surrogate models</td>
</tr>
<tr>
<td>Optional</td>
<td>seed</td>
<td>Seed of the random number generator</td>
</tr>
<tr>
<td>Optional</td>
<td>rng</td>
<td>Selection of a random number generator</td>
</tr>
<tr>
<td>Optional</td>
<td>response_levels</td>
<td>Values at which to estimate desired statistics for each response</td>
</tr>
</tbody>
</table>
### Description

These methods do not support forward/inverse mappings involving `reliability_levels`, since they never form a reliability index based on distance in u-space. Rather they use a Gaussian process model to form an approximation to the limit state (based either in x-space via the `x_gaussian_process` specification or in u-space via the `u_gaussian_process` specification), followed by probability estimation based on multimodal adaptive importance sampling (see [11]) and [12]). These probability estimates may then be transformed into generalized reliability levels if desired. At this time, inverse reliability analysis (mapping probability or generalized reliability levels into response levels) is not implemented.

The Gaussian process model approximation to the limit state is formed over the aleatory uncertain variables by default, but may be extended to also capture the effect of design, epistemic uncertain, and state variables. If this is desired, one must use the appropriate controls to specify the active variables in the variables specification block. Refer to `variable_support` for additional information on supported variable types.

| Optional | max_iterations | Number of iterations allowed for optimizers and adaptive UQ methods |
| Optional | convergence_tolerance | Stopping criterion based on convergence of the objective function or statistics |
| Optional | distribution | Selection of cumulative or complementary cumulative functions |
| Optional | probability_levels | Specify probability levels at which to estimate the corresponding response value |
| Optional | gen_reliability_levels | Specify generalized reliability levels at which to estimate the corresponding response value |
| Optional | model_pointer | Identifier for model block to be used by a method |
6.2. METHOD

See Also

These keywords may also be of interest:

- adaptive_sampling
- gpais
- local_reliability
- sampling
- importance_sampling
- polynomial_chaos
- stoch_collocation

_initial_samples

- Keywords Area
- method
- global_reliability
- initial_samples

Initial number of samples for sampling-based methods

Specification

**Alias:** none

**Argument(s):** INTEGER

**Default:** \((d+1)(d+2)/2\)

Description

The initial_samples keyword is used to define the number of initial samples (i.e., randomly chosen sets of variable values) at which to execute a model. The initial samples may later be augmented in an iterative process.

**Default Behavior**

By default, Dakota will use the minimum number of samples required by the chosen method.

**Usage Tips**

To obtain linear sensitivities or to construct a linear response surface, at least \(d+1\) samples should be used, where "dim" is the number of variables. For sensitivities to quadratic terms or quadratic response surfaces, at least \((d+1)(d+2)/2\) samples are needed. For uncertainty quantification, we recommend at least \(10 \times \text{dim}\) samples. For variance_based_decomp, we recommend hundreds to thousands of samples. Note that for variance-based_decomp, the number of simulations performed will be \(N \times (d+2)\).

Examples

```plaintext
method sampling
    sample_type random
    initial_samples = 20
    refinement_samples = 5
```
x_gaussian_process

- Keywords Area
- method
- global_reliability
- x_gaussian_process

Create GP surrogate in x-space

Topics

This keyword is related to the topics:
- reliability_methods

Specification

Alias: x_kriging
Argument(s): none

u_gaussian_process

- Keywords Area
- method
- global_reliability
- u_gaussian_process

Create GP surrogate in u-space

Topics

This keyword is related to the topics:
- reliability_methods

Specification

Alias: u_kriging
Argument(s): none

surfpack

- Keywords Area
- method
- global_reliability
- surfpack

Use the Surfpack version of Gaussian Process surrogates
6.2. METHOD

Specification

Alias: none
Argument(s): none

Description

This keyword specifies the use of the Gaussian process that is incorporated in our surface fitting library called Surfpack.

Several user options are available:

1. Optimization methods:
   Maximum Likelihood Estimation (MLE) is used to find the optimal values of the hyper-parameters governing the trend and correlation functions. By default the global optimization method DIRECT is used for MLE, but other options for the optimization method are available. See optimization_method.
   The total number of evaluations of the likelihood function can be controlled using the max_trials keyword followed by a positive integer. Note that the likelihood function does not require running the "truth" model, and is relatively inexpensive to compute.

2. Trend Function:
   The GP models incorporate a parametric trend function whose purpose is to capture large-scale variations. See trend.

3. Correlation Lengths:
   Correlation lengths are usually optimized by Surfpack, however, the user can specify the lengths manually. See correlation_lengths.

4. Ill-conditioning
   One of the major problems in determining the governing values for a Gaussian process or Kriging model is the fact that the correlation matrix can easily become ill-conditioned when there are too many input points close together. Since the predictions from the Gaussian process model involve inverting the correlation matrix, ill-conditioning can lead to poor predictive capability and should be avoided.
   Note that a sufficiently bad sample design could require correlation lengths to be so short that any interpolatory GP model would become inept at extrapolation and interpolation.
   The surfpack model handles ill-conditioning internally by default, but behavior can be modified using

5. Gradient Enhanced Kriging (GEK).
   The use_derivatives keyword will cause the Surfpack GP to be constructed from a combination of function value and gradient information (if available).
   See notes in the Theory section.

Theory

Gradient Enhanced Kriging

Incorporating gradient information will only be beneficial if accurate and inexpensive derivative information is available, and the derivatives are not infinite or nearly so. Here "inexpensive" means that the cost of evaluating a function value plus gradient is comparable to the cost of evaluating only the function value, for example gradients computed by analytical, automatic differentiation, or continuous adjoint techniques. It is not cost effective to use derivatives computed by finite differences. In tests, GEK models built from finite difference derivatives were also
significantly less accurate than those built from analytical derivatives. Note that GEK’s correlation matrix tends to have a significantly worse condition number than Kriging for the same sample design.

This issue was addressed by using a pivoted Cholesky factorization of Kriging’s correlation matrix (which is a small sub-matrix within GEK’s correlation matrix) to rank points by how much unique information they contain. This reordering is then applied to whole points (the function value at a point immediately followed by gradient information at the same point) in GEK’s correlation matrix. A standard non-pivoted Cholesky is then applied to the reordered GEK correlation matrix and a bisection search is used to find the last equation that meets the constraint on the (estimate of) condition number. The cost of performing pivoted Cholesky on Kriging’s correlation matrix is usually negligible compared to the cost of the non-pivoted Cholesky factorization of GEK’s correlation matrix. In tests, it also resulted in more accurate GEK models than when pivoted Cholesky or whole-point-block pivoted Cholesky was performed on GEK’s correlation matrix.

dakota

- Keywords Area
- method
- global_reliability
- dakota

Select the built in Gaussian Process surrogate

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

A second version of GP surrogates was available in prior versions of Dakota. For now, both versions are supported but the dakota version is deprecated and intended to be removed in a future release.

Historically these models were drastically different, but in Dakota 5.1, they became quite similar. They now differ in that the Surfpack GP has a richer set of features/options and tends to be more accurate than the Dakota version. Due to how the Surfpack GP handles ill-conditioned correlation matrices (which significantly contributes to its greater accuracy), the Surfpack GP can be a factor of two or three slower than Dakota’s. As of Dakota 5.2, the Surfpack implementation is the default in all contexts except Bayesian calibration.

More details on the gaussian_process dakota model can be found in[58].

Dakota’s GP deals with ill-conditioning in two ways. First, when it encounters a non-invertible correlation matrix it iteratively increases the size of a “nugget,” but in such cases the resulting approximation smooths rather than interpolates the data. Second, it has a point_selection option (default off) that uses a greedy algorithm to select a well-spaced subset of points prior to the construction of the GP. In this case, the GP will only interpolate the selected subset. Typically, one should not need point selection in trust-region methods because a small number of points are used to develop a surrogate within each trust region. Point selection is most beneficial when constructing with a large number of points, typically more than order one hundred, though this depends on the number of variables and spacing of the sample points.

This differs from the point_selection option of the Dakota GP which initially chooses a well-spaced subset of points and finds the correlation parameters that are most likely for that one subset.
6.2. METHOD

**import_build_points_file**

- **Keywords Area**
- **method**
- **global_reliability**
- **import_build_points_file**

File containing points you wish to use to build a surrogate

**Specification**

**Alias:** import_points_file

**Argument(s):** STRING

**Default:** no point import from a file

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional/Choose One</td>
<td>Tabular Format (Group 1)</td>
<td>annotated</td>
<td>Selects annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>custom_annotated</td>
<td>Selects custom-annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>freeform</td>
<td>Selects freeform file format</td>
</tr>
<tr>
<td>Optional</td>
<td>active_only</td>
<td></td>
<td>Import only active variables from tabular data file</td>
</tr>
</tbody>
</table>

**Description**

The **import_build_points_file** allows the user to specify a file that contains a list of points and truth model responses used to construct a surrogate model. These can be used by all methods that (explicitly, e.g. surrogate-based optimization, or implicitly, e.g. efficient global optimization) operate on a surrogate. In particular, these points and responses are used in place of truth model evaluations to construct the initial surrogate. When used to construct surrogate models or emulators these are often called build points or training data.

**Default Behavior**

By default, methods do not import points from a file.

**Usage Tips**

Dakota parses input files without regard to whitespace, but the **import_build_points_file** must be in one of three formats:

- **annotated** (default)
- **custom_annotated**
- **freeform**
Examples

```bash
method
  polynomial_chaos
    expansion_order = 4
  import_build_points_file = 'dakota_uq_rosenbrock_pce_import.annot.pts.dat'

annotated
  - Keywords Area
  - method
  - global_reliability
  - import_build_points_file
  - annotated

Selects annotated tabular file format
```

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none
  - Argument(s): none
  - Default: annotated format

Description

An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

**Default Behavior**

By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

**Usage Tips**

- To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify custom_annotated_header eval_id

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.
6.2. METHOD

Examples
Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```python
environment
    tabular_data
        tabular_data_file = 'dakota_summary.dat'
annotated

Resulting tabular file:

<table>
<thead>
<tr>
<th>eval_id</th>
<th>interface</th>
<th>x1</th>
<th>x2</th>
<th>obj_fn</th>
<th>nln_ineq_con_1</th>
<th>nln_ineq_con_2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>NO_ID</td>
<td>0.9</td>
<td>1.1</td>
<td>0.0002</td>
<td>0.26</td>
<td>0.76</td>
</tr>
<tr>
<td>2</td>
<td>NO_ID</td>
<td>0.90009</td>
<td>1.1</td>
<td>0.0001996404857</td>
<td>0.2601620081</td>
<td>0.759955</td>
</tr>
<tr>
<td>3</td>
<td>NO_ID</td>
<td>0.89991</td>
<td>1.1</td>
<td>0.0002003604863</td>
<td>0.2598380081</td>
<td>0.760045</td>
</tr>
</tbody>
</table>

... 

custom_annotated

- **Keywords Area**
- **method**
- **global_reliability**
- **import_build_points_file**
- **custom_annotated**

Selects custom-annotated tabular file format

Topics
This keyword is related to the topics:

- **file_formats**

Specification

**Alias:** none

**Argument(s):** none

**Default:** annotated format

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>header</td>
<td>Enable header row in custom-annotated tabular file</td>
</tr>
</tbody>
</table>
Optional \( \text{eval\_id} \) Enable evaluation ID column in custom-annotated tabular file

Optional \( \text{interface\_id} \) Enable interface ID column in custom-annotated tabular file

**Description**

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, \( \text{eval\_id} \) column, and \( \text{interface\_id} \) column appear in the tabular file, thus bridging freeform and (fully) annotated.

**Default Behavior**

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

**Usage Tips**

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

**Examples**

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and \( \text{eval\_id} \) (no \( \text{interface\_id} \)), and data for variables and responses. Input file fragment:

```plaintext
environment
  tabular_data
    tabular_data_file = 'dakota_summary.dat'
    custom_annotated header eval_id
```

Resulting tabular file:

```plaintext
%eval_id  x1  x2  obj_fn  nln_ineq_con_1  nln_ineq_con_2
1 0.9 1.1 0.0002 0.26 0.76
2 0.90009 1.1 0.0001996404857 0.2601620081 0.759955
3 0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...
```

**header**

- Keywords Area
- method
- global_reliability
6.2. METHOD

- import_build_points_file
- custom_annotated
- header

Enable header row in custom-annotated tabular file

**Specification**

**Alias:** none

- **Argument(s):** none
- **Default:** no header

**Description**

See description of parent `custom_annotated`

- `eval_id`
  - **Keywords Area**
  - method
  - global_reliability
  - import_build_points_file
  - custom_annotated
  - `eval_id`

Enable evaluation ID column in custom-annotated tabular file

**Specification**

**Alias:** none

- **Argument(s):** none
- **Default:** no eval_id column

**Description**

See description of parent `custom_annotated`

- `interface_id`
  - **Keywords Area**
  - method
  - global_reliability
  - import_build_points_file
  - custom_annotated
  - `interface_id`

Enable interface ID column in custom-annotated tabular file
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): none

Default: no interface_id column

Description

See description of parent custom_annotated

freeform

- Keywords Area
- method
- global_reliability
- import_build_points_file
- freeform

Selects freeform file format

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none

Argument(s): none

Default: annotated format

Description

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior

The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips

- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
6.2. METHOD

- In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```python
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
freeform

Resulting tabular file:

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>0.9</td>
<td>1.1</td>
<td>0.0002</td>
<td>0.26</td>
<td>0.76</td>
</tr>
<tr>
<td>0.90009</td>
<td>1.1</td>
<td>0.0001996404857</td>
<td>0.2601620081</td>
<td>0.759955</td>
</tr>
<tr>
<td>0.89991</td>
<td>1.1</td>
<td>0.0002003604863</td>
<td>0.2598380081</td>
<td>0.760045</td>
</tr>
</tbody>
</table>

...```

active_only

- Keywords Area
- method
- global_reliability
- import_build_points_file
- active_only

Import only active variables from tabular data file

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none

Argument(s): none

Description

By default, files for tabular data imports are expected to contain columns for all variables, active and inactive. The keyword active_only indicates that the file to import contains only the active variables.

This option should only be used in contexts where the inactive variables have no influence, for example, building a surrogate over active variables, with the state variables held at nominal. It should not be used in more complex nested contexts, where the values of inactive variables are relevant to the function evaluations used to build the surrogate.
export(approx)points(file
  
  **Keywords Area**
  
  **method**
  
  **global_reliability**
  
  **export(approx)points(file**

Output file for evaluations of a surrogate model

**Specification**

**Alias:** export_points_file  
**Argument(s):** STRING  
**Default:** no point export to a file

<table>
<thead>
<tr>
<th>Required/Optional Optional</th>
<th>Description of Group Tabular Format (Group 1)</th>
<th>Dakota Keyword annotated</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>ComboBox: annotated, custom_annotated, freeform</td>
<td>annotated</td>
<td>Selects annotated tabular file format</td>
</tr>
<tr>
<td>custom_annotated</td>
<td></td>
<td></td>
<td>Selects custom-annotated tabular file format</td>
</tr>
<tr>
<td>freeform</td>
<td></td>
<td></td>
<td>Selects freeform file format</td>
</tr>
</tbody>
</table>

**Description**

The `export(approx)points(file` keyword allows the user to specify a file in which the points (input variable values) at which the surrogate model is evaluated and corresponding response values computed by the surrogate model will be written. The response values are the surrogate’s predicted approximation to the truth model responses at those points.

**Usage Tips**

Dakota exports tabular data in one of three formats:

- **annotated** (default)
- **custom_annotated**
- **freeform**

**annotated**

- **Keywords Area**
- **method**
- **global_reliability**
- **export(approx)points(file**
6.2. METHOD

- **annotated**

  Selects annotated tabular file format

**Topics**

This keyword is related to the topics:

- **file_formats**

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** annotated format

**Description**

An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

**Default Behavior**

By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

**Usage Tips**

- To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify custom_annotated header eval_id

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

**Examples**

Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
tabular_data_file = ‘dakota_summary.dat’
annotated
```

**Resulting tabular file:**

```plaintext
%eval_id interface x1 x2 obj_fn nln_ineq_con_1 nln_ineq_con_2
1  NO_ID 0.9 1.1 0.0002 0.26 0.76
2  NO_ID 0.90009 1.1 0.0001996404857 0.2601620081 0.759955
3  NO_ID 0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...```
custom_annotated

- Keywords Area
- method
- global_reliability
- export_approx_points_file
- custom_annotated

Selects custom-annotated tabular file format

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none
Argument(s): none
Default: annotated format

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>header</td>
<td>header</td>
<td>Enable header row in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td>eval_id</td>
<td>eval_id</td>
<td>Enable evaluation ID column in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td>interface_id</td>
<td>interface_id</td>
<td>Enable interface ID column in custom-annotated tabular file</td>
</tr>
</tbody>
</table>

Description

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

Default Behavior

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

Usage Tips
6.2. METHOD

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
  tabular_data_file = 'dakota_summary.dat'
custom_annotated header eval_id
```

Resulting tabular file:

```
%eval_id  x1    x2  obj_fn nln_ineq_con_1 nln_ineq_con_2
1 0.9    1.1  0.0002  0.26   0.76
2 0.90009 1.1 0.001996404857 0.2601620081 0.759955
3 0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...
```

header

- Keywords Area
- method
- global_reliability
- export_approx_points_file
- custom_annotated
- header

Enable header row in custom-annotated tabular file

Specification

Alias: none
Argument(s): none
Default: no header

Description

See description of parent custom_annotated
eval_id
- Keywords Area
- method
- global_reliability
- export_approx_points_file
- custom_annotated
- eval_id

Enable evaluation ID column in custom-annotated tabular file

**Specification**

*Alias:* none

*Argument(s):* none

*Default:* no eval_id column

**Description**

See description of parent custom_annotated

interface_id
- Keywords Area
- method
- global_reliability
- export_approx_points_file
- custom_annotated
- interface_id

Enable interface ID column in custom-annotated tabular file

**Specification**

*Alias:* none

*Argument(s):* none

*Default:* no interface_id column

**Description**

See description of parent custom_annotated
freeform

- Keywords Area
- method
- global_reliability
- export_approx_points_file
- freeform

Selects freeform file format

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none

Argument(s): none

Default: annotated format

Description

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior

The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips

- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.
Examples
Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
  tabular_data_file = 'dakota_summary.dat'
freeform

Resulting tabular file:

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>0.9</td>
<td>1.1</td>
<td>0.0002</td>
<td>0.26</td>
<td>0.76</td>
</tr>
<tr>
<td>0.9009</td>
<td>1.1</td>
<td>0.0001996404857</td>
<td>0.2601620081</td>
<td>0.759955</td>
</tr>
<tr>
<td>0.89991</td>
<td>1.1</td>
<td>0.0002003604863</td>
<td>0.2598380081</td>
<td>0.760045</td>
</tr>
</tbody>
</table>
...
```

use_derivatives

- Keywords Area
- method
- global_reliability
- use_derivatives

Use derivative data to construct surrogate models

Specification

Alias: none

- Argument(s): none
- Default: use function values only

Description

The `use_derivatives` flag specifies that any available derivative information should be used in global approximation builds, for those global surrogate types that support it (currently, polynomial regression and the Surfpack Gaussian process).

However, its use with Surfpack Gaussian process is not recommended.

seed

- Keywords Area
- method
- global_reliability
- seed

Seed of the random number generator

Specification

Alias: none

- Argument(s): INTEGER
- Default: system-generated (non-repeatable)
6.2. METHOD

Description
The random seed control provides a mechanism for making a stochastic method repeatable. That is, the use of the same random seed in identical studies will generate identical results.

Default Behavior
If not specified, the seed is randomly generated.

Expected Output
If seed is specified, a stochastic study will generate identical results when repeated using the same seed value. Otherwise, results are not guaranteed to be the same.

Usage Tips
If a stochastic study was run without seed specified, and the user later wishes to repeat the study using the same seed, the value of the seed used in the original study can be found in the output Dakota prints to the screen. That value can then be added to the Dakota input file.

Examples
```
method
  sampling
    sample_type lhs
    samples = 10
    seed = 15347
```

rng

- Keywords Area
- method
- global_reliability
- rng

Selection of a random number generator

Specification
Alias: none
Argument(s): none
Default: Mersenne twister ( mt19937 )

<table>
<thead>
<tr>
<th>Required/-Optional Required(Choose One)</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Group 1</td>
<td>mt19937</td>
<td>Generates random numbers using the Mersenne twister</td>
</tr>
</tbody>
</table>
The `rng` keyword is used to indicate a choice of random number generator.

**Default Behavior**
If specified, the `rng` keyword must be accompanied by either `rnum2` (pseudo-random numbers) or `mt19937` (random numbers generated by the Mersenne twister). Otherwise, `mt19937`, the Mersenne twister is used by default.

**Usage Tips**
The default is recommended, as the Mersenne twister is a higher quality random number generator.

**Examples**
```plaintext
method
  sampling
    sample_type lhs
    samples = 10
    seed = 98765
    rng rnum2

mt19937
  - Keywords Area
  - method
  - global_reliability
  - rng
  - mt19937

Generates random numbers using the Mersenne twister
```

**Specification**

* Alias: none
  * Argument(s): none

**Description**
The `mt19937` keyword directs Dakota to use the Mersenne twister to generate random numbers. Additional information can be found on wikipedia: [http://en.wikipedia.org/wiki/Mersenne_twister](http://en.wikipedia.org/wiki/Mersenne_twister).

**Default Behavior**
`mt19937` is the default random number generator. To specify it explicitly in the Dakota input file, however, it must be specified in conjunction with the `rng` keyword.

**Usage Tips**
Use of the Mersenne twister random number generator (`mt19937`) is recommended.
6.2. METHOD

Examples

```dakota
method sampling
  sample_type lhs
  samples = 10
  seed = 98765
  rng mt19937
```

`rnum2`

- Keywords Area
- method
- global_reliability
- rng
- rnum2

Generates pseudo-random numbers using the Pecos package

Specification

Alias: none
Argument(s): none

Description

The `rnum2` keyword directs Dakota to use pseudo-random numbers generated by the Pecos package.

**Default Behavior**

`rnum2` is not used by default. To change this behavior, it must be specified in conjunction with the `rng` keyword.

**Usage Tips**

Use of the Mersenne twister random number generator (`mt19937`) is recommended over `rnum2`.

Examples

```dakota
method sampling
  sample_type lhs
  samples = 10
  seed = 98765
  rng rnum2
```

`response_levels`

- Keywords Area
- method
- global_reliability
- response_levels

Values at which to estimate desired statistics for each response
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none  
Argument(s): REALLIST  
Default: No CDF/CCDF probabilities/reliabilities to compute

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>num_response_levels</td>
<td>Number of values at which to estimate desired statistics for each response</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>compute</td>
<td>Selection of statistics to compute at each response level</td>
</tr>
</tbody>
</table>

Description

The `response_levels` specification provides the target response values for which to compute probabilities, reliabilities, or generalized reliabilities (forward mapping).

Default Behavior

If `response_levels` are not specified, no statistics will be computed. If they are, probabilities will be computed by default.

Expected Outputs

If `response_levels` are specified, Dakota will create two tables in the standard output: a Probability Density function (PDF) histogram and a Cumulative Distribution Function (CDF) table. The PDF histogram has the lower and upper endpoints of each bin and the corresponding density of that bin. Note that the PDF histogram has bins defined by the `probability_levels` and/or `response_levels` in the Dakota input file. If there are not very many levels, the histogram will be coarse. Dakota does not do anything to optimize the bin size or spacing. The CDF table has the list of response levels and the corresponding probability that the response value is less than or equal to each response level threshold.

Usage Tips

The `num_response_levels` is used to specify which arguments of the `response_level` correspond to which response.

Examples

For example, specifying a `response_level` of 52.3 followed with `compute probabilities` will result in the calculation of the probability that the response value is less than or equal to 52.3, given the uncertain distributions on the inputs.

For an example with multiple responses, the following specification

```plaintext
response_levels = 1. 2. .1 .2 .3 .4 10. 20. 30.  
num_response_levels = 2 4 3
```

would assign the first two response levels (1., 2.) to response function 1, the next four response levels (.1, .2, .3, .4) to response function 2, and the final three response levels (10., 20., 30.) to response function 3. If the `num_response_levels` key were omitted from this example, then the response levels would be evenly distributed among the response functions (three levels each in this case).
The Dakota input file below specifies a sampling method with response levels of interest.

```
method,
sampling,
samples = 100 seed = 1
complementary distribution
response_levels = 3.6e+11 4.0e+11 4.4e+11
6.0e+04 6.5e+04 7.0e+04
3.5e+05 4.0e+05 4.5e+05
variables,
normal_uncertain = 2
means = 248.89, 593.33
std_deviations = 12.4, 29.7
descriptors = 'TF1n' 'TF2n'
uniform_uncertain = 2
lower_bounds = 199.3, 474.63
upper_bounds = 298.5, 712.
descriptors = 'TF1u' 'TF2u'
weibull_uncertain = 2
alphas = 12., 30.
betas = 250., 590.
descriptors = 'TF1w' 'TF2w'
histogram_bin_uncertain = 2
num_pairs = 3 4
abscissas = 5 8 10 .1 .2 .3 .4
counts = 17 21 0 12 24 12 0
descriptors = 'TF1h' 'TF2h'
histogram_point_uncertain
real = 1
num_pairs = 2
abscissas = 3 4
counts = 1 1
descriptors = 'TF3h'
```

Given the above Dakota input file, the following excerpt from the output shows the PDF and CCDF generated. Note that the bounds on the bins of the PDF are the response values specified in the input file. The probability levels corresponding to those response values are shown in the CCDF.

```
Probability Density Function (PDF) histograms for each response function:
PDF for response_fn_1:
<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.7604749078e+11</td>
<td>3.6000000000e+11</td>
<td>5.3601733194e-12</td>
</tr>
<tr>
<td>3.6000000000e+11</td>
<td>4.0000000000e+11</td>
<td>4.2500000000e-12</td>
</tr>
<tr>
<td>4.0000000000e+11</td>
<td>4.4000000000e+11</td>
<td>3.7500000000e-12</td>
</tr>
<tr>
<td>4.4000000000e+11</td>
<td>5.4196114379e+11</td>
<td>2.2557612778e-12</td>
</tr>
</tbody>
</table>
PDF for response_fn_2:
<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.6431154744e+04</td>
<td>6.0000000000e+04</td>
<td>2.8742313192e-05</td>
</tr>
<tr>
<td>6.0000000000e+04</td>
<td>6.5000000000e+04</td>
<td>6.4000000000e-05</td>
</tr>
<tr>
<td>6.5000000000e+04</td>
<td>7.0000000000e+04</td>
<td>4.0000000000e-05</td>
</tr>
</tbody>
</table>
```
PDF for response_fn_3:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.3796737090e+05</td>
<td>3.5000000000e+05</td>
<td>4.284460868e-06</td>
</tr>
<tr>
<td>3.5000000000e+05</td>
<td>4.0000000000e+05</td>
<td>8.6000000000e-06</td>
</tr>
<tr>
<td>4.0000000000e+05</td>
<td>4.5000000000e+05</td>
<td>1.8000000000e-06</td>
</tr>
</tbody>
</table>

Level mappings for each response function:

Complementary Cumulative Distribution Function (CCDF) for response_fn_1:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.6000000000e+11</td>
<td>5.5000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.0000000000e+11</td>
<td>3.8000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.4000000000e+11</td>
<td>2.3000000000e-01</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Complementary Cumulative Distribution Function (CCDF) for response_fn_2:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.0000000000e+04</td>
<td>6.1000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6.5000000000e+04</td>
<td>2.9000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7.0000000000e+04</td>
<td>9.0000000000e-02</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Complementary Cumulative Distribution Function (CCDF) for response_fn_3:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.5000000000e+05</td>
<td>5.2000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.0000000000e+05</td>
<td>9.0000000000e-02</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.5000000000e+05</td>
<td>0.0000000000e+00</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Theory

Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.

In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

A forward mapping involves computing the belief and plausibility probability level for a specified response level.

num_response_levels

- Keywords Area
- method
- global_reliability
- response_levels
- num_response_levels

Number of values at which to estimate desired statistics for each response

Specification

Alias: none

Argument(s): INTEGERLIST

Default: response_levels evenly distributed among response functions
Description

The `num_response_levels` keyword allows the user to specify the number of response values, for each response, at which estimated statistics are of interest. Statistics that can be computed are probabilities and reliabilities, both according to either a cumulative distribution function or a complementary cumulative distribution function.

**Default Behavior**

If `num_response_levels` is not specified, the response levels will be evenly distributed among the responses.

**Expected Outputs**

The specific output will be determined by the type of statistics that are specified. In a general sense, the output will be a list of response level-statistic pairs that show the estimated value of the desired statistic for each response level specified.

**Examples**

```dakota
method sampling
   samples = 100
   seed = 34785
   num_response_levels = 1 1 1
   response_levels = 0.5 0.5 0.5
compute
```

- **Keywords Area**
- **method**
- **global_reliability**
- **response_levels**
- **compute**

Selection of statistics to compute at each response level

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** probabilities

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>Group 1</td>
<td>probabilities</td>
<td>Description</td>
</tr>
<tr>
<td><strong>Required</strong></td>
<td><strong>Choose</strong> One</td>
<td>Group 1</td>
<td><strong>Statistic</strong></td>
</tr>
</tbody>
</table>

Computes probabilities associated with response levels
### Description

The `compute` keyword is used to select which forward statistical mapping is calculated at each response level.

#### Default Behavior

- If `response_levels` is not specified, no statistics are computed.
- If `response_levels` is specified but `compute` is not, probabilities will be computed by default.
- If both `response_levels` and `compute` are specified, then one of the following must be specified: `probabilities`, `reliabilities`, or `gen_reliabilities`.

#### Expected Output

The type of statistics specified by `compute` will be reported for each response level.

#### Usage Tips

CDF/CCDF probabilities are calculated for specified response levels using a simple binning approach.

CDF/CCDF reliabilities are calculated for specified response levels by computing the number of sample standard deviations separating the sample mean from the response level.

#### Examples

```plaintext
method
  sampling
    sample_type random
    samples = 100 seed = 1
    complementary distribution
    response_levels = 3.6e+11 4.0e+11 4.4e+11
                     6.0e+04 6.5e+04 7.0e+04
                     3.5e+05 4.0e+05 4.5e+05
    compute reliabilities
```

### Table

<table>
<thead>
<tr>
<th>Optional</th>
<th>system</th>
<th>gen_reliabilities</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Computes generalized reliabilities associated with response levels</td>
</tr>
</tbody>
</table>

### Keywords Area

- `method`
- `global_reliability`
- `response_levels`
- `compute`
- `probabilities`

Computes probabilities associated with response levels
6.2. METHOD

Specification

Alias: none
Argument(s): none

Description

The **probabilities** keyword directs Dakota to compute the probability that the model response will be below (cumulative) or above (complementary cumulative) a specified response value. This is done for every response level designated for each response.

**Default Behavior**

If **response_levels** is specified, the probabilities are computed by default. To explicitly specify it in the Dakota input file, though, the **probabilities** keyword should be specified in conjunction with the **compute** keyword.

**Expected Outputs**

The Dakota output is a set of response level-probability pairs that give the probability that the model response will be below or above the corresponding response level, depending on the distribution defined.

Examples

```
method
  sampling
  sample_type random
  samples = 100 seed = 1
  complementary distribution
  response_levels = 3.6e+11 4.0e+11 4.4e+11
                    6.0e+04 6.5e+04 7.0e+04
                    3.5e+05 4.0e+05 4.5e+05
  compute probabilities

gen_reliabilities
```

**Keywords Area**

- **method**
- **global_reliability**
- **response_levels**
- **compute**
- **gen_reliabilities**

Computes generalized reliabilities associated with response levels

Specification

Alias: none
Argument(s): none
**Description**

The `gen_reliabilities` keyword directs Dakota to compute generalized reliabilities according to the specified distribution for a specified response value. This is done for every response level designated for each response.

**Default Behavior**

If `response_levels` is specified, the generalized reliabilities are not computed by default. To change this behavior, the `gen_reliabilities` keyword should be specified in conjunction with the `compute` keyword.

**Expected Outputs**

The Dakota output is a set of response level-generalized reliability pairs according to the distribution defined.

**Examples**

```plaintext
method
  sampling
    sample_type random
    samples = 100 seed = 1
    complementary distribution
    response_levels = 3.6e+11 4.0e+11 4.4e+11
                      6.0e+04 6.5e+04 7.0e+04
                      3.5e+05 4.0e+05 4.5e+05
    compute gen_reliabilities

system
```

- **Keywords Area**
- **method**
- **global_reliability**
- **response_levels**
- **compute**
- **system**

Compute system reliability (series or parallel)

**Specification**

**Alias:** none

**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/Optional Required (Choose One)</th>
<th>Description of Group 1</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>series</td>
<td>Aggregate response statistics assuming a series system</td>
<td></td>
</tr>
</tbody>
</table>
6.2. METHOD

| parallel | Aggregate response statistics assuming a parallel system |

Description

With the system probability/reliability option, statistics for specified response levels are calculated and reported assuming the response functions combine either in series or parallel to produce a total system response.

For a series system, the system fails when any one component (response) fails. The probability of failure is the complement of the product of the individual response success probabilities.

For a parallel system, the system fails only when all components (responses) fail. The probability of failure is the product of the individual response failure probabilities.

series

- Keywords Area
- method
- global_reliability
- response_levels
- compute
- system
- series

Aggregate response statistics assuming a series system

Specification

Alias: none
Argument(s): none

Description

See parent keyword system for description.

parallel

- Keywords Area
- method
- global_reliability
- response_levels
- compute
- system
**parallel**

Aggregate response statistics assuming a parallel system

**Specification**

*Alias*: none

*Argument(s)*: none

**Description**

See parent keyword `system` for description.

**max_iterations**

- Keywords Area
- method
- global_reliability
- max_iterations

Number of iterations allowed for optimizers and adaptive UQ methods

**Topics**

This keyword is related to the topics:

- method_independent Controls

**Specification**

*Alias*: none

*Argument(s)*: INTEGER

*Default*: 100 (exceptions: `fsu_cvt`, local_reliability: 25; global `{reliability, interval_est, evidence}` / `efficient_global`: 25*n)

**Description**

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed `max_iterations` iterations. See also `max_function_evaluations`.

**Default Behavior**

Default value is 100.
6.2. METHOD

convergence_tolerance

- Keywords Area
- method
- global_reliability
- convergence_tolerance

Stopping criterion based on convergence of the objective function or statistics

Topics

This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none

Argument(s): REAL

Default: 1.e-4

Description

The convergence_tolerance specification provides a real value for controlling the termination of iteration.

For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by convergence_tolerance, then this convergence criterion is satisfied on the current iteration.

Therefore, permissible values are between 0 and 1, non-inclusive.

Behavior Varies by Package/Library

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NLSSOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- DOT: must be satisfied for two consecutive iterations

- NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of convergence_tolerance approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., convergence_tolerance = 1.e-6 will result in approximately six digits of accuracy in the final objective function).

- NL2SOL: See nl2sol
CHAPTER 6. KEYWORDS AREA

distribution

- Keywords Area
- method
- global_reliability
- distribution

Selection of cumulative or complementary cumulative functions

Specification

Alias: none
Argument(s): none
Default: cumulative (CDF)

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Choose One</td>
<td></td>
<td>cumulative</td>
<td>Computes statistics according to cumulative functions</td>
</tr>
<tr>
<td>complementary</td>
<td></td>
<td>complement</td>
<td>Computes statistics according to complementary cumulative functions</td>
</tr>
</tbody>
</table>

Description

The distribution keyword allows the user to select between a cumulative distribution/belief/plausibility function and a complementary cumulative distribution/belief/plausibility function. This choice affects how probabilities and reliability indices are reported.

Default Behavior

If the distribution keyword is present, it must be accompanied by either cumulative or complementary. Otherwise, a cumulative distribution will be used by default.

Expected Outputs

Output will be a set of model response-probability pairs determined according to the choice of distribution. The choice of distribution also defines the sign of the reliability or generalized reliability indices.

Examples

method
sampling
sample_type lhs
samples = 10
distribution cumulative
6.2. **METHOD**

**cumulative**

- **Keywords Area**
- **method**
- **global_reliability**
- **distribution**
- **cumulative**

Computes statistics according to cumulative functions

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

Statistics on model responses will be computed according to a cumulative distribution/belief/plausibility function.

**Default Behavior**

By default, a cumulative distribution/belief/plausibility function will be used. To explicitly specify it in the Dakota input file, however, the **cumulative** keyword must appear in conjunction with the **distribution** keyword.

**Expected Outputs**

Output will be a set of model response-probability pairs determined according to a cumulative distribution/belief/plausibility function. The probabilities reported are the probabilities that the model response falls below given response thresholds.

**Examples**

```dakota
method
sampling
  sample_type lhs
  samples = 10
  distribution cumulative
```

**complementary**

- **Keywords Area**
- **method**
- **global_reliability**
- **distribution**
- **complementary**

Computes statistics according to complementary cumulative functions
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): none

Description

Statistics on model responses will be computed according to a complementary cumulative distribution/belief/plausibility function.

Default Behavior
By default, a complementary cumulative distribution/belief/plausibility function will not be used. To change that behavior, the complementary keyword must be appear in conjunction with the distribution keyword.

Expected Outputs
Output will be a set of model response-probability pairs determined according to a complementary cumulative distribution/belief/plausibility function. The probabilities reported are the probabilities that the model response falls above given response thresholds.

Examples

method
  sampling
    sample_type lhs
    samples = 10
    distribution complementary

probability_levels

- Keywords Area
- method
- global_reliability
- probability_levels

Specify probability levels at which to estimate the corresponding response value

Specification

Alias: none

Argument(s): REALLIST

Default: No CDF/CCDF response levels to compute

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>Optional</td>
<td>num_probability_levels</td>
<td>Specify which probability_levels correspond to which response</td>
</tr>
</tbody>
</table>
6.2. METHOD

Description

Response levels are calculated for specified CDF/CCDF probabilities by indexing into a sorted samples array (the response levels computed are not interpolated and will correspond to one of the sampled values).

Expected Output

If probability_levels are specified, Dakota will create two tables in the standard output: a Probability Density function (PDF) histogram and a Cumulative Distribution Function (CDF) table. The PDF histogram has the lower and upper endpoints of each bin and the corresponding density of that bin. Note that the PDF histogram has bins defined by the probability_levels and/or response_levels in the Dakota input file. If there are not very many levels, the histogram will be coarse. Dakota does not do anything to optimize the bin size or spacing. The CDF table has the list of response levels and the corresponding probability that the response value is less than or equal to each response level threshold.

Examples

The Dakota input file below specifies a sampling method with probability levels of interest.

```
method,
    sampling,
    samples = 100 seed = 1
    complementary distribution
    probability_levels = 1.  .66  .33  0.
                  1. .8 .9 0.
                  1. .3 .2 0.
variables,
    normal_uncertain = 2
    means = 248.89, 593.33
    std_deviations = 12.4, 29.7
    descriptors = 'TF1n' 'TF2n'
    uniform_uncertain = 2
    lower_bounds = 199.3, 474.63
    upper_bounds = 298.5, 712.
    descriptors = 'TF1u' 'TF2u'
    weibull_uncertain = 2
    alphas = 12., 30.
    betas = 250., 590.
    descriptors = 'TF1w' 'TF2w'
histogram_bin_uncertain = 2
    num_pairs = 3 4
    abscissas = 5 8 10 .1 .2 .3 .4
    counts = 17 21 0 12 24 12 0
    descriptors = 'TF1h' 'TF2h'
histogram_point_uncertain
    real = 1
    num_pairs = 2
    abscissas = 3 4
    counts = 11
    descriptors = 'TF3h'
interface,
    system asynch evaluation_concurrency = 5
    analysis_driver = 'text_book'
responses,
    response_functions = 3
    no_gradients
    no_hessians
```
Given the above Dakota input file, the following excerpt from the output shows the PDF and CCDF generated. Note that the bounds on the bins of the PDF are the response values that correspond the probability levels specified in the input file. Those response values are also shown in the CCDF.

### Probability Density Function (PDF) histograms for each response function:

#### PDF for response_fn_1:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.7604749078e+11</td>
<td>3.4221494996e+11</td>
<td>5.1384774972e-12</td>
</tr>
<tr>
<td>3.4221494996e+11</td>
<td>4.0634975300e+11</td>
<td>5.145122311e-12</td>
</tr>
<tr>
<td>4.0634975300e+11</td>
<td>5.4196114379e+11</td>
<td>2.4334239039e-12</td>
</tr>
</tbody>
</table>

#### PDF for response_fn_2:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.6431154744e+04</td>
<td>5.6511827775e+04</td>
<td>1.9839945149e-05</td>
</tr>
<tr>
<td>5.6511827775e+04</td>
<td>6.1603813790e+04</td>
<td>5.8916108390e-05</td>
</tr>
<tr>
<td>6.1603813790e+04</td>
<td>7.8702465755e+04</td>
<td>2.9242071306e-05</td>
</tr>
</tbody>
</table>

#### PDF for response_fn_3:

<table>
<thead>
<tr>
<th>Bin Lower</th>
<th>Bin Upper</th>
<th>Density Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.3796370900e+05</td>
<td>3.6997214153e+05</td>
<td>3.0828386523e-06</td>
</tr>
<tr>
<td>3.6997214153e+05</td>
<td>3.8100966235e+05</td>
<td>9.060055534e-06</td>
</tr>
<tr>
<td>3.8100966235e+05</td>
<td>4.411498127e+05</td>
<td>3.3274925348e-06</td>
</tr>
</tbody>
</table>

### Level mappings for each response function:

#### Complementary Cumulative Distribution Function (CCDF) for response_fn_1:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.7604749078e+11</td>
<td>1.0000000000e+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.4221494996e+11</td>
<td>6.6000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.0634975300e+11</td>
<td>3.0000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5.4196114379e+11</td>
<td>0.0000000000e+00</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

#### Complementary Cumulative Distribution Function (CCDF) for response_fn_2:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.6431154744e+04</td>
<td>1.0000000000e+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5.6511827775e+04</td>
<td>8.0000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6.1603813790e+04</td>
<td>5.0000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7.8702465755e+04</td>
<td>0.0000000000e+00</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

#### Complementary Cumulative Distribution Function (CCDF) for response_fn_3:

<table>
<thead>
<tr>
<th>Response Level</th>
<th>Probability Level</th>
<th>Reliability Index</th>
<th>General Rel Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.3796370900e+05</td>
<td>1.0000000000e+00</td>
<td></td>
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</tr>
<tr>
<td>3.6997214153e+05</td>
<td>3.0000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.8100966235e+05</td>
<td>2.0000000000e-01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.411498127e+05</td>
<td>0.0000000000e+00</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Theory

Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.

In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

An inverse mapping involves computing the belief and plausibility response level for either a specified probability level or a specified generalized reliability level (two results for each level mapping in the evidence-based epistemic case, instead of the one result for each level mapping in the aleatory case).

**num_probability_levels**
6.2. Method

- Keywords Area
- method
- global_reliability
- probability_levels
- num_probability_levels

Specify which probability_levels correspond to which response

**Specification**

**Alias:** none

**Argument(s):** INTEGERLIST

**Default:** probability_levels evenly distributed among response functions

**Description**

See parent page

**gen_reliability_levels**

- Keywords Area
- method
- global_reliability
- gen_reliability_levels

Specify generalized reliability levels at which to estimate the corresponding response value

**Specification**

**Alias:** none

**Argument(s):** REALLIST

**Default:** No CDF/CCDF response levels to compute

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>num_gen_reliability_levels</td>
<td>Specify which gen_reliability_levels correspond to which response</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Description**

Response levels are calculated for specified generalized reliabilities by indexing into a sorted samples array (the response levels computed are not interpolated and will correspond to one of the sampled values).
Theory

Sets of response-probability pairs computed with the forward/inverse mappings define either a cumulative distribution function (CDF) or a complementary cumulative distribution function (CCDF) for each response function.

In the case of evidence-based epistemic methods, this is generalized to define either cumulative belief and plausibility functions (CBF and CPF) or complementary cumulative belief and plausibility functions (CCBF and CCPF) for each response function.

An inverse mapping involves computing the belief and plausibility response level for either a specified probability level or a specified generalized reliability level (two results for each level mapping in the evidence-based epistemic case, instead of the one result for each level mapping in the aleatory case).

\texttt{num\_gen\_reliability\_levels}

- Keywords Area
- method
- \texttt{global\_reliability}
- \texttt{gen\_reliability\_levels}
- \texttt{num\_gen\_reliability\_levels}

Specify which \texttt{gen\_reliability\_levels} correspond to which response

Specification

Alias: none

\textbf{Argument(s):} INTEGERLIST

\textbf{Default:} gen\_reliability\_levels evenly distributed among response functions

Description

See parent page

\texttt{model\_pointer}

- Keywords Area
- method
- \texttt{global\_reliability}
- \texttt{model\_pointer}

Identifier for model block to be used by a method

Topics

This keyword is related to the topics:

- \texttt{block\_pointer}
6.2. METHOD

Specification

Alias: none

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)

Description

The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.

Usage Tips

When doing advanced analyses that involve using multiple methods and multiple models, defining a model-pointer for each method is imperative.

See block_pointer for details about pointers.

Examples

environment
  tabular_graphics_data
  method_pointer = 'UQ'

method
  id_method = 'UQ'
  model_pointer = 'SURR'
  sampling,
    samples = 10
    seed = 98765 rng rnum2
    response_levels = 0.1 0.2 0.6
      0.1 0.2 0.6
      0.1 0.2 0.6
    sample_type lhs
    distribution cumulative

model
  id_model = 'SURR'
  surrogate global,
  dace_method_pointer = 'DACE'
  polynomial quadratic

method
  id_method = 'DACE'
  model_pointer = 'DACE_M'
  sampling sample_type lhs
    samples = 121 seed = 5034 rng rnum2

model
  id_model = 'DACE_M'
  single
  interface_pointer = 'I1'

variables
  uniform_uncertain = 2
    lower_bounds = 0. 0.
    upper_bounds = 1. 1.
    descriptors = 'x1' 'x2'
interface
    id_interface = 'I1'
    system async evaluation_concurrency = 5
    analysis_driver = 'text_book'

responses
    response_functions = 3
    no_gradients
    no_hessians

6.2.67 fsu_quasi_mc

- Keywords Area
- method
- fsu_quasi_mc

Design of Computer Experiments - Quasi-Monte Carlo sampling

Topics
This keyword is related to the topics:
- package.fsudace
- design_and_analysis_of_computer_experiments

Specification
Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of Group sequence type (Group 1)</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
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<tbody>
<tr>
<td>Optional</td>
<td>halton</td>
<td></td>
<td>Generate samples from a Halton sequence</td>
</tr>
<tr>
<td>Optional</td>
<td>hammersley</td>
<td></td>
<td>Use Hammersley sequences</td>
</tr>
<tr>
<td>Optional</td>
<td>latinize</td>
<td></td>
<td>Adjust samples to improve the discrepancy of the marginal distributions</td>
</tr>
</tbody>
</table>
### Optional

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>quality_metrics</td>
<td>Calculate metrics to assess the quality of quasi-Monte Carlo samples</td>
</tr>
<tr>
<td>variance_based_decomp</td>
<td>Activates global sensitivity analysis based on decomposition of response variance into contributions from variables</td>
</tr>
<tr>
<td>samples</td>
<td>Number of samples for sampling-based methods</td>
</tr>
<tr>
<td>fixed_sequence</td>
<td>Reuse the same sequence and samples for multiple sampling sets</td>
</tr>
<tr>
<td>sequence_start</td>
<td>Choose where to start sampling the sequence</td>
</tr>
<tr>
<td>sequence_leap</td>
<td>Specify how often the sequence is sampled</td>
</tr>
<tr>
<td>prime_base</td>
<td>The prime numbers used to generate the sequence</td>
</tr>
<tr>
<td>max_iterations</td>
<td>Number of iterations allowed for optimizers and adaptive UQ methods</td>
</tr>
</tbody>
</table>
Optional | model_pointer | Identifier for model block to be used by a method

### Description

Quasi-Monte Carlo methods produce low discrepancy sequences, especially if one is interested in the uniformity of projections of the point sets onto lower dimensional faces of the hypercube (usually 1-D: how well do the marginal distributions approximate a uniform?)

This method generates sets of uniform random variables on the interval $[0,1]$. If the user specifies lower and upper bounds for a variable, the $[0,1]$ samples are mapped to the [lower, upper] interval.

The user must first choose the sequence type:

- `halton` or
- `hammersley`

Then three keywords are used to define the sequence and how it is sampled:

- `prime_base`
- `sequence_start`
- `sequence_leap`

Each of these has defaults, so specification is optional.

### Theory

The quasi-Monte Carlo sequences of Halton and Hammersley are deterministic sequences determined by a set of prime bases. Generally, we recommend that the user leave the default setting for the bases, which are the lowest primes. Thus, if one wants to generate a sample set for 3 random variables, the default bases used are 2, 3, and 5 in the Halton sequence. To give an example of how these sequences look, the Halton sequence in base 2 starts with points 0.5, 0.25, 0.75, 0.125, 0.625, etc. The first few points in a Halton base 3 sequence are 0.33333, 0.66667, 0.11111, 0.44444, 0.77777, etc. Notice that the Halton sequence tends to alternate back and forth, generating a point closer to zero then a point closer to one. An individual sequence is based on a radix inverse function defined on a prime base. The prime base determines how quickly the $[0,1]$ interval is filled in. Generally, the lowest primes are recommended.

The Hammersley sequence is the same as the Halton sequence, except the values for the first random variable are equal to $1/N$, where $N$ is the number of samples. Thus, if one wants to generate a sample set of 100 samples for 3 random variables, the first random variable has values $1/100$, $2/100$, $3/100$, etc. and the second and third variables are generated according to a Halton sequence with bases 2 and 3, respectively.

For more information about these sequences, see [43], [44], and [1].

### See Also

These keywords may also be of interest:

- `dace`
- `fsu_cvt`
- `psuade_moat`
6.2. **METHOD**

**halton**

- Keywords Area
- method
- fsu_quasi_mc
- halton

Generate samples from a Halton sequence

**Topics**

This keyword is related to the topics:

- package_fsudace

**Specification**

Alias: none

Argument(s): none

**Description**

The quasi-Monte Carlo sequences of Halton are deterministic sequences determined by a set of prime bases. These sequences generate random numbers with the goal of filling a unit hypercube uniformly.

Generally, we recommend that the user leave the default setting for the bases, which are the lowest primes. Thus, if one wants to generate a sample set for 3 random variables, the default bases used are 2, 3, and 5 in the Halton sequence. To give an example of how these sequences look, the Halton sequence in base 2 starts with points 0.5, 0.25, 0.75, 0.125, 0.625, etc. The first few points in a Halton base 3 sequence are 0.33333, 0.66667, 0.11111, 0.44444, 0.77777, etc. Notice that the Halton sequence tends to alternate back and forth, generating a point closer to zero then a point closer to one. An individual sequence is based on a radix inverse function defined on a prime base. The prime base determines how quickly the [0,1] interval is filled in.

**Theory**

For more information about these sequences, see[43], [44], and [1].

**hammersley**

- Keywords Area
- method
- fsu_quasi_mc
- hammersley

Use Hammersley sequences
Topics
This keyword is related to the topics:

- package_f Sudace
- design_and_analysis_of_computer_experiments

Specification
Alias: none
Argument(s): none

Description
The Hammersley sequence is the same as the Halton sequence, except the values for the first random variable are equal to 1/N, where N is the number of samples. Thus, if one wants to generate a sample set of 100 samples for 3 random variables, the first random variable has values 1/100, 2/100, 3/100, etc. and the second and third variables are generated according to a Halton sequence with bases 2 and 3, respectively.

See Also
These keywords may also be of interest:

- fsu_quasi_mc

latinize

- Keywords Area
- method
- fsu_quasi_mc
- latinize

Adjust samples to improve the discrepancy of the marginal distributions

Specification
Alias: none
Argument(s): none
Default: No latinization

Description
The latinize control takes the samples and "latinizes" them, meaning that each original sample is moved so that it falls into one strata or bin in each dimension as in Latin Hypercube sampling. The default setting is NOT to latinize. However, one may be interested in doing this in situations where one wants better discrepancy of the 1-dimensional projections (the marginal distributions).
6.2. METHOD

**quality_metrics**

- **Keywords Area**
- **method**
- **fsu_quasi_mc**
- **quality_metrics**

Calculate metrics to assess the quality of quasi-Monte Carlo samples

**Topics**

This keyword is related to the topics:

- **package_fsudace**

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** No quality_metrics

**Description**

`quality_metrics` calculates four quality metrics relating to the volumetric spacing of the samples. The four quality metrics measure different aspects relating to the uniformity of point samples in hypercubes. Desirable properties of such point samples are:

- are the points equally spaced
- do the points cover the region
- and are they isotropically distributed
- with no directional bias in the spacing

The four quality metrics we report are:

- **h:** the point distribution norm, which is a measure of uniformity of the point distribution
- **chi:** a regularity measure, and provides a measure of local uniformity of a set of points
- **tau:** the second moment trace measure
- **d:** the second moment determinant measure

All of these values are scaled so that smaller is better (the smaller the metric, the better the uniformity of the point distribution).

**Examples**

Complete explanation of these measures can be found in [38].
variance_based_decomp

- Keywords Area
- method
- fsu_quasi_mc
- variance_based_decomp

Activates global sensitivity analysis based on decomposition of response variance into contributions from variables

**Specification**

*Alias:* none

*Argument(s):* none

*Default:* no variance-based decomposition

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<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>drop_tolerance</td>
<td>Suppresses output of sensitivity indices with values lower than this tolerance</td>
</tr>
</tbody>
</table>

**Description**

Dakota can calculate sensitivity indices through variance based decomposition using the keyword `variance_based_decomp`. These indicate how important the uncertainty in each input variable is in contributing to the output variance.

**Default Behavior**

Because of the computational cost, `variance_based_decomp` is turned off as a default.

If the user specified a number of samples, N, and a number of nondeterministic variables, M, variance-based decomposition requires the evaluation of $N \times (M+2)$ samples. **Note that specifying this keyword will increase the number of function evaluations above the number requested with the `samples` keyword since replicated sets of sample values are evaluated.**

**Expected Outputs**

When `variance_based_decomp` is specified, sensitivity indices for main effects and total effects will be reported. Main effects (roughly) represent the percent contribution of each individual variable to the variance in the model response. Total effects represent the percent contribution of each individual variable in combination with all other variables to the variance in the model response.

**Usage Tips**

To obtain sensitivity indices that are reasonably accurate, we recommend that N, the number of samples, be at least one hundred and preferably several hundred or thousands.

**Examples**

```plaintext
method,
  sampling
    sample_type lhs
```
6.2. METHOD

samples = 100
variance_based_decomp

Theory
In this context, we take sensitivity analysis to be global, not local as when calculating derivatives of output variables with respect to input variables. Our definition is similar to that of[73]: “The study of how uncertainty in the output of a model can be apportioned to different sources of uncertainty in the model input.”

Variance based decomposition is a way of using sets of samples to understand how the variance of the output behaves, with respect to each input variable. A larger value of the sensitivity index, $S_i$, means that the uncertainty in the input variable i has a larger effect on the variance of the output. More details on the calculations and interpretation of the sensitivity indices can be found in[73] and[87].

drop_tolerance

- Keywords Area
- method
- fsu_quasi_mc
- variance_based_decomp
- drop_tolerance

Suppresses output of sensitivity indices with values lower than this tolerance

Specification

Alias: none

Argument(s): REAL
Default: All VBD indices displayed

Description

The drop_tolerance keyword allows the user to specify a value below which sensitivity indices generated by variance_based_decomp are not displayed.

Default Behavior
By default, all sensitivity indices generated by variance_based_decomp are displayed.

Usage Tips
For polynomial_chaos, which outputs main, interaction, and total effects by default, the univariate_effects may be a more appropriate option. It allows suppression of the interaction effects since the output volume of these results can be prohibitive for high dimensional problems. Similar to suppression of these interactions is the covariance control, which can be selected to be diagonal_covariance or full_covariance, with the former supporting suppression of the off-diagonal covariance terms (to save compute and memory resources and reduce output volume).

Examples

method,
sampling
  sample_type lhs
  samples = 100
  variance_based_decomp
drop_tolerance = 0.001
samples

- **Keywords Area**
- **method**
- **fsu_quasi_mc**
- **samples**

Number of samples for sampling-based methods

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** 0

**Description**

The `samples` keyword is used to define the number of samples (i.e., randomly chosen sets of variable values) at which to execute a model.

**Default Behavior**

By default, Dakota will use the minimum number of samples required by the chosen method.

**Usage Tips**

To obtain linear sensitivities or to construct a linear response surface, at least `dim+1` samples should be used, where “`dim`” is the number of variables. For sensitivities to quadratic terms or quadratic response surfaces, at least `((dim+1)(dim+2))/2` samples are needed. For uncertainty quantification, we recommend at least `10*dim` samples. For `variance_based_decomp`, we recommend hundreds to thousands of samples. Note that for `variance_based_decomp`, the number of simulations performed will be `N*(dim+2)`.

**Examples**

```plaintext
method
  sampling
    sample_type lhs
    samples = 20
```

**fixed_sequence**

- **Keywords Area**
- **method**
- **fsu_quasi_mc**
- **fixed_sequence**

Reuse the same sequence and samples for multiple sampling sets

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** sequence not fixed: sampling patterns are variable among multiple QMC runs
6.2. METHOD

Description

The fixed_sequence control is similar to fixed_seed for other sampling methods. If fixed_sequence is specified, the user will get the same sequence (meaning the same set of samples) for subsequent calls of the QMC sampling method (for example, this might be used in a surrogate based optimization method or a parameter study where one wants to fix the uncertain variables).

sequence_start

- Keywords Area
- method
- fsu_quasi_mc
- sequence_start

Choose where to start sampling the sequence

Specification

Alias: none

Argument(s): INTEGERLIST
Default: Vector of zeroes

Description

sequence_start determines where in the sequence the samples will start.

The default sequence_start is a vector with 0 for each variable, specifying that each sequence start with the first term.

Examples

For example, for the Halton sequence in base 2, if the user specifies sequence_start = 2, the sequence would not include 0.5 and 0.25, but instead would start at 0.75.

sequence_leap

- Keywords Area
- method
- fsu_quasi_mc
- sequence_leap

Specify how often the sequence is sampled

Specification

Alias: none

Argument(s): INTEGERLIST
Default: Vector of ones
Description

`sequence_leap` controls the "leaping" of terms in the sequence. The default is 1 for each variable, meaning that each term in the sequence be returned.

Examples

If the user specifies a `sequence_leap` of 2 for a variable, the points returned would be every other term from the QMC sequence.

Theory

The advantage to using a leap value greater than one is mainly for high-dimensional sets of random deviates. In this case, setting a leap value to the next prime number larger than the largest prime base can help maintain uniformity when generating sample sets for high dimensions. For more information about the efficacy of leaped Halton sequences, see[71].

`prime_base`

- Keywords Area
- method
- `fsu_quasi_mc`
- `prime_base`

The prime numbers used to generate the sequence

Specification

Alias: none

Argument(s): INTEGERLIST

Default: Vector of the first s primes for s-dimensions in Halton, First (s-1) primes for Hammersley

Description

It is recommended that the user not specify this and use the default values.

- For the Halton sequence, the default bases are primes in increasing order, starting with 2, 3, 5, etc.
- For the Hammersley sequence, the user specifies (s-1) primes if one is generating an s-dimensional set of random variables.

`max_iterations`

- Keywords Area
- method
- `fsu_quasi_mc`
- `max_iterations`

Number of iterations allowed for optimizers and adaptive UQ methods
6.2. METHOD

Topics
This keyword is related to the topics:

- method independent controls

Specification
Alias: none
Argument(s): INTEGER
Default: 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence} / efficient_global: 25*n)

Description
The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed max_iterations iterations. See also max_function_evaluations.

Default Behavior
Default value is 100.

model_pointer

- Keywords Area
- method
- fsu_quasi_mc
- model_pointer

Identifier for model block to be used by a method

Topics
This keyword is related to the topics:

- block_pointer

Specification
Alias: none
Argument(s): STRING
Default: method use of last model parsed (or use of default model if none parsed)

Description
The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior
If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.
CHAPTER 6. KEYWORDS AREA

Usage Tips
When doing advanced analyses that involve using multiple methods and multiple models, defining a model-pointer for each method is imperative.
See block_pointer for details about pointers.

Examples

environment
   tabular_graphics_data
   method_pointer = 'UQ'

method
   id_method = 'UQ'
   model_pointer = 'SURR'
   sampling,
      samples = 10
      seed = 98765 rng rnum2
      response_levels = 0.1 0.2 0.6
      0.1 0.2 0.6
      0.1 0.2 0.6
      sample_type lhs
      distribution cumulative

model
   id_model = 'SURR'
   surrogate global,
   dace_method_pointer = 'DACE'
   polynomial quadratic

method
   id_method = 'DACE'
   model_pointer = 'DACE_M'
   sampling sample_type lhs
   samples = 121 seed = 5034 rng rnum2

model
   id_model = 'DACE_M'
   single
   interface_pointer = 'I1'

variables
   uniform_uncertain = 2
   lower_bounds = 0. 0.
   upper_bounds = 1. 1.
   descriptors = 'x1' 'x2'

interface
   id_interface = 'I1'
   system asynch evaluation_concurrency = 5
   analysis_driver = 'text_book'

responses
   response_functions = 3
   no_gradients
   no_hessians

6.2.68  vector_parameter_study

   • Keywords Area
6.2. METHOD

- method
- vector-parameter_study

Samples variables along a user-defined vector

Topics

This keyword is related to the topics:

- parameter_studies

Specification

Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional (Choose One)</td>
<td></td>
<td>final_point</td>
<td>Final variable values defining vector in vector parameter study</td>
</tr>
<tr>
<td></td>
<td></td>
<td>step_vector</td>
<td>Size of step for each variable</td>
</tr>
<tr>
<td>Required</td>
<td></td>
<td>num_steps</td>
<td>Number of sampling steps along the vector in a vector parameter study</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>model_pointer</td>
<td>Identifier for model block to be used by a method</td>
</tr>
</tbody>
</table>

Description

Dakota’s vector parameter study computes response data sets at selected intervals along a vector in parameter space. It is often used for single-coordinate parameter studies (to study the effect of a single variable on a response set), but it can be used more generally for multiple coordinate vector studies (to investigate the response variations along some n-dimensional vector such as an optimizer search direction).

**Default Behavior**

By default, the multidimensional parameter study operates over all types of variables.

**Expected Outputs**

A multidimensional parameter study produces a set of responses for each parameter set that is generated.

**Usage Tips**

**Group 1** is used to define the vector along which the parameters are varied. Both cases also rely on the variables specification of an initial value, through:

- the initial_point keyword
• the initial_state keyword
• relying on the default initial value, based on the rest of the variables specification

From the initial value, the vector can be defined using one of the two keyword choices.
Once the vector is defined, the samples are then fully specified by num_steps.

Examples
The following example is a good comparison to the examples on multidim.parameter.study and centered.parameter.study.

```dakota
# tested on Dakota 6.0 on 140501
environment
  tabular_data
    tabular_data_file = 'rosen_vector.dat'

method
  vector_parameter_study
    num_steps = 10
    final_point = 2.0  2.0

model
  single

variables
  continuous_design = 2
    initial_point = -2.0 -2.0
    descriptors = 'x1'  'x2'

interface
  analysis_driver = 'rosenbrock'
    fork

responses
  response_functions = 1
    no_gradients
    no_hessians
```

See Also
These keywords may also be of interest:

• centered.parameter.study
• multidim.parameter.study
• list.parameter.study

final_point

• Keywords Area
• method
• vector.parameter.study
• final_point

Final variable values defining vector in vector parameter study
### Specification

**Alias:** none  
**Argument(s):** REALLIST

#### Description

The final_point keyword is used to define the final values for each variable on the vector to be used in the vector parameter study. The vector’s direction and magnitude are determined by the initial value from the variables specification, and the final_point.

**Default Behavior**

The user is required to specify either final_point or step_vector. There is no default definition for the vector.

**Usage Tips**

The actual points are determined based on this vector and the number of points chosen is given in num-points.

### Examples

```plaintext
method
  vector_parameter_study
  num_steps = 10
  final_point = 2.0 2.0

step_vector
  • Keywords Area
  • method
  • vector_parameter_study
  • step_vector

Size of step for each variable
```

### Specification

**Alias:** none  
**Argument(s):** REALLIST

#### Description

The step_vector keyword specifies how much each variable will be incremented in a single step.

step_vector works in conjunction with num_steps, which determines the number of steps taken during the vector_parameter_study. If instead of step_vector, final_point is specified with num_steps, Dakota will infer the step sizes.

Entries in the step_vector are the actual amounts by which continuous and range variables are incremented. For set variables, step_vector entries are interpreted as indexes into the underlying set.

**Default Behavior**

The user is required to specify either final_point or step_vector. There is no default definition for the vector.
CHAPTER 6. KEYWORDS AREA

Examples

variables
  continuous_design 1
  initial_point 1.0
  descriptors 'x1'
discrete_design_set
  string 1
    elements 'bar' 'baz' 'foo' 'fuzz'
    initial_point 'bar'
    descriptors 's1'

method
  vector_parameter_study
  num_steps = 3
  # Add 2.0 to x1 and increment s1 by 1 element in each step
  step_vector = 2.0 1

num_steps
  * Keywords Area
  * method
  * vector_parameter_study
  * num_steps

  Number of sampling steps along the vector in a vector parameter study

Specification

Alias: none
  Argument(s): INTEGER

Description

num_steps defines the number of steps that are taken in the direction of the vector. The magnitude of each step is determined in conjunction with the rest of the method specification.

  Default Behavior
  The user is required to specify num_steps for a vector parameter study. There is no default value.
  This study performs function evaluations at both ends, making the total number of evaluations equal to num_steps+1.

  Usage Tips
  The study has stringent requirements on performing appropriate steps with any discrete range and discrete set variables. A num_steps specification must result in discrete range and set index steps that are integers: no remainder is currently permitted in the integer step calculation and no rounding to integer steps will occur.

Examples

method
  vector_parameter_study
  num_steps = 10
  final_point = 2.0 2.0
6.2. METHOD

model_pointer

- Keywords Area
- method
- vector_parameter_study
- model_pointer

Identifier for model block to be used by a method

Topics

This keyword is related to the topics:

- block_pointer

Specification

Alias: none

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)

Description

The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.

Usage Tips

When doing advanced analyses that involve using multiple methods and multiple models, defining a model-pointer for each method is imperative.

See block_pointer for details about pointers.

Examples

environment
  tabular_graphics_data
  method_pointer = ‘UQ’

method
  id_method = ‘UQ’
  model_pointer = ‘SURR’
  sampling,
  samples = 10
  seed = 98765 rng rnum2
  response_levels = 0.1 0.2 0.6
    0.1 0.2 0.6
    0.1 0.2 0.6
  sample_type lhs
  distribution cumulative

model
  id_model = ‘SURR’
surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
id_method = 'DACE'
model_pointer = 'DACE_M'
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = 'DACE_M'
single
interface_pointer = 'I1'

variables
uniform_uncertain = 2
lower_bounds = 0.0.
upper_bounds = 1.1.
descriptors = 'x1' 'x2'

interface
id_interface = 'I1'
system asynch evaluation_concurrency = 5
analysis_driver = 'text_book'

responses
response_functions = 3
no_gradients
no_hessians

6.2.69 list_parameter_study

- Keywords Area
- method
- list_parameter_study

Samples variables as a specified values

Topics
This keyword is related to the topics:

- parameter_studies

Specification
Alias: none

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
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<tr>
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<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
6.2. METHOD

<table>
<thead>
<tr>
<th>Required (Choose One)</th>
<th>Group 1</th>
<th>list_of_points</th>
<th>List of variable values to evaluate in a list parameter study</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>import_points_file</td>
<td>File containing list of variable values to evaluate in a list parameter study</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>model_pointer</td>
<td>Identifier for model block to be used by a method</td>
</tr>
</tbody>
</table>

**Description**

Dakota’s list parameter study allows for evaluations at user selected points of interest.

**Default Behavior**

By default, the list parameter study operates over all types of variables.

The number of real values in the list_of_points specification or file referenced by import_points_file must be a multiple of the total number of variables (including continuous and discrete types) contained in the variables specification.

**Expected Outputs**

A list parameter study produces a set of responses for each parameter set that is specified.

**Usage Tips**

- This parameter study simply performs simulations for the first parameter set (the first \( n \) entries in the list), followed by the next parameter set (the next \( n \) entries), and so on, until the list of points has been exhausted.

- Since the initial values from the variables specification will not be used, they need not be specified.

- When the points are specified in the Dakota input file using the list_of_points keyword, discrete set values must be referred to using 0-based indexes, and not the values themselves. However, when using import_points_file, refer to discrete set values directly, not by index.

- For both list_of_points and import_points_file, Dakota expects the values for each evaluation to be ordered by type. The type ordering matches that of the variables section of this Reference Manual and of the listing in the Parameters file format section of the Dakota User’s Manual[4]. When multiple variables are present for a single type, the ordering within that type must match the order specified by the user in the variables section of her input file.

**Examples**

This shows the method and variables block of a Dakota input file that runs a list_parameter_study.

```plaintext
method
  list_parameter_study
  list_of_points =
    3.1e6   0.0029   0.31
    3.2e6   0.0028   0.32
    3.3e6   0.0027   0.34
    3.3e6   0.0026   0.36
```
variables
  continuous_design = 3
  descriptors = 'E' 'MASS' 'DENSITY'

Note that because of the way Dakota treats whitespace, the above example is equivalent to:

method
  list_parameter_study
  list_of_points =
  3.1e6 0.0029 0.31 3.2e6 0.0028
  0.32 3.3e6 0.0027
  0.34 3.3e6 0.0026 0.36

variables
  continuous_design = 3
  descriptors = 'E' 'MASS' 'DENSITY'

Although the first example is much more readable.
And here’s a full input file:

# tested on Dakota 6.0 on 140501
environment
  tabular_data
    tabular_data_file 'List_param_study.dat'
method
  list_parameter_study
    list_of_points =  0.1 0.1
                    0.2 0.1
                    0.3 0.0
                    0.3 1.0

model
  single
variables
  active design
  continuous_design = 2
    descriptors ‘x1’ ‘x2’
  continuous_state = 1
    descriptors = ‘constant1’
    initial_state = 100
interface
  analysis_drivers 'text_book'
  fork
    asynchronous
      evaluation_concurrency 2
responses
  response_functions = 1
  no_gradients
  no_hessians

This example illustrates the list_parameter_study.

- The function evaluations are independent, so any level of evaluation_concurrency can be used.
- Default behavior for parameter studies is to iterate on all variables. However, because active design is specified, this study will only iterate on the continuous_design variables.
6.2. METHOD

See Also

These keywords may also be of interest:

- centered_parameter_study
- multidim_parameter_study
- vector_parameter_study

list_of_points

- Keywords Area
- method
- list_parameter_study
- list_of_points

List of variable values to evaluate in a list parameter study

Specification

Alias: none

Argument(s): REALLIST

Description

The list_of_points keyword allows the user to specify, in a freeform format, a list of variable values at which to compute a model response.

Default Behavior

The user is required to provide a list of points for a list parameter study either by specifying it with list_of_points or by providing a file from which such a list can be read via import_points_file. There is no default list of points.

Usage Tips

The number of values in the list must be an integer multiple of the number of variables. Dakota will verify that this condition is met.

Examples

method
list_parameter_study
list_of_points =
  3.1e6  0.0029  0.31
  3.2e6  0.0028  0.32
  3.3e6  0.0027  0.34
  3.3e6  0.0026  0.36
import_points_file

- **Keywords Area**
- **method**
- **list_parameter_study**
- **import_points_file**

File containing list of variable values to evaluate in a list parameter study

### Specification

**Alias:** none  
**Argument(s):** STRING  
**Default:** no point import from a file

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Optional (Choose One)</strong></td>
<td>tabular_format (Group 1)</td>
<td>annotated</td>
<td>Selects annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>custom_annotated</td>
<td>Selects custom-annotated tabular file format</td>
</tr>
<tr>
<td></td>
<td></td>
<td>freeform</td>
<td>Selects freeform file format</td>
</tr>
<tr>
<td>Optional</td>
<td>active_only</td>
<td></td>
<td>Import only active variables from tabular data file</td>
</tr>
</tbody>
</table>

### Description

The `import_points_file` specifies a file containing a list of variable values at which to compute a model response.

**Default Behavior**

By default, methods do not import points from a file.

**Usage Tips**

Dakota parses input files without regard to whitespace, but the `import_points_file` must be in one of three formats:

- `annotated` (default)
- `custom_annotated`
- `freeform`
6.2. METHOD

Examples

```python
method
  list_parameter_study
  import_points_file = 'dakota_pstudy.3.dat'

annotated

- Keywords Area
- method
- list_parameter_study
- import_points_file
- annotated

Selects annotated tabular file format
```

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none

Argument(s): none

Default: annotated

Description

An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior

By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips

- To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify custom_annotated header eval_id

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.
Examples
Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```environment
    tabular_data
    tabular_data_file = 'dakota_summary.dat'
```

```
annotated
```

Resulting tabular file:

```
%eval_id interface x1 x2 obj_fn nln_ineq_con_1 nln_ineq_con_2
1 NO_ID 0.9 1.1 0.0002 0.26 0.76
2 NO_ID 0.90009 1.1 0.0001996404857 0.2601620081 0.759955
3 NO_ID 0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...
```

custom_annotated

- Keywords Area
- method
- list_parameter_study
- import_points_file
- custom_annotated

Selects custom-annotated tabular file format

Topics
This keyword is related to the topics:

- file_formats

Specification
Alias: none

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword header</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td></td>
<td>Enable header row in custom-annotated tabular file</td>
</tr>
</tbody>
</table>
**6.2. METHOD**

<table>
<thead>
<tr>
<th>Optional</th>
<th>eval_id</th>
<th>Enable evaluation ID column in custom-annotated tabular file</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>interface_id</td>
<td>Enable interface ID column in custom-annotated tabular file</td>
</tr>
</tbody>
</table>

**Description**

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

**Default Behavior**

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

**Usage Tips**

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

**Examples**

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:

```
environment
  tabular_data
    tabular_data_file = ‘dakota_summary.dat’
    custom_annotated header eval_id
```

Resulting tabular file:

```
%eval_id  x1  x2  obj_fn  nln_ineq_con_1  nln_ineq_con_2
1          0.9  1.1  0.0002  0.26     0.76
2  0.90009  1.1  0.0001996404857  0.2601620081  0.759955
3  0.89991  1.1  0.0002003604863  0.2598380081  0.760045
...
```

**header**

- Keywords Area
- method
- list_parameter_study
• import_points_file
• custom.annotated
• header

Enable header row in custom-annotated tabular file

Specification
Alias: none
Argument(s): none

Description
See description of parent custom.annotated

eval_id
• Keywords Area
• method
• list_parameter_study
• import_points_file
• custom.annotated
• eval_id

Enable evaluation ID column in custom-annotated tabular file

Specification
Alias: none
Argument(s): none

Description
See description of parent custom.annotated

interface_id
• Keywords Area
• method
• list_parameter_study
• import_points_file
• custom.annotated
• interface_id

Enable interface ID column in custom-annotated tabular file
6.2. METHOD

Specification
Alias: none
Argument(s): none

Description
See description of parent custom_annotated

freeform
- Keywords Area
- method
- list_parameter_study
- import_points_file
- freeform
  Selects freeform file format

Topics
This keyword is related to the topics:
- fileformats

Specification
Alias: none
Argument(s): none

Description
A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior
The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips
- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.
Examples
Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```python
environment
  tabular_data
    tabular_data_file = 'dakota_summary.dat'
  freeform

Resulting tabular file:

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>0.9</td>
<td>1.1</td>
<td>0.002</td>
<td>0.26</td>
<td>0.76</td>
</tr>
<tr>
<td>0.9009</td>
<td>1.1</td>
<td>0.0001996404857</td>
<td>0.2601620081</td>
<td>0.759955</td>
</tr>
<tr>
<td>0.89991</td>
<td>1.1</td>
<td>0.0002003604863</td>
<td>0.2598380081</td>
<td>0.760045</td>
</tr>
</tbody>
</table>
...
```

active_only

- Keywords Area
- method
- list_parameter_study
- import_points_file
- active_only

Import only active variables from tabular data file

Topics
This keyword is related to the topics:

- file_formats

Specification
Alias: none
Argument(s): none

Description
By default, files for tabular data imports are expected to contain columns for all variables, active and inactive. The keyword `active_only` indicates that the file to import contains only the active variables.

This option should only be used in contexts where the inactive variables have no influence, for example, building a surrogate over active variables, with the state variables held at nominal. It should not be used in more complex nested contexts, where the values of inactive variables are relevant to the function evaluations used to build the surrogate.
6.2. METHOD

model_pointer

- Keywords Area
- method
- list_parameter_study
- model_pointer

Identifier for model block to be used by a method

Topics

This keyword is related to the topics:
- block_pointer

Specification

Alias: none

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)

Description

The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.

Usage Tips

When doing advanced analyses that involve using multiple methods and multiple models, defining a model_pointer for each method is imperative.

See block_pointer for details about pointers.

Examples

```
environment
    tabular_graphics_data
    method_pointer = 'UQ'

method
    id_method = 'UQ'
    model_pointer = 'SURR'
    sampling,
        samples = 10
        seed = 98765 rng rnum2
        response_levels = 0.1 0.2 0.6
        0.1 0.2 0.6
        0.1 0.2 0.6
    sample_type lhs
    distribution cumulative

model
    id_model = 'SURR'
```
surrogate global,
dace_method_pointer = ‘DACE’
polynomial quadratic

method
id_method = ‘DACE’
model_pointer = ‘DACE_M’
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = ‘DACE_M’
single
interface_pointer = ‘I1’

variables
uniform_uncertain = 2
lower_bounds = 0. 0.
upper_bounds = 1. 1.
descriptors = ‘x1’ ‘x2’

interface
id_interface = ‘I1’
system asynch evaluation_concurrency = 5
analysis_driver = ‘text_book’

responses
response_functions = 3
no_gradients
no_hessians

6.2.70 centered_parameter_study

- Keywords Area
- method
- centered_parameter_study

Samples variables along points moving out from a center point

Topics
This keyword is related to the topics:

- parameter_studies

Specification

Alias: none

<table>
<thead>
<tr>
<th>Argument(s): none</th>
<th>Required/Opt:</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
</table>
6.2. METHOD

<table>
<thead>
<tr>
<th>Required</th>
<th>step_vector</th>
<th>Size of steps to be taken in each dimension of a centered parameter study</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required</td>
<td>steps_per_variable</td>
<td>Number of steps to take in each dimension of a centered parameter study</td>
</tr>
<tr>
<td>Optional</td>
<td>model_pointer</td>
<td>Identifier for model block to be used by a method</td>
</tr>
</tbody>
</table>

### Description

Dakota’s centered parameter study computes response data sets along multiple coordinate-based vectors, one per parameter, centered about the initial values from the variables specification. This is useful for investigation of function contours with respect to each parameter individually in the vicinity of a specific point (e.g., post-optimality analysis for verification of a minimum), thereby avoiding the cost associated with a multidimensional grid.

**Default Behavior**

By default, the centered parameter study operates over all types of variables. The centered_parameter_study takes steps along each orthogonal dimension. Each dimension is treated independently. The number of steps are taken in each direction, so that the total number of points in the parameter study is $1 + 2 \sum n$.

### Expected Outputs

A centered parameter study produces a set of responses for each parameter set that is generated.

### Examples

The following example is a good comparison to the examples on multidim_parameter_study and vector_parameter_study.

```plaintext
# tested on Dakota 6.0 on 140501 environment
  tabular_data = 'rosen_centered.dat'

method
  centered_parameter_study
  steps_per_variable = 5 4
  step_vector = 0.4 0.5

model
  single

variables
  continuous_design = 2
  initial_point = 0 0
  descriptors = 'x1' "x2"
```
interface
    analysis_driver = 'rosenbrock'
    fork

responses
    response_functions = 1
    no_gradients
    no_hessians

See Also
These keywords may also be of interest:

- multidim_parameter_study
- list_parameter_study
- vector_parameter_study

step_vector

- Keywords Area
- method
- centered_parameter_study
- step_vector

Size of steps to be taken in each dimension of a centered parameter study

Specification

Alias: none
Argument(s): REALLIST

Description
The step_vector keyword defines the individual step size in each dimension, treated separately.

Default Behavior
The user is required to define the number of step sizes for a centered parameter study. There are no default values.

Steps are taken in the plus and minus directions, and are defined in either actual values (continuous and discrete range) or index offsets (discrete set).

Examples

method
    centered_parameter_study
    steps_per_variable = 5 4
    step_vector = 0.4 0.5
steps_per_variable

- Keywords Area
- method
- centered_parameter_study
- steps_per_variable

Number of steps to take in each dimension of a centered parameter study

Specification

Alias: deltas_per_variable

Argument(s): INTEGERLIST

Description

The \texttt{steps_per_variable} keyword allows the user to define the number of steps in each dimension of a centered parameter study. Because they are taken independently, the number of steps can be specified for each.

Default Behavior

The user is required to define the number of steps per variable for a centered parameter study. There are no default values.

Steps are taken in the plus and minus directions, and are defined in either actual values (continuous and discrete range) or index offsets (discrete set).

Examples

\begin{verbatim}
method
  centered_parameter_study
  steps_per_variable = 5 4
  step_vector = 0.4 0.5
\end{verbatim}

model_pointer

- Keywords Area
- method
- centered_parameter_study
- model_pointer

Identifier for model block to be used by a method

Topics

This keyword is related to the topics:

- block_pointer
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)

Description

The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.

Usage Tips

When doing advanced analyses that involve using multiple methods and multiple models, defining a model_pointer for each method is imperative.

See block_pointer for details about pointers.

Examples

environment
  tabular_graphics_data
  method_pointer = 'UQ'

method
  id_method = ‘UQ’
  model_pointer = ‘SURR’
  sampling,
    samples = 10
    seed = 98765 rng rnum2
    response_levels = 0.1 0.2 0.6
                       0.1 0.2 0.6
                       0.1 0.2 0.6
    sample_type lhs
    distribution cumulative

model
  id_model = ‘SURR’
  surrogate global,
  dace_method_pointer = ‘DACE’
  polynomial quadratic

method
  id_method = ‘DACE’
  model_pointer = ‘DACE_M’
  sampling sample_type lhs
  samples = 121 seed = 5034 rng rnum2

model
  id_model = ‘DACE_M’
  single
  interface_pointer = ’I1’

variables
  uniform_uncertain = 2
  lower_bounds = 0. 0.
  upper_bounds = 1. 1.
  descriptors = ’x1’ ’x2’
6.2. METHOD

interface
  id_interface = 'I1'
system asynch evaluation_concurrency = 5
  analysis_driver = 'text_book'

responses
  response_functions = 3
  no_gradients
  no_hessians

6.2.71 multidim_parameter_study

- Keywords Area
- method
- multidim_parameter_study

Samples variables on full factorial grid of study points

Topics

This keyword is related to the topics:

- parameter_studies

Specification

Alias: none

Argument(s): none

| Required/- | Description of Group | Dakota Keyword | Dakota Keyword Description |
| Optional Required | partitions | model_pointer | Samples variables on full factorial grid of study points | Identifier for model block to be used by a method |

Description

Dakota’s multidimensional parameter study computes response data sets for an n-dimensional grid of points. Each continuous and discrete range variable is partitioned into equally spaced intervals between its upper and lower bounds, each discrete set variable is partitioned into equally spaced index intervals. The partition boundaries in n-dimensional space define a grid of points, and every point is evaluated.

Default Behavior
By default, the multidimensional parameter study operates over all types of variables.

Expected Outputs
A multidimensional parameter study produces a set of responses for each parameter set that is generated.

Usage Tips
Since the initial values from the variables specification will not be used, they need not be specified.
Examples

This example is taken from the Users Manual and is a good comparison to the examples on centered\_parameter\_study and vector\_parameter\_study.

```dakota
# tested on Dakota 6.0 on 140501
environment
tabular_data
tabular_data_file = 'rosen_multidim.dat'

method
multidim\_parameter\_study
partitions = 10 8

model
single

variables
continuous\_design = 2
lower\_bounds -2.0 -2.0
upper\_bounds 2.0 2.0
descriptors ‘x1’ “x2”

interface
analysis\_driver = ‘rosenbrock’
fork

responses
response\_functions = 1
no\_gradients
no\_hessians
```

This example illustrates the full factorial combinations of parameter values created by the multidim\_parameter\_study. With 10 and 8 partitions, there are actually 11 and 9 values for each variable. This means that $11 \times 9 = 99$ function evaluations will be required.

See Also

These keywords may also be of interest:

- centered\_parameter\_study
- list\_parameter\_study
- vector\_parameter\_study

partitions

- Keywords Area
- method
- multidim\_parameter\_study
- partitions

Samples variables on full factorial grid of study points
6.2. METHOD

Topics
This keyword is related to the topics:

- parameter_studies

Specification

Alias: none
Argument(s): INTEGERLIST

Description
Dakota’s multidimensional parameter study computes response data sets for an n-dimensional grid of points. Each continuous and discrete range variable is partitioned into equally spaced intervals between its upper and lower bounds, each discrete set variable is partitioned into equally spaced index intervals. The partition boundaries in n-dimensional space define a grid of points, and every point is evaluated.

Default Behavior
By default, the multidimensional parameter study operates over all types of variables.

Expected Outputs
A multidimensional parameter study produces a set of responses for each parameter set that is generated.

Usage Tips
Since the initial values from the variables specification will not be used, they need not be specified.

Examples
This example is taken from the Users Manual and is a good comparison to the examples on centered_parameter_study and vector_parameter_study.

```plaintext
# tested on Dakota 6.0 on 140501
environment
tabular_data
tabular_data_file = 'rosen_multidim.dat'
method
multidim_parameter_study
partitions = 10 8
model
single
variables
  continuous_design = 2
  lower_bounds -2.0 -2.0
  upper_bounds 2.0 2.0
  descriptors 'x1' "x2"
interface
  analysis_driver = 'rosenbrock'
  fork
responses
  response_functions = 1
  no_gradients
  no_hessians
```
This example illustrates the full factorial combinations of parameter values created by the multidim_parameter_study. With 10 and 8 partitions, there are actually 11 and 9 values for each variable. This means that $11 \times 9 = 99$ function evaluations will be required.

See Also
These keywords may also be of interest:

- centered_parameter_study
- list_parameter_study
- vector_parameter_study

model_pointer

- Keywords Area
- method
- multidim_parameter_study
- model_pointer

Identifier for model block to be used by a method

Topics
This keyword is related to the topics:

- block_pointer

Specification
Alias: none
Argument(s): STRING
Default: method use of last model parsed (or use of default model if none parsed)

Description
The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior
If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.

Usage Tips
When doing advanced analyses that involve using multiple methods and multiple models, defining a model_pointer for each method is imperative.

See block_pointer for details about pointers.
6.2. METHOD

Examples

```plaintext
environment
tabular_graphics_data
method_pointer = 'UQ'

method
id_method = 'UQ'
model_pointer = 'SURR'
sampling,
samples = 10
seed = 98765 rng rnum2
response_levels = 0.1 0.2 0.6
0.1 0.2 0.6
0.1 0.2 0.6
sample_type lhs
distribution cumulative

model
id_model = 'SURR'
surrogate global,
dace_method_pointer = 'DACE'
polynomial quadratic

method
id_method = 'DACE'
model_pointer = 'DACE_M'
sampling sample_type lhs
samples = 121 seed = 5034 rng rnum2

model
id_model = 'DACE_M'
single
interface_pointer = 'I1'

variables
uniform_uncertain = 2
lower_bounds = 0. 0.
upper_bounds = 1. 1.
descriptors = 'x1' 'x2'

interface
id_interface = 'I1'
system asynch evaluationConcurrency = 5
analysis_driver = 'text_book'

responses
response_functions = 3
no_gradients
no_hessians
```

6.2.72 richardson_extrap

- Keywords Area
- method
- richardson_extrap

Estimate order of convergence of a response as model fidelity increases
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<tr>
<td>Required (Choose One)</td>
<td>Group 1</td>
<td>estimate_order</td>
<td>Compute the best estimate of the convergence order from three points</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>converge_order</td>
<td>Refine until the estimated convergence order converges</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>converge_qoi</td>
<td>Refine until the response converges</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>refinement_rate</td>
<td>Rate at which the state variables are refined</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>convergence_tolerance</td>
<td>Stopping criterion based on convergence of the objective function or statistics</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>max_iterations</td>
<td>Number of iterations allowed for optimizers and adaptive UQ methods</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>model_pointer</td>
<td>Identifier for model block to be used by a method</td>
</tr>
</tbody>
</table>

Description

Solution verification procedures estimate the order of convergence of the simulation response data during the course of a refinement study. This branch of methods is new and currently only contains one algorithm: Richardson extrapolation.

**Refinement of the model**

The model fidelity must be parameterized by one or more continuous state variable(s).

The refinement path is determined from the initial state of the continuous state variables specification in combination with the refinement_rate, where each of the state variables is treated as an independent refinement factor and each of the initial state values is repeatedly divided by the refinement rate value to define new discretization states.

**Results**

Three algorithm options are currently provided:

1. estimate_order
2. converge_order
3. converge_qoi

Stopping Criteria
The method employs the max_iterations and convergence_tolerance method independent controls as stopping criteria.

Theory
In each of these cases, convergence order for a response quantity of interest (QoI) is estimated from

\[ p = \ln \left( \frac{QoI_3 - QoI_2}{QoI_2 - QoI_1} \right) / \ln(r) \]

where \( r \) is the uniform refinement rate specified by refinement_rate.

estimate_order
- Keywords: Area, method, richardson_extrap, estimate_order

Compute the best estimate of the convergence order from three points

Specification
Alias: none
Argument(s): none

Description
The estimate_order option is the simplest option. For each of the refinement factors, it evaluates three points along the refinement path and uses these results to perform an estimate of the convergence order for each response function.

converge_order
- Keywords: Area, method, richardson_extrap, converge_order

Refine until the estimated coverage order converges
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none
   Argument(s): none

Description

The **converge_order** option is initialized using the **estimate_order** approach, and additional refinements are performed along the refinement path until the convergence order estimates converge (two-norm of the change in response orders is less than the convergence tolerance).

**converge_qoi**

- **Keywords Area**
- **method**
- **richardson_extrap**
- **converge_qoi**

Refine until the response converges

Specification

Alias: none
   Argument(s): none

Description

The **converge_qoi** option is similar to the **converge_order** option, except that the convergence criterion is that the two-norm of the response discretization errors (computed from extrapolation) must be less than the convergence tolerance.

**refinement_rate**

- **Keywords Area**
- **method**
- **richardson_extrap**
- **refinement_rate**

Rate at which the state variables are refined

Specification

Alias: none
   Argument(s): REAL
   Default: 2.
6.2. METHOD

Description

Described on parent page

convergence_tolerance

- Keywords Area
- method
- richardson_extrap
- convergence_tolerance

Stopping criterion based on convergence of the objective function or statistics

Topics

This keyword is related to the topics:

- method_independent_controls

Specification

Alias: none

Argument(s): REAL

Default: 1.e-4

Description

The convergence_tolerance specification provides a real value for controlling the termination of iteration.

For optimization, it is most commonly a relative convergence tolerance for the objective function; i.e., if the change in the objective function between successive iterations divided by the previous objective function is less than the amount specified by convergence_tolerance, then this convergence criterion is satisfied on the current iteration.

Therefore, permissible values are between 0 and 1, non-inclusive.

Behavior Varies by Package/Library

This control is used with most optimization and least squares iterators (DOT, CONMIN, NPSOL, NL2SOL, OPT++, and SCOLIB). Most other Dakota methods (such as DACE or parameter studies) do not use this control, but some adaptive methods, such as adaptive UQ, do.

Since no progress may be made on one iteration followed by significant progress on a subsequent iteration, some libraries require that the convergence tolerance be satisfied on two or more consecutive iterations prior to termination of iteration.

Notes on each library:

- DOT: must be satisfied for two consecutive iterations
- NPSOL: defines an internal optimality tolerance which is used in evaluating if an iterate satisfies the first-order Kuhn-Tucker conditions for a minimum. The magnitude of convergence_tolerance approximately specifies the number of significant digits of accuracy desired in the final objective function (e.g., convergence_tolerance = 1.e-6 will result in approximately six digits of accuracy in the final objective function).
- NL2SOL: See nl2sol
max_iterations

- Keywords Area
- method
- richardson_extrap
- max_iterations

Number of iterations allowed for optimizers and adaptive UQ methods

Topics

This keyword is related to the topics:
- method_independent_controls

Specification

Alias: none
Argument(s): INTEGER
Default: 100 (exceptions: fsu_cvt, local_reliability: 25; global_{reliability, interval_est, evidence} / efficient_global: 25*n)

Description

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed max_iterations iterations. See also max_function_evaluations.

Default Behavior
Default value is 100.

model_pointer

- Keywords Area
- method
- richardson_extrap
- model_pointer

Identifier for model block to be used by a method

Topics

This keyword is related to the topics:
- block_pointer
6.2. METHOD

Specification

Alias: none

Argument(s): STRING

Default: method use of last model parsed (or use of default model if none parsed)

Description

The model_pointer is used to specify which model block will be used to perform the function evaluations needed by the Dakota method.

Default Behavior

If not specified, a Dakota method will use the last model block parsed. If specified, there must be a model block in the Dakota input file that has a corresponding id_model with the same name.

Usage Tips

When doing advanced analyses that involve using multiple methods and multiple models, defining a model_pointer for each method is imperative.

See block_pointer for details about pointers.

Examples

environment
  tabular_graphics_data
  method_pointer = 'UQ'

method
  id_method = 'UQ'
  model_pointer = 'SURR'
  sampling,
  samples = 10
  seed = 98765 rng rnum2
  response_levels = 0.1 0.2 0.6
  0.1 0.2 0.6
  0.1 0.2 0.6
  sample_type lhs
  distribution cumulative

model
  id_model = 'SURR'
  surrogate global,
  dace_method_pointer = 'DACE'
  polynomial quadratic

method
  id_method = 'DACE'
  model_pointer = 'DACE_M'
  sampling sample_type lhs
  samples = 121 seed = 5034 rng rnum2

model
  id_model = 'DACE_M'
  single
  interface_pointer = 'I1'

variables
  uniform_uncertain = 2
  lower_bounds = 0. 0.
  upper_bounds = 1. 1.
  descriptors = 'x1' 'x2'
interface
  id_interface = 'I1'
system async evaluation_concurrency = 5
  analysis_driver = 'text_book'

responses
  response_functions = 3
  no_gradients
  no_hessians

6.3 model

- Keywords Area
- model

Specifies how variables are mapped into a set of responses

Topics

This keyword is related to the topics:

- block

Specification

Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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</thead>
<tbody>
<tr>
<td>id</td>
<td></td>
<td>id_model</td>
<td>Give the model block an identifying name, in case of multiple model blocks</td>
</tr>
<tr>
<td>single</td>
<td></td>
<td></td>
<td>A model with one of each block: variable, interface, and response</td>
</tr>
<tr>
<td>surrogate</td>
<td></td>
<td></td>
<td>An empirical model that is created from data or the results of a submodel</td>
</tr>
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</table>

<table>
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<tr>
<th>Required(Choose One)</th>
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<th></th>
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<tr>
<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>surrogate</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
**nested**  
A model whose responses are computed through the use of a sub-iterator

**active_subspace**  
Active (variable) subspace model

**adapted_basis**  
Unused (reserved for future Adapted Basis Model)

**random_field**  
Experimental capability to generate a random field representation from data, from simulation runs, or from a covariance matrix. The representation may then be sampled for use as a random field input to another simulation. **THIS IS AN EXPERIMENTAL CAPABILITY.**
CHAPTER 6. KEYWORDS AREA

Optional | variables_pointer | Specify which variables block will be included with this model block. Specify which responses block will be used by this model block. Enables hierarchical evaluation tagging.

Optional | responses_pointer |

Optional | hierarchical_tagging |

Description

A model is comprised of a mapping from variables, through an interface, to responses.

**Model Group 1** The type of model can be:

1. single (default)
2. surrogate
3. nested
4. subspace
5. random_field

The input file must specify one of these types. If the type is not specified, Dakota will assume a single model.

**Block Pointers and ID**

Each of these model types supports variables_pointer and responses_pointer strings for identifying the variables and responses specifications used in constructing the model by cross-referencing with id_variables and id_responses strings from particular variables and responses keyword specifications.

These pointers are valid for each model type since each model contains a set of variables that is mapped into a set of responses – only the specifics of the mapping differ.

Additional pointers are used for each model type for constructing the components of the variable to response mapping. As an environment specification identifies a top-level method and a method specification identifies a model, a model specification identifies variables, responses, and (for some types) interface specifications. This top-down flow specifies all of the object interrelationships.

Examples

The first example shows a minimal specification for a single model, which is the default model when no models are explicitly specified by the user.

```
model
  single
```

The next example displays a surrogate model specification which selects a quadratic polynomial from among the global approximation methods. It uses a pointer to a design of experiments method for generating the data needed for building the global approximation, reuses any old data available for the current approximation region, and employs the first-order multiplicative approach to correcting the approximation each time correction is requested.
6.3. **MODEL**

```python
model,
    id_model = 'M1'
variables_pointer = 'V1'
responses_pointer = 'R1'
surrogate
global
    polynomial quadratic
dace_method_pointer = 'DACE'
reuse_samples region
correction multiplicative first_order
```

This example demonstrates the use of identifiers and pointers. It provides the optional model independent specifications for model identifier, variables pointer, and responses pointer as well as model dependent specifications for global surrogates (see `global`).

Finally, an advanced nested model example would be

```python
model
    id_model = 'M1'
variables_pointer = 'V1'
responses_pointer = 'R1'
nested
    optional_interface_pointer = 'OI1'
        optional_interface_responses_pointer = 'OIR1'
sub_method_pointer = 'SM1'
    primary_variable_mapping = 'X' 'Y'
    secondary_variable_mapping = 'mean' 'mean'
    primary_response_mapping = 1. 0. 0. 0. 0. 0. 0. 0. 0.
    secondary_response_mapping = 0. 0. 0. 1. 3. 0. 0. 0. 0.
        0. 0. 0. 0. 0. 0. 1. 3. 0.
```

This example illustrates controls for model identifier, variables pointer, and responses pointer and for specifying details of the nested mapping.

### 6.3.1 id_model

- **Keywords Area**
- **model**
- **id_model**

Give the model block an identifying name, in case of multiple model blocks

**Topics**

This keyword is related to the topics:

- **block_identifier**

**Specification**

- **Alias:** none
- **Argument(s):** STRING
- **Default:** method use of last model parsed
CHAPTER 6. KEYWORDS AREA

Description

The model identifier string is supplied with id_model and is used to provide a unique identifier string for use within method specifications (refer to the keyword model_pointer in any of the methods in the method block, for example: model_pointer).

This is used to determine which model the method will run.

See Also

These keywords may also be of interest:

- model_pointer

6.3.2 single

- Keywords Area
- model
- single

A model with one of each block: variable, interface, and response

Specification

Alias: simulation
Argument(s): none
Default: N/A (single if no model specification)

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>interface_pointer</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>solution_level_control</td>
<td></td>
</tr>
</tbody>
</table>

Description

The single model is the simplest model type. It uses a single interface instance to map variables into responses. There is no recursion in this case.

The optional interface_pointer specification identifies the interface block by cross-referencing with the id-interface string input from a particular interface keyword specification. This is only necessary when the input file has multiple interface blocks, and you wish to explicitly point to the desired block. The same logic follows for responses and variables blocks and pointers.
Examples
The example shows a minimal specification for a single model, which is the default model when no models are specified by the user.

```
model
  single
```

This example does not provide any pointer strings and therefore relies on the default behavior of constructing the model with the last variables, interface, and responses specifications parsed.

See Also
These keywords may also be of interest:

- surrogate
- nested

**interface_pointer**

- Keywords Area
- model
- single
- interface_pointer

Interface block pointer for the single model type

Topics
This keyword is related to the topics:

- block_pointer

Specification
 Alias: none
 Argument(s): STRING
 Default: model use of last interface parsed

Description
In the single model case, a single interface is used to map the variables into responses. The optional interface-pointer specification identifies this interface by cross-referencing with the id_interface string input from a particular interface keyword specification.

See block_pointer for details about pointers.

When an interface pointer is not specified, the model will use the last interface block parsed from the input file.
solution_level_control

- Keywords Area
- model
- single
- solution_level_control

Identifier for variable that manages solution control levels.

**Specification**

**Alias:** none  
**Argument(s):** STRING  
**Default:** use of single default solution level

| Required/- | Description of | Dakota Keyword | Dakota Keyword |
| Optional | Group | | Description |
| Required | | solution_level_control | Relative cost profile for solution levels |

**Description**

This string specification identifies a descriptor/tag for the variable that controls the solution level hierarchy. In current usage, the variable is assumed to be a discrete set or discrete range variable.

**Examples**

The discrete variable identified by the descriptor `N_x` should have four values in its set or range, corresponding to the length of the cost specification.

```plaintext
code
model,
  id_model = 'SIM1'
simulation
  solution_level_control = 'N_x'
solution_level_cost = 630. 1260. 2100. 4200.
```

**See Also**

These keywords may also be of interest:

- multilevel_sampling
- polynomial_chaos


6.3. MODEL

- solution_level_control
- solution_level_cost

Relative cost profile for solution levels

Specification

Alias: none
Argument(s): REALLIST

Description

This specification provides a profile of relative costs corresponding to an ordered hierarchy of solution control values (e.g., discretization levels).

Usage Tips

The order of the cost values should correspond to the order of the discrete set or range values that can be assumed by the variable identified by solution_level_control.

Examples

The discrete variable identified by the descriptor 'N_x' should have four values in its set or range, corresponding to the length of the cost specification. The solution_level_cost is neither strictly ascending or descending, rather it should match the order of the discrete values assumed by 'N_x'.

```model,
  id_model = 'SIM1'
  simulation
    solution_level_control = 'N_x'
    solution_level_cost = 630. 1260. 2100. 4200.
```

See Also

These keywords may also be of interest:

- multilevel_sampling
- polynomial_chaos

6.3.3 surrogate

- Keywords Area
- model
- surrogate

An empirical model that is created from data or the results of a submodel

Specification

Alias: none
Argument(s): none
### Description

Surrogate models are inexpensive approximate models that are intended to capture the salient features of an expensive high-fidelity model. They can be used to explore the variations in response quantities over regions of the parameter space, or they can serve as inexpensive stand-ins for optimization or uncertainty quantification studies (see, for example, the surrogate-based optimization methods, surrogate_based_global and surrogate_based_local).

Surrogate models supported in Dakota are categorized as Data Fitting or Hierarchical, as shown below. Each of these surrogate types provides an approximate representation of a "truth" model which is used to perform the parameter to response mappings. This approximation is built and updated using results from the truth model, called the "training data".

- **Data fits:**
  
  *Known Issue*: When using discrete variables, there have been sometimes significant differences in surrogate behavior observed across computing platforms in some cases. The cause has not yet been fully diagnosed and is currently under investigation. In addition, guidance on appropriate construction and use of surrogates with discrete variables is under development. In the meantime, users should therefore be aware that there is a risk of inaccurate results when using surrogates with discrete variables.

  Data fitting methods involve construction of an approximation or surrogate model using data (response values, gradients, and Hessians) generated from the original truth model. Data fit methods can be further...
categorized as local, multipoint, and global approximation techniques, based on the number of points used in generating the data fit.

1. Local: built from response data from a single point in parameter space
   - Taylor series expansion: `taylor_series`
     Training data consists of a single point, plus gradient and Hessian information.

2. Multipoint: built from two or more points in parameter space, often involving the current and previous iterates of a minimization algorithm.
   - TANA-3: `tana`
     Training Data comes from a few previously evaluated points

3. Global full space response surface methods:
   - Polynomial regression: `polynomial`
   - Gaussian process (Kriging): `gaussian_process`
   - Artificial neutral network: `neural_network`
   - MARS: `mars`
   - Radial Basis Functions: `radial_basis`
   - Orthogonal polynomials (only supported in PCE/SC for now): `polynomial_chaos` and `stoch_collocation`

   Training data is generated using either a design of experiments method applied to the truth model (specified by `dace_method_pointer`), or from saved data (specified by `reuse_points`) in a restart database, or an import file.

- Multifidelity/hierarchical:

  Multifidelity modeling involves the use of a low-fidelity physics-based model as a surrogate for the original high-fidelity model. The low-fidelity model typically involves a coarser mesh, looser convergence tolerances, reduced element order, or omitted physics.

  See `hierarchical`.

  The global and hierarchical surrogates have a correction feature in order to improve the local accuracy of the surrogate models. The correction factors force the surrogate models to match the true function values and possibly true function derivatives at the center point of each trust region. Details can be found on global correction or hierarchical correction.

**Theory**

Surrogate models are used extensively in the surrogate-based optimization and least squares methods, in which the goals are to reduce expense by minimizing the number of truth function evaluations and to smooth out noisy data with a global data fit. However, the use of surrogate models is not restricted to optimization techniques; uncertainty quantification and optimization under uncertainty methods are other primary users.

**Data Fit Surrogate Models**

A surrogate of the \{data fit\} type is a non-physics-based approximation typically involving interpolation or regression of a set of data generated from the original model. Data fit surrogates can be further characterized by the number of data points used in the fit, where a local approximation (e.g., first or second-order Taylor series) uses data from a single point, a multipoint approximation (e.g., two-point exponential approximations (TPEA) or two-point adaptive nonlinearity approximations (TANA)) uses a small number of data points often drawn from the previous iterates of a particular algorithm, and a global approximation (e.g., polynomial response surfaces, kriging/gaussian_process, neural networks, radial basis functions, splines) uses a set of data points distributed over the domain of interest, often generated using a design of computer experiments.
Dakota contains several types of surface fitting methods that can be used with optimization and uncertainty quantification methods and strategies such as surrogate-based optimization and optimization under uncertainty. These are: polynomial models (linear, quadratic, and cubic), first-order Taylor series expansion, kriging spatial interpolation, artificial neural networks, multivariate adaptive regression splines, radial basis functions, and moving least squares. With the exception of Taylor series methods, all of the above methods listed in the previous sentence are accessed in Dakota through the Surpack library. All of these surface fitting methods can be applied to problems having an arbitrary number of design parameters. However, surface fitting methods usually are practical only for problems where there are a small number of parameters (e.g., a maximum of somewhere in the range of 30-50 design parameters). The mathematical models created by surface fitting methods have a variety of names in the engineering community. These include surrogate models, meta-models, approximation models, and response surfaces. For this manual, the terms surface fit model and surrogate model are used.

The data fitting methods in Dakota include software developed by Sandia researchers and by various researchers in the academic community.

**Multifidelity Surrogate Models**

A second type of surrogate is the \{model hierarchy\} type (also called multifidelity, variable fidelity, variable complexity, etc.). In this case, a model that is still physics-based but is of lower fidelity (e.g., coarser discretization, reduced element order, looser convergence tolerances, omitted physics) is used as the surrogate in place of the high-fidelity model. For example, an inviscid, incompressible Euler CFD model on a coarse discretization could be used as a low-fidelity surrogate for a high-fidelity Navier-Stokes model on a fine discretization.

**Surrogate Model Selection**

This section offers some guidance on choosing from among the available surrogate model types.

- For Surrogate Based Local Optimization, using the `surrogate_based_local` method with a trust region: using the keywords:

  1. `surrogate local taylor_series` or
  2. `surrogate multipoint tana`

  will probably work best.

  If for some reason you wish or need to use a global surrogate (not recommended) then the best of these options is likely to be either:

  1. `surrogate global gaussian_process surfpack` or
  2. `surrogate global moving_least_squares`.

- For Efficient Global Optimization (EGO), the `efficient_global` method:

  the default surrogate is: `gaussian_process surfpack` which is likely to find a more optimal value and/or require fewer true function evaluations than the alternative, `gaussian_process dakota`. However, the surfpack will likely take more time to build than the dakota version. Note that currently the `use_derivatives` keyword is not recommended for use with EGO based methods.

- For EGO based global interval estimation, the `global_interval_est ego` method:

  the default `gaussian_process surfpack` will likely work better than the alternative `gaussian_process dakota`.

- For Efficient Global Reliability Analysis (EGRA), the `global_reliability` method:

  the `surfpack` and `dakota` versions of the gaussian process tend to give similar answers with the `dakota` version tending to use fewer true function evaluations. Since this is based on EGO, it is likely that the default `surfpack` is more accurate, although this has not been rigorously demonstrated.
For EGO based Dempster-Shafer Theory of Evidence, i.e. the global_evidence ego method, the default gaussian_process surfpack often use significantly fewer true function evaluations than the alternative gaussian_process dakota.

When using a global surrogate to extrapolate, any of the surrogates:

- gaussian_process surfpack
- polynomial quadratic
- polynomial cubic

are recommended.

When there is over roughly two or three thousand data points and you wish to interpolate (or approximately interpolate) then a Taylor series, Radial Basis Function Network, or Moving Least Squares fit is recommended. The only reason that the gaussian_process surfpack is not recommended is that it can take a considerable amount of time to construct when the number of data points is very large. Use of the third party MARS package included in Dakota is generally discouraged.

In other situations that call for a global surrogate, the gaussian_process surfpack is generally recommended. The use_derivatives keyword will only be useful if accurate and inexpensive derivatives are available. Finite difference derivatives are disqualified on both counts. However, derivatives generated by analytical, automatic differentiation, or continuous adjoint techniques can be appropriate. Currently, first order derivatives, i.e. gradients, are the highest order derivatives that can be used to construct the gaussian_process surfpack model; Hessians will not be used even if they are available.

See Also

These keywords may also be of interest:

- single
- nested

id_surrogates

Keywords Area

- model
- surrogate
- id_surrogates

Identifies the subset of the response functions by number that are to be approximated (the default is all functions).

Specification

Alias: none

Argument(s): INTEGERLIST

Default: All response functions are approximated
Description

In the surrogate model case, the specification first allows a mixture of surrogate and actual response mappings through the use of the optional `id_surrogates` specification. This identifies the subset of the response functions by number that are to be approximated (the default is all functions). The valid response function identifiers range from 1 through the total number of response functions (see `response_functions`).

global

- Keywords Area
- model
- surrogate
- global

Select a surrogate model with global support

Specification

Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<tr>
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<td>gaussian_process</td>
<td>Gaussian Process surrogate model</td>
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<td></td>
<td>marts</td>
<td></td>
<td>Multivariate Adaptive Regression Spline (MARS)</td>
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<td></td>
<td>moving_least_squares</td>
<td></td>
<td>Moving Least Squares surrogate models</td>
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<tr>
<td></td>
<td>neural_network</td>
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<td>Artificial neural network model</td>
</tr>
<tr>
<td></td>
<td>radial_basis</td>
<td></td>
<td>Radial basis function (RBF) model</td>
</tr>
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### 6.3. MODEL

<table>
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<tr>
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<td>Polynomial surrogate model</td>
</tr>
<tr>
<td>Optional/Choose One</td>
<td>Piecewise Domain Decomposition for Global Surrogate Models</td>
</tr>
<tr>
<td>Optional/Choose One</td>
<td>Specified number of training points</td>
</tr>
<tr>
<td>Optional/Choose One</td>
<td>Construct surrogate with minimum number of points</td>
</tr>
<tr>
<td>Optional/Choose One</td>
<td>Construct surrogate with recommended number of points</td>
</tr>
<tr>
<td>Optional/Choose One</td>
<td>Specify a method to gather training data</td>
</tr>
<tr>
<td>Optional/Choose One</td>
<td>A surrogate model pointer that guides a method to whether it should use a surrogate model or compute truth function evaluations</td>
</tr>
<tr>
<td>Optional</td>
<td>Surrogate model training data reuse control</td>
</tr>
<tr>
<td>Optional</td>
<td>File containing points you wish to use to build a surrogate</td>
</tr>
</tbody>
</table>
CHAPTER 6. KEYWORDS AREA

| Optional | export_approx_points_file | Output file for evaluations of a surrogate model |
| Optional | use_derivatives | Use derivative data to construct surrogate models |
| Optional | correction | Correction approaches for surrogate models |
| Optional | metrics | Compute surrogate quality metrics |
| Optional | import_challenge_points_file | Datafile of points to assess surrogate quality |

**Description**

The global surrogate model requires specification of one of the following approximation types:

1. Polynomial
2. Gaussian process (Kriging interpolation)
3. Layered perceptron artificial neural network approximation
4. MARS
5. Moving least squares
6. Radial basis function
7. Voronoi Piecewise Surrogate (VPS)

All these approximations are implemented in SurfPack[36], except for VPS. In addition, a second version of Gaussian process is implemented directly in Dakota.

**Training Data**

Training data can be taken from prior runs, stored in a datafile, or by running a Design of Experiments method. The keywords listed below are used to determine how to collect training data:

- `dace_method_pointer`
- `reuse_points`
- `import_points_file`
- `use_derivatives` The source of training data is determined by the contents of a provided `import_points_file`, whether `reuse_points` and `use_derivatives` are specified, and the contents of the method block specified by `dace_method_pointer`. `use_derivatives` is a special case, the other keywords are discussed below.
The number of training data points used in building a global approximation is determined by specifying one of three point counts:

1. **minimum_points**: minimum required or minimum "reasonable" amount of training data. Defaults to \(d+1\) for \(d\) input dimensions for most models, e.g., polynomials override to the number of coefficients required to estimate the requested order.

2. **recommended_points**: recommended number of training data, (this is the default option, if none of the keywords is specified). Defaults to \(5\times d\), except for polynomials where it’s equal to the minimum.

3. **total_points**: specify the number of training data points. However, if the total_points value is less than the default minimum_points value, the minimum_points value is used.

The sources of training data depend on the number of training points, \(N_{tp}\), the number of points in the import file, \(N_{if}\), and the value of `reuse_points`.

- If there is no import file, all training data come from the DACE method
- If there is an import file, all \(N_{if}\) points from the file are used, and the remaining \(N_{tp} - N_{if}\) points come from the DACE method
- If there is an import file and `reuse_points` is:
  - `none` - all \(N_{tp}\) points from DACE method
  - `region` - only the points within a trust region are taken from the import file, and all remaining points are from the DACE method.
  - `all` - (Default) all \(N_{if}\) points from the file are used, and the remaining \(N_{tp} - N_{if}\) points come from the DACE method

**Surrogate Correction**

A correction model can be added to the constructed surrogate in order to better match the training data. The specified correction method will be applied to the surrogate, and then the corrected surrogate model is used by the method.

Finally, the quality of the surrogate can be tested using the `metrics` and `challenge_points_file` keywords.

**Theory**

Global methods, also referred to as response surface methods, involve many points spread over the parameter ranges of interest. These surface fitting methods work in conjunction with the sampling methods and design of experiments methods.

**Procedures for Surface Fitting**

The surface fitting process consists of three steps:

1. selection of a set of design points
2. evaluation of the true response quantities (e.g., from a user-supplied simulation code) at these design points,
3. using the response data to solve for the unknown coefficients (e.g., polynomial coefficients, neural network weights, kriging correlation factors) in the surface fit model.
In cases where there is more than one response quantity (e.g., an objective function plus one or more constraints), then a separate surface is built for each response quantity. Currently, the surface fit models are built using only 0th-order information (function values only), although extensions to using higher-order information (gradients and Hessians) are possible.

Each surface fitting method employs a different numerical method for computing its internal coefficients. For example, the polynomial surface uses a least-squares approach that employs a singular value decomposition to compute the polynomial coefficients, whereas the kriging surface uses Maximum Likelihood Estimation to compute its correlation coefficients. More information on the numerical methods used in the surface fitting codes is provided in the Dakota Developers Manual.

**See Also**

These keywords may also be of interest:

- local
- hierarchical
- multipoint

**gaussian_process**

- Keywords Area
- model
- surrogate
- global
- gaussian_process

Gaussian Process surrogate model

**Specification**

Alias: kriging

**Argument(s):** none

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<thead>
<tr>
<th>Required/-Optional Required (Choose One)</th>
<th>Description of Group GP Implementation (Group 1)</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<td>dakota</td>
<td>Select the built-in Gaussian Process surrogate</td>
</tr>
<tr>
<td></td>
<td></td>
<td>surfpack</td>
<td>Use the Surfpack version of Gaussian Process surrogates</td>
</tr>
</tbody>
</table>
Description

Use the Gaussian process (GP) surrogate from Surfpack, which is specified using the surfpack keyword.

An alternate version of GP surrogates was available in prior versions of Dakota. **For now, both versions are supported but the dakota version is deprecated and intended to be removed in a future release.**

**Known Issue:** When using discrete variables, there have been sometimes significant differences in surrogate behavior observed across computing platforms in some cases. The cause has not yet been fully diagnosed and is currently under investigation. In addition, guidance on appropriate construction and use of surrogates with discrete variables is under development. In the meantime, users should therefore be aware that there is a risk of inaccurate results when using surrogates with discrete variables.

<table>
<thead>
<tr>
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</tr>
</thead>
<tbody>
<tr>
<td>• Keywords Area</td>
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<td>• surrogate</td>
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<td>• global</td>
</tr>
<tr>
<td>• gaussian_process</td>
</tr>
<tr>
<td>• dakota</td>
</tr>
</tbody>
</table>

Select the built in Gaussian Process surrogate

Specification

**Alias:** none

**Argument(s):** none

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<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
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<tr>
<td>Optional</td>
<td>point_selection</td>
<td>Enable greedy selection of well-spaced build points</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>trend</td>
<td>Choose a trend function for a Gaussian process surrogate</td>
<td></td>
</tr>
</tbody>
</table>

Description

A second version of GP surrogates was available in prior versions of Dakota. **For now, both versions are supported but the dakota version is deprecated and intended to be removed in a future release.**

Historically these models were drastically different, but in Dakota 5.1, they became quite similar. They now differ in that the Surfpack GP has a richer set of features/options and tends to be more accurate than the Dakota version. Due to how the Surfpack GP handles ill-conditioned correlation matrices (which significantly contributes to its greater accuracy), the Surfpack GP can be a factor of two or three slower than Dakota’s. As of Dakota 5.2, the Surfpack implementation is the default in all contexts except Bayesian calibration.
More details on the `gaussian_process` dakota model can be found in [58].

Dakota’s GP deals with ill-conditioning in two ways. First, when it encounters a non-invertible correlation matrix it iteratively increases the size of a “nugget,” but in such cases the resulting approximation smooths rather than interpolates the data. Second, it has a `point_selection` option (default off) that uses a greedy algorithm to select a well-spaced subset of points prior to the construction of the GP. In this case, the GP will only interpolate the selected subset. Typically, one should not need point selection in trust-region methods because a small number of points are used to develop a surrogate within each trust region. Point selection is most beneficial when constructing with a large number of points, typically more than order one hundred, though this depends on the number of variables and spacing of the sample points.

This differs from the `point_selection` option of the Dakota GP which initially chooses a well-spaced subset of points and finds the correlation parameters that are most likely for that one subset.

**point_selection**

- Keywords Area
- model
- surrogate
- global
- `gaussian_process`
- `dakota`
- `point_selection`

Enable greedy selection of well-spaced build points

**Topics**

This keyword is related to the topics:

- `surrogate_models`

**Specification**

Alias: none

Argument(s): none

Default: no point selection

**Description**

The Dakota Gaussian Process model has a `point_selection` option (default off) that uses a greedy algorithm to select a well-spaced subset of points prior to the construction of the GP. In this case, the GP will only interpolate the selected subset. Typically, one should not need point selection in trust-region methods because a small number of points are used to develop a surrogate within each trust region. Point selection is most beneficial when constructing with a large number of points, typically more than order one hundred, though this depends on the number of variables and spacing of the sample points.
Choose a trend function for a Gaussian process surrogate

**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** reduced_quadratic

<table>
<thead>
<tr>
<th>Required/-Optional Required (Choose One)</th>
<th>Description of Group Trend Order (Group 1)</th>
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<td>Constant trend function</td>
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<tr>
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<td></td>
<td>linear</td>
<td>Use a linear polynomial or trend function</td>
</tr>
<tr>
<td></td>
<td></td>
<td>reduced_quadratic</td>
<td>Quadratic polynomials - main effects only</td>
</tr>
</tbody>
</table>

**Description**

The only trend functions that are currently supported are polynomials.

The trend function is selected using the `trend` keyword, with options `constant`, `linear`, or `reduced_quadratic`. The `reduced_quadratic` trend function includes the main effects, but not mixed/interaction terms. The Surfpack GP (See surfpack) has the additional option of (a full) quadratic.

**constant**

- Keywords Area
- model
- surrogate
- global
• gaussian_process
• dakota
• trend
• constant

Constant trend function

**Specification**
Alias: none
Argument(s): none

**Description**
See parent page

**linear**
• Keywords Area
• model
• surrogate
• global
• gaussian_process
• dakota
• trend
• linear

Use a linear polynomial or trend function

**Specification**
Alias: none
Argument(s): none

**Description**
See parent page
reduced_quadratic

- Keywords Area
- model
- surrogate
- global
- gaussian_process
- dakota
- trend
- reduced_quadratic

Quadratic polynomials - main effects only

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

In 2 or more dimensions, this polynomial omits the interaction, or mixed, terms.

**surfpack**

- Keywords Area
- model
- surrogate
- global
- gaussian_process
- surfpack

Use the Surfpack version of Gaussian Process surrogates

**Specification**

**Alias:** none

**Argument(s):** none
<table>
<thead>
<tr>
<th>Optional</th>
<th>trend</th>
<th>Choose a trend function for a Gaussian process surrogate</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>optimization_method</td>
<td>Change the optimization method used to compute hyperparameters</td>
</tr>
<tr>
<td>Optional</td>
<td>max_trials</td>
<td>Max number of likelihood function evaluations</td>
</tr>
<tr>
<td>Optional (Choose One)</td>
<td>Nugget (Group 1)</td>
<td>nugget</td>
</tr>
<tr>
<td>Optional</td>
<td>find_nugget</td>
<td>Have Surfpack compute a nugget to handle ill-conditioning</td>
</tr>
<tr>
<td>Optional</td>
<td>correlation_lengths</td>
<td>Specify the correlation lengths for the Gaussian process</td>
</tr>
<tr>
<td>Optional</td>
<td>export_model</td>
<td>Exports surrogate model in user-selected format</td>
</tr>
</tbody>
</table>

**Description**

This keyword specifies the use of the Gaussian process that is incorporated in our surface fitting library called Surfpack.

Several user options are available:

1. **Optimization methods:**

   Maximum Likelihood Estimation (MLE) is used to find the optimal values of the hyper-parameters governing the trend and correlation functions. By default the global optimization method DIRECT is used for MLE, but other options for the optimization method are available. See `optimization_method`.

   The total number of evaluations of the likelihood function can be controlled using the `max_trials` keyword followed by a positive integer. Note that the likelihood function does not require running the "truth" model, and is relatively inexpensive to compute.

2. **Trend Function:**

   The GP models incorporate a parametric trend function whose purpose is to capture large-scale variations. See `trend`.

3. **Correlation Lengths:**

   Correlation lengths are usually optimized by Surfpack, however, the user can specify the lengths manually. See `correlation_lengths`.
4. Ill-conditioning

One of the major problems in determining the governing values for a Gaussian process or Kriging model is the fact that the correlation matrix can easily become ill-conditioned when there are too many input points close together. Since the predictions from the Gaussian process model involve inverting the correlation matrix, ill-conditioning can lead to poor predictive capability and should be avoided.

Note that a sufficiently bad sample design could require correlation lengths to be so short that any interpolatory GP model would become inept at extrapolation and interpolation.

The surfpack model handles ill-conditioning internally by default, but behavior can be modified using

5. Gradient Enhanced Kriging (GEK).

The use_derivatives keyword will cause the Surfpack GP to be constructed from a combination of function value and gradient information (if available).

See notes in the Theory section.

Theory

Gradient Enhanced Kriging

Incorporating gradient information will only be beneficial if accurate and inexpensive derivative information is available, and the derivatives are not infinite or nearly so. Here "inexpensive" means that the cost of evaluating a function value plus gradient is comparable to the cost of evaluating only the function value, for example gradients computed by analytical, automatic differentiation, or continuous adjoint techniques. It is not cost effective to use derivatives computed by finite differences. In tests, GEK models built from finite difference derivatives were also significantly less accurate than those built from analytical derivatives. Note that GEK’s correlation matrix tends to have a significantly worse condition number than Kriging for the same sample design.

This issue was addressed by using a pivoted Cholesky factorization of Kriging’s correlation matrix (which is a small sub-matrix within GEK’s correlation matrix) to rank points by how much unique information they contain. This reordering is then applied to whole points (the function value at a point immediately followed by gradient information at the same point) in GEK’s correlation matrix. A standard non-pivoted Cholesky is then applied to the reordered GEK correlation matrix and a bisection search is used to find the last equation that meets the constraint on the (estimate of) condition number. The cost of performing pivoted Cholesky on Kriging’s correlation matrix is usually negligible compared to the cost of the non-pivoted Cholesky factorization of GEK’s correlation matrix. In tests, it also resulted in more accurate GEK models than when pivoted Cholesky or whole-point-block pivoted Cholesky was performed on GEK’s correlation matrix.

trend

- Keywords Area
- model
- surrogate
- global
- gaussian_process
- surfpack
- trend

Choose a trend function for a Gaussian process surrogate
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none
Argument(s): none
Default: reduced_quadratic

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
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</tr>
<tr>
<td>linear</td>
<td></td>
<td>Use a linear polynomial or trend function</td>
</tr>
<tr>
<td>reduced_quadratic</td>
<td></td>
<td>Quadratic polynomials - main effects only</td>
</tr>
<tr>
<td>quadratic</td>
<td></td>
<td>Use a quadratic polynomial or trend function</td>
</tr>
</tbody>
</table>

Description

The only trend functions that are currently supported are polynomials.

The trend function is selected using the trend keyword, with options constant, linear, or reduced_quadratic. The reduced_quadratic trend function includes the main effects, but not mixed/interaction terms. The Surfpack GP (See surfpack) has the additional option of (a full) quadratic.

constant
  - Keywords Area
  - model
  - surrogate
  - global
  - gaussian_process
  - surfpack
  - trend
  - constant

Constant trend function

Specification

Alias: none
Argument(s): none
6.3. MODEL

Description
See parent page

- linear
  - Keywords Area
  - model
  - surrogate
  - global
  - gaussian_process
  - surfpack
  - trend
  - linear
  Use a linear polynomial or trend function

Specification
Alias: none
Argument(s): none

Description
See parent page

- reduced_quadratic
  - Keywords Area
  - model
  - surrogate
  - global
  - gaussian_process
  - surfpack
  - trend
  - reduced_quadratic
  Quadratic polynomials - main effects only

Specification
Alias: none
Argument(s): none
CHAPTER 6. KEYWORDS AREA

Description
In 2 or more dimensions, this polynomial omits the interaction, or mixed, terms.

- **quadratic**
  - Keywords Area
  - model
  - surrogate
  - global
  - gaussian_process
  - surfpack
  - trend
  - quadratic

Use a quadratic polynomial or trend function

Specification
Alias: none
Argument(s): none

Description
See parent page

- **optimization_method**
  - Keywords Area
  - model
  - surrogate
  - global
  - gaussian_process
  - surfpack
  - optimization_method

Change the optimization method used to compute hyperparameters

Specification
Alias: none
Argument(s): STRING
Default: global
6.3. MODEL

Description
Select the optimization method to compute hyperparameters of the Gaussian Process by specifying one of these arguments:

- **global** (default) - DIRECT method
- **local** - CONMIN method
- **sampling** - generates several random guesses and picks the candidate with greatest likelihood
- **none** - no optimization, pick the center of the feasible region

The **none** option, and the starting location of the **local** optimization, default to the center, in log(correlation length) scale, of the feasible region. Surfpack picks a small feasible region of correlation parameters. Note that we have found the **global** optimization method to be the most robust.

**max_trials**

- **Keywords Area**
- **Model**
- **surrogate**
- **global**
- **gaussian_process**
- **surfpack**
- **max_trials**

Max number of likelihood function evaluations

Specification
**Alias:** none
**Argument(s):** INTEGER

Description
See parent page

**nugget**

- **Keywords Area**
- **model**
- **surrogate**
- **global**
- **gaussian_process**
CHAPTER 6. KEYWORDS AREA

- surfpack
- nugget

Specify a nugget to handle ill-conditioning

**Specification**

**Alias:** none

**Argument(s):** REAL

**Default:** None

**Description**

By default, the Surfpack GP handles ill-conditioning and does not use a nugget. If the user wishes to specify a nugget, there are two approaches.

- The user can specify the value of a nugget with `nugget`.
- Have Surfpack find the optimal value of the nugget. This is specified by `find_nugget`. There are two options for `find_nugget`.
  
  - `find_nugget = 1`: assume that the reciprocal condition number of the correlation matrix $R$, $\text{rcond}_R$, is zero and calculate the nugget needed to make the worst case of $R$ not ill-conditioned.
  
  - `find_nugget = 2`: calculate $\text{rcond}_R$, which requires a Cholesky factorization. If $\text{rcond}_R$ indicates that $R$ is not ill-conditioned, then kriging uses the Cholesky factorization. Otherwise, if $\text{rcond}_R$ says $R$ is ill conditioned, then kriging will calculate the nugget needed to make the worst case of $R$ not ill conditioned.

`find_nugget = 1` and `2` are similar, the second option just takes more computation (the initial Cholesky factorization) for larger problems.

**find_nugget**

- Keywords Area
- model
- surrogate
- global
- gaussian_process
- surfpack
- `find_nugget`

Have Surfpack compute a nugget to handle ill-conditioning

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** None
6.3. **MODEL**

**Description**

By default, the Surfpack GP handles ill-conditioning and does not use a nugget. If the user wishes to specify a nugget, there are two approaches.

- The user can specify the value of a nugget with `nugget`.
- Have Surfpack find the optimal value of the nugget. This is specified by `find_nugget`. There are two options for `find_nugget`.
  - `find_nugget = 1`: assume that the reciprocal condition number of the correlation matrix R, rcondR, is zero and calculate the nugget needed to make the worst case of R not ill-conditioned.
  - `find_nugget = 2`: calculate rcondR, which requires a Cholesky factorization. If rcondR indicates that R is not ill-conditioned, then kriging uses the Cholesky factorization. Otherwise, if rcondR says R is ill conditioned, then kriging will calculate the nugget needed to make the worst case of R not ill-conditioned.

`find_nugget = 1` and `2` are similar, the second option just takes more computation (the initial Cholesky factorization) for larger problems.

**correlation_lengths**

- **Keywords Area**
- **model**
- **surrogate**
- **global**
- **gaussian_process**
- **surfpack**
- **correlation_lengths**

Specify the correlation lengths for the Gaussian process

**Specification**

**Alias**: none

**Argument(s)**: REALLIST

**Default**: internally computed `correlation_lengths`

**Description**

Directly specify `correlation_lengths` as a list of N real numbers where N is the number of input dimensions.
**export_model**

- Keywords Area
- model
- surrogate
- global
- gaussian_process
- surfpack
- export_model

Exports surrogate model in user-selected format

**Topics**

This keyword is related to the topics:

- surrogate_models

**Specification**

Alias: none  
Argument(s): none

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<tr>
<th>Required/Optional Optional</th>
<th>Description of Group</th>
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<th>Dakota Keyword Description</th>
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<tbody>
<tr>
<td>Required</td>
<td>filename_prefix</td>
<td>formats</td>
<td>formats for surrogate model export</td>
</tr>
</tbody>
</table>

**Description**

Export the surrogate for later evaluation using the surfpack executable (bin/surfpack) or a user-developed tool. Export format is controlled using the *formats* specification. Four formats are available in Dakota; however, not all have been enabled for all surrogates.

The four formats are:

- **text_archive** - Plain-text, machine-readable archive for use with the surfpack executable
- **binary_archive** - Binary, machine-readable archive for use with the surfpack executable
- **algebraic_file** - Plain-text, human-readable file intended for use with user-created tools; not compatible with the surfpack executable
- **algebraic_console** - Print the model in algebraic format to the screen; not compatible with the surfpack executable
Most global surrogates can be exported in all four formats. These include:

- Gaussian process (keyword `gaussian_process surfpack`)
- Artificial neural network (keyword `neural_network`)
- Radial basis Functions (keyword `radial_basis`)
- Polynomial (keyword `polynomial`)

However, for Multivariate Adaptive Regression Spline (keyword `mars`) and moving least squares (keyword `moving_least_squares`) models, only `text_archive` and `binary_archive` formats may be used. Currently, no other surrogate models can be exported. In addition, Dakota cannot import models that have been exported. They are strictly for use with external tools.

**Default Behavior**
No export.

**Expected Output**
Output depends on selected format; see the `formats` specification.

**Additional Discussion**
The Dakota examples folder includes a demonstration of using the surfpack executable with an exported model file.

**filename_prefix**

- **Keywords Area**
- model
- surrogate
- global
- `gaussian_process`
- surfpack
- `export_model`
- `filename_prefix`

User-customizable portion of exported model filenames

**Topics**
This keyword is related to the topics:

- surrogate_models

**Specification**

Alias: none

Argument(s): STRING

Default: `exported_surrogate`
Description

When a file-based export of a surrogate model is specified, Dakota writes one file per response, per requested format. The files are named using the pattern \{prefix\}.{response_descriptor}.{extension}.

The response descriptor portion of the pattern is filled in using the response descriptors provided by the user (or, if none are specified, descriptors automatically generated by Dakota). Extension is a three or four letter string that depends on the format. The filename_prefix keyword is used to supply the prefix portion of the pattern.

Examples

This input snippet directs Dakota to write one algebraic format file and one binary archive file for each response. The names of the files will follow the patterns my_surrogate.{response_descriptor}.alg (for the algebraic files) and my_surrogate.{response_descriptor}.bps (for the binary files).

```python
surrogate global gaussian_process surfpack
   export_model
      filename_prefix = 'my_surrogate'
      formats
         algebraic_file
         binary_archive
```
### Description

Select from among the 2-4 available export formats available for this surrogate. Multiple selections are permitted. See `export_model` and the entries for the format selection keywords for further information.

**text_archive**

- Keywords Area
  - model
  - surrogate
  - global
  - gaussian_process
  - surfpack
  - export_model
  - formats
  - text_archive

Export surrogate model to a plain-text archive file

### Topics

This keyword is related to the topics:

- surrogate_models

### Specification

**Alias:** none

**Argument(s):** none
Description

After the surrogate model has been built, Dakota will export it to a plain-text archival file suitable only for use with the surfpack executable (bin/surfpack). The file is named using the pattern \{prefix\}.\{response_descriptor\}.sps, in which ‘sps’ stands for Surfpack Surrogate. See filename.prefix for further information about exported surrogate file naming.

The Dakota examples folder includes a demonstration of using the surfpack executable with an exported model file.

**binary_archive**

- Keywords Area
- model
- surrogate
- global
- gaussian_process
- surfpack
- export_model
- formats
- binary_archive

Export surrogate model to a binary archive file

Topics

This keyword is related to the topics:

- surrogate_models

Specification

Alias: none

Argument(s): none

Description

After the surrogate model has been built, Dakota will export it to a binary archival file suitable only for use with the surfpack executable (bin/surfpack). The file is named using the pattern \{prefix\}.\{response_descriptor\}.bsps, in which ‘bsps’ stands for Binary Surfpack Surrogate. See filename.prefix for further information about exported surrogate file naming.

The Dakota examples folder includes a demonstration of using the surfpack executable with an exported model file.
6.3. MODEL

algebraic_file

- Keywords Area
- model
- surrogate
- global
- gaussian_process
- surfpack
- export_model
- formats
- algebraic_file

Export surrogate model in algebraic format to a file

Topics
This keyword is related to the topics:

- surrogate_models

Specification
Alias: none
Argument(s): none

Description
After the surrogate model has been built, Dakota will export it to a file in a human-readable "algebraic" format. The file is named using the pattern \{prefix\}.{response_descriptor}.alg. See filename_prefix for further information about exported surrogate file naming. The file contains sufficient information for the user to (re)construct and evaluate the model outside of Dakota.

Expected Output
The format depends on the type of surrogate model, but in general will include a LaTeX-like representation of the analytic form of the model to aid tool development, all needed model hyperparameters, and headers describing the shape or dimension of the provided data.

The output written to the file matches exactly the output written to the console when algebraic_console is specified.

algebraic_console

- Keywords Area
- model
- surrogate
- global
Export surrogate model in algebraic format to the console

Topics
This keyword is related to the topics:

- surrogate_models

Specification
Alias: none
Argument(s): none

Description
After the surrogate model has been built, Dakota will export it to the console (screen, or output file if Dakota was run using the -o option) in a human-readable "algebraic" format. The output contains sufficient information for the user to (re)construct and evaluate the model outside of Dakota.

Expected Output
The format depends on the type of surrogate model, but in general will include a LaTeX-like representation of the analytic form of the model to aid tool development, all needed model hyperparameters, and headers describing the shape or dimension of the provided data.

The output written to the screen for the exported model matches exactly the output written to file when algebraic_file is specified. Use of algebraic_file is preferred over algebraic_console, which exists largely to provide a measure of backward compatibility.

mars

- Keywords Area
- model
- surrogate
- global
- mars

Multivariate Adaptive Regression Spline (MARS)

Specification
Alias: none
Argument(s): none
### Description

This surface fitting method uses multivariate adaptive regression splines from the MARS3.5 package [27] developed at Stanford University.

The MARS reference material does not indicate the minimum number of data points that are needed to create a MARS surface model. However, in practice it has been found that at least $n_{\text{quad}}$, and sometimes as many as 2 to 4 times $n_{\text{quad}}$, data points are needed to keep the MARS software from terminating. Provided that sufficient data samples can be obtained, MARS surface models can be useful in SBO and OUU applications, as well as in the prediction of global trends throughout the parameter space.

**Known Issue:** When using discrete variables, there have been sometimes significant differences in surrogate behavior observed across computing platforms in some cases. The cause has not yet been fully diagnosed and is currently under investigation. In addition, guidance on appropriate construction and use of surrogates with discrete variables is under development. In the meantime, users should therefore be aware that there is a risk of inaccurate results when using surrogates with discrete variables.

### Theory

The form of the MARS model is based on the following expression:

$$\hat{f}(x) = \sum_{m=1}^{M} a_m B_m(x)$$

where the $a_m$ are the coefficients of the truncated power basis functions $B_m$, and $M$ is the number of basis functions. The MARS software partitions the parameter space into subregions, and then applies forward and backward regression methods to create a local surface model in each subregion. The result is that each subregion contains its own basis functions and coefficients, and the subregions are joined together to produce a smooth, $C^2$-continuous surface model.

MARS is a nonparametric surface fitting method and can represent complex multimodal data trends. The regression component of MARS generates a surface model that is not guaranteed to pass through all of the response data values. Thus, like the quadratic polynomial model, it provides some smoothing of the data.
CHAPTER 6. KEYWORDS AREA

- surrogate
- global
- mars
- max_bases

Maximum number of MARS bases

**Specification**

**Alias:** none  
**Argument(s):** INTEGER

**Description**

The maximum number of basis functions allowed in the MARS approximation model.

**interpolation**

- **Keywords Area**
- model
- surrogate
- global
- mars
- **interpolation**

MARS model interpolation type

**Specification**

**Alias:** none  
**Argument(s):** none

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<tr>
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<th>Description of Group Interpolation Order (Group 1)</th>
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<th>Dakota Keyword Description</th>
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<td>Linear interpolation</td>
</tr>
<tr>
<td></td>
<td></td>
<td>cubic</td>
<td>Cubic interpolation</td>
</tr>
</tbody>
</table>

**Description**

The MARS model interpolation type: linear or cubic.
6.3. MODEL

**linear**
- Keywords Area
- model
- surrogate
- global
- mars
- interpolation
- linear

Linear interpolation

**Specification**

**Alias:** none
- **Argument(s):** none

**Description**

Use linear interpolation in the MARS model.

**cubic**
- Keywords Area
- model
- surrogate
- global
- mars
- interpolation
- cubic

Cubic interpolation

**Specification**

**Alias:** none
- **Argument(s):** none

**Description**

Use cubic interpolation in the MARS model.
**export_model**

- **Keywords Area**
- **model**
- **surrogate**
- **global**
- **mars**
- **export_model**

Exports surrogate model in user-selected format

**Topics**

This keyword is related to the topics:

- **surrogate_models**

**Specification**

**Alias:** none  
**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
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<th>Dakota Keyword Description</th>
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<tbody>
<tr>
<td>Optional</td>
<td>filename_prefix</td>
<td>formats</td>
<td>User-customizable portion of exported model filenames</td>
</tr>
<tr>
<td>Required</td>
<td></td>
<td></td>
<td>Formats for surrogate model export</td>
</tr>
</tbody>
</table>

**Description**

Export the surrogate for later evaluation using the surfpack executable (bin/surfpack) or a user-developed tool. Export format is controlled using the `formats` specification. Four formats are available in Dakota; however, not all have been enabled for all surrogates.

The four formats are:

- **text_archive** - Plain-text, machine-readable archive for use with the surfpack executable
- **binary_archive** - Binary, machine-readable archive for use with the surfpack executable
- **algebraic_file** - Plain-text, human-readable file intended for use with user-created tools; not compatible with the surfpack executable
- **algebraic_console** - Print the model in algebraic format to the screen; not compatible with the surfpack executable

Most global surrogates can be exported in all four formats. These include:
6.3. \textit{MODEL}

- Gaussian process (keyword \texttt{gaussian\_process surfpack})
- Artificial neural network (keyword \texttt{neural\_network})
- Radial basis Functions (keyword \texttt{radial\_basis})
- Polynomial (keyword \texttt{polynomial})

However, for Multivariate Adaptive Regression Spline (keyword \texttt{mars}) and moving least squares (keyword \texttt{moving\_least\_squares}) models, only text archive and binary archive formats may be used. Currently, no other surrogate models can be exported. In addition, Dakota cannot import models that have been exported. They are strictly for use with external tools.

\textbf{Default Behavior}
No export.

\textbf{Expected Output}
Output depends on selected format; see the formats specification.

\textbf{Additional Discussion}
The Dakota examples folder includes a demonstration of using the surfpack executable with an exported model file.

\textit{filename\_prefix}

- Keywords Area
- model
- surrogate
- global
- mars
- export\_model
- filename\_prefix

User-customizable portion of exported model filenames

\textbf{Topics}
This keyword is related to the topics:

- surrogate\_models

\textbf{Specification}
\textit{Alias}: none
\textit{Argument(s)}: \texttt{STRING}
\textit{Default}: exported\_surrogate
CHAPTER 6. KEYWORDS AREA

Description
When a file-based export of a surrogate model is specified, Dakota writes one file per response, per requested format. The files are named using the pattern `{prefix}.{response_descriptor}.{extension}`.

The `response_descriptor` portion of the pattern is filled in using the response descriptors provided by the user (or, if none are specified, descriptors automatically generated by Dakota). Extension is a three or four letter string that depends on the format. The `filename_prefix` keyword is used to supply the prefix portion of the pattern.

Examples
This input snippet directs Dakota to write one algebraic format file and one binary archive file for each response. The names of the files will follow the patterns `my_surrogate.{response_descriptor}.alg` (for the algebraic files) and `my_surrogate.{response_descriptor}.bsps` (for the binary files).

```
surrogate global gaussian_process surfpack
export_model
    filename_prefix = 'my_surrogate'
    formats
        algebraic_file
        binary_archive
```

Formats for surrogate model export

Topics
This keyword is related to the topics:

• surrogate_models

Specification
Alias: none
Argument(s): none

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<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<tbody>
<tr>
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<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
6.3. MODEL

<table>
<thead>
<tr>
<th>Optional</th>
<th>text_archive</th>
<th>Export surrogate model to a plain-text archive file</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>binary_archive</td>
<td>Export surrogate model to a binary archive file</td>
</tr>
</tbody>
</table>

**Description**

Select from among the 2-4 available export formats available for this surrogate. Multiple selections are permitted. See `export_model` and the entries for the format selection keywords for further information.

- **text_archive**
  - Keywords Area
  - model
  - surrogate
  - global
  - mars
  - export_model
  - formats
  - text_archive

  Export surrogate model to a plain-text archive file

**Topics**

This keyword is related to the topics:

- surrogate_models

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

After the surrogate model has been built, Dakota will export it to a plain-text archival file suitable only for use with the surfpack executable (`bin/surfpack`). The file is named using the pattern `{prefix}.{response_descriptor}.sps`, in which `sps` stands for Surfpack Surrogate. See `filename_prefix` for further information about exported surrogate file naming.

The Dakota examples folder includes a demonstration of using the surfpack executable with an exported model file.
Export surrogate model to a binary archive file

**Topics**

This keyword is related to the topics:

- surrogate_models

**Specification**

Alias: none

Argument(s): none

**Description**

After the surrogate model has been built, Dakota will export it to a binary archival file suitable only for use with the surfpack executable (bin/surfpack). The file is named using the pattern `{prefix}.response-descriptor.bsp`, in which 'bsp' stands for Binary Surfpack Surrogate. See `filename.prefix` for further information about exported surrogate file naming.

The Dakota examples folder includes a demonstration of using the surfpack executable with an exported model file.

**moving_least_squares**

- Keywords Area
- model
- surrogate
- global
- moving_least_squares

Moving Least Squares surrogate models

**Specification**

Alias: none

Argument(s): none
## Description

Moving least squares is a further generalization of weighted least squares where the weighting is "moved" or recalculated for every new point where a prediction is desired[64].

**The implementation of moving least squares is still under development.** It tends to work well in trust region optimization methods where the surrogate model is constructed in a constrained region over a few points. The present implementation may not work as well globally.

**Known Issue:** When using discrete variables, there have been sometimes significant differences in surrogate behavior observed across computing platforms in some cases. The cause has not yet been fully diagnosed and is currently under investigation. In addition, guidance on appropriate construction and use of surrogates with discrete variables is under development. In the meantime, users should therefore be aware that there is a risk of inaccurate results when using surrogates with discrete variables.

## Theory

Moving Least Squares can be considered a more specialized version of linear regression models. In linear regression, one usually attempts to minimize the sum of the squared residuals, where the residual is defined as the difference between the surrogate model and the true model at a fixed number of points.

In weighted least squares, the residual terms are weighted so the determination of the optimal coefficients governing the polynomial regression function, denoted by \( \hat{f}(x) \), are obtained by minimizing the weighted sum of squares at \( N \) data points:

\[
\sum_{n=1}^{N} w_n(\| \hat{f}(x_n) - f(x_n) \|)
\]

**basis_order**

- **Keywords Area**
- model
- surrogate
- **global**

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<tr>
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<th>Description of Group</th>
<th>Dakota Keyword</th>
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<tr>
<td>Optional</td>
<td></td>
<td>basis_order</td>
<td>Polynomial order for the MLS bases</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>weight_function</td>
<td>Selects the weight function for the MLS model</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>export_model</td>
<td>Exports surrogate model in user-selected format</td>
</tr>
</tbody>
</table>
• moving_least_squares
• basis_order

Polynomial order for the MLS bases

**Specification**

Alias: poly_order

Argument(s): INTEGER

**Description**

The polynomial order for the moving least squares basis function (default = 2).

weight_function

• Keywords Area

• model

• surrogate

• global

• moving_least_squares

• weight_function

Selects the weight function for the MLS model

**Specification**

Alias: none

Argument(s): INTEGER

**Description**

The weight function decays as a function of distance from the training data. Specify one of:

• 1 (default): exponential decay in weight function; once differentiable MLS model

• 2: twice differentiable MLS model

• 3: three times differentiable MLS model
6.3. MODEL

export_model

- Keywords Area
- model
- surrogate
- global
- moving_least_squares
- export_model

Exports surrogate model in user-selected format

Topics

This keyword is related to the topics:

- surrogate_models

Specification

Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
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<td>formats</td>
<td>User-customizable portion of exported model filenames</td>
</tr>
<tr>
<td>Required</td>
<td></td>
<td>formats</td>
<td>Formats for surrogate model export</td>
</tr>
</tbody>
</table>

Description

Export the surrogate for later evaluation using the surfpack executable (bin/surfpack) or a user-developed tool. Export format is controlled using the formats specification. Four formats are available in Dakota; however, not all have been enabled for all surrogates.

The four formats are:

- **text_archive** - Plain-text, machine-readable archive for use with the surfpack executable
- **binary_archive** - Binary, machine-readable archive for use with the surfpack executable
- **algebraic_file** - Plain-text, human-readable file intended for use with user-created tools; not compatible with the surfpack executable
- **algebraic_console** - Print the model in algebraic format to the screen; not compatible with the surfpack executable

Most global surrogates can be exported in all four formats. These include:
CHAPTER 6. KEYWORDS AREA

- Gaussian process (keyword `gaussian_process surfpack`)
- Artificial neural network (keyword `neural_network`)
- Radial basis Functions (keyword `radial_basis`)
- Polynomial (keyword `polynomial`)

However, for Multivariate Adaptive Regression Spline (keyword `mars`) and moving least squares (keyword `moving_least_squares`) models, only `text_archive` and `binary_archive` formats may be used. Currently, no other surrogate models can be exported. In addition, Dakota cannot import models that have been exported. They are strictly for use with external tools.

**Default Behavior**
No export.

**Expected Output**
Output depends on selected format; see the `formats` specification.

**Additional Discussion**
The Dakota examples folder includes a demonstration of using the surfpack executable with an exported model file.

**filename_prefix**

- Keywords Area
- model
- surrogate
- global
- moving_least_squares
- export_model
- filename_prefix

User-customizable portion of exported model filenames

**Topics**
This keyword is related to the topics:

- surrogate_models

**Specification**

**Alias:** none

**Argument(s):** STRING

**Default:** exported_surrogate
6.3. MODEL

Description

When a file-based export of a surrogate model is specified, Dakota writes one file per response, per requested format. The files are named using the pattern \{prefix\}.{response_descriptor}.{extension}.

The response_descriptor portion of the pattern is filled in using the response descriptors provided by the user (or, if none are specified, descriptors automatically generated by Dakota). Extension is a three or four letter string that depends on the format. The filename_prefix keyword is used to supply the prefix portion of the pattern.

Examples

This input snippet directs Dakota to write one algebraic format file and one binary archive file for each response. The names of the files will follow the patterns my_surrogate.{response_descriptor}.alg (for the algebraic files) and my_surrogate.{response_descriptor}.bsps (for the binary files).

```
surrogate global gaussian_process surfpack
    export_model
        filename_prefix = 'my_surrogate'
        formats
            algebraic_file
            binary_archive
```

Formats

- Keywords Area
- model
- surrogate
- global
- moving_least_squares
- export_model
- formats

Formats for surrogate model export

Topics

This keyword is related to the topics:

- surrogate_models

Specification

Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
CHAPTER 6. KEYWORDS AREA

Optional | **text_archive** | Export surrogate model to a plain-text archive file
Optional | **binary_archive** | Export surrogate model to a binary archive file

**Description**

Select from among the 2-4 available export formats available for this surrogate. Multiple selections are permitted. See `export_model` and the entries for the format selection keywords for further information.

- **text_archive**
  - Keywords Area
  - model
  - surrogate
  - global
  - moving_least_squares
  - export_model
  - formats
  - text_archive

Export surrogate model to a plain-text archive file

**Topics**

This keyword is related to the topics:

- surrogate_models

**Specification**

*Alias*: none

*Argument(s)*: none

**Description**

After the surrogate model has been built, Dakota will export it to a plain-text archival file suitable only for use with the surfpack executable (`bin/surfpack`). The file is named using the pattern `{prefix}.{response_descriptor}.sps`, in which `sps` stands for Surfpack Surrogate. See `filename_prefix` for further information about exported surrogate file naming.

The Dakota examples folder includes a demonstration of using the surfpack executable with an exported model file.
6.3. MODEL

binary_archive

- Keywords Area
- model
- surrogate
- global
- moving_least_squares
- export_model
- formats
- binary_archive

Export surrogate model to a binary archive file

Topics
This keyword is related to the topics:
- surrogate_models

Specification

Alias: none
Argument(s): none

Description
After the surrogate model has been built, Dakota will export it to a binary archival file suitable only for use with the surfpack executable (bin/surfpack). The file is named using the pattern {prefix}.{response_descriptor}.bsps, in which 'bsps' stands for Binary Surfpack Surrogate. See filename_prefix for further information about exported surrogate file naming.

The Dakota examples folder includes a demonstration of using the surfpack executable with an exported model file.

neural_network

- Keywords Area
- model
- surrogate
- global
- neural_network

Artificial neural network model

Specification

Alias: none
Argument(s): none
### Description

Dakota’s artificial neural network surrogate is a stochastic layered perceptron network, with a single hidden layer. Weights for the input layer are chosen randomly, while those in the hidden layer are estimated from data using a variant of the Zimmerman direct training approach\[93\].

This typically yields lower training cost than traditional neural networks, yet good out-of-sample performance. This is helpful in surrogate-based optimization and optimization under uncertainty, where multiple surrogates may be repeatedly constructed during the optimization process, e.g., a surrogate per response function, and a new surrogate for each optimization iteration.

The neural network is a non parametric surface fitting method. Thus, along with Kriging (Gaussian Process) and MARS, it can be used to model data trends that have slope discontinuities as well as multiple maxima and minima. However, unlike Kriging, the neural network surrogate is not guaranteed to interpolate the data from which it was constructed.

This surrogate can be constructed from fewer than $n_{\text{quad}}$ data points, however, it is a good rule of thumb to use at least $n_{\text{quad}}$ data points when possible.

**Known Issue:** When using discrete variables, there have been sometimes significant differences in surrogate behavior observed across computing platforms in some cases. The cause has not yet been fully diagnosed and is currently under investigation. In addition, guidance on appropriate construction and use of surrogates with discrete variables is under development. In the meantime, users should therefore be aware that there is a risk of inaccurate results when using surrogates with discrete variables.

### Theory

The form of the neural network model is

$$\hat{f}(x) \approx \tanh \{ A_1 \tanh (A_0^T x + \theta_0^T) + \theta_1 \}$$

where $x$ is the evaluation point in $n$-dimensional parameter space; the terms $A_0, \theta_0$ are the random input layer weight matrix and bias vector, respectively; and $A_1, \theta_1$ are a weight vector and bias scalar, respectively, estimated from training data. These coefficients are analogous to the polynomial coefficients obtained from regression to training data. The neural network uses a cross validation-based orthogonal matching pursuit solver to determine the optimal number of nodes and to solve for the weights and offsets.

### Table

<table>
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<tr>
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<td>Maximum number of hidden layer nodes</td>
</tr>
<tr>
<td>Optional</td>
<td>range</td>
<td>range</td>
<td>Range for neural network random weights</td>
</tr>
<tr>
<td>Optional</td>
<td>random_weight</td>
<td>random_weight</td>
<td>(Inactive) Random weight control</td>
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<tr>
<td>Optional</td>
<td>export_model</td>
<td>export_model</td>
<td>Exports surrogate model in user-selected format</td>
</tr>
</tbody>
</table>
max_nodes

- Keywords Area
- model
- surrogate
- global
- neural_network
- max_nodes

Maximum number of hidden layer nodes

Topics
This keyword is related to the topics:
- surrogate_models

Specification
Alias: nodes
Argument(s): INTEGER
Default: numTrainingData - 1

Description
Limits the maximum number of hidden layer nodes in the neural network model. The default is to use one less node than the number of available training data points yielding a fully-determined linear least squares problem. However, reducing the number of nodes can help reduce overfitting and more importantly, can drastically reduce surrogate construction time when building from a large data set. (Historically, Dakota limited the number of nodes to 100.)

The keyword max_nodes provides an upper bound. Dakota’s orthogonal matching pursuit algorithm may further reduce the effective number of nodes in the final model to achieve better generalization to unseen points.

range

- Keywords Area
- model
- surrogate
- global
- neural_network
- range

Range for neural network random weights
Topics
This keyword is related to the topics:

- surrogate_models

Specification
Alias: none
Argument(s): REAL

Description
Controls the range of the input layer random weights in the neural network model. The default range is 2.0, resulting in weights in (-1, 1). These weights are applied after the training inputs have been scaled into [-0.8, 0.8].

random_weight

- Keywords Area
- model
- surrogate
- global
- neural_network
- random_weight

(Inactive) Random weight control

Topics
This keyword is related to the topics:

- surrogate_models

Specification
Alias: none
Argument(s): INTEGER

Description
This option is not currently in use and is likely to be removed
6.3. **MODEL**

**export_model**

- **Keywords Area**
- **model**
- **surrogate**
- **global**
- **neural_network**
- **export_model**

Exports surrogate model in user-selected format

**Topics**

This keyword is related to the topics:

- **surrogate_models**

**Specification**

**Alias:** none

**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>filename &amp; prefix</td>
<td>Dakota Keyword</td>
<td>formats</td>
<td>User-customizable portion of exported model filenames</td>
</tr>
<tr>
<td>Optional</td>
<td>filename &amp; prefix</td>
<td>formats</td>
<td>Formats for surrogate model export</td>
</tr>
</tbody>
</table>

**Description**

Export the surrogate for later evaluation using the surfpack executable (bin/surfpack) or a user-developed tool. Export format is controlled using the *formats* specification. Four formats are available in Dakota; however, not all have been enabled for all surrogates.

The four formats are:

- **text_archive** - Plain-text, machine-readable archive for use with the surfpack executable
- **binary_archive** - Binary, machine-readable archive for use with the surfpack executable
- **algebraic_file** - Plain-text, human-readable file intended for use with user-created tools; not compatible with the surfpack executable
- **algebraic_console** - Print the model in algebraic format to the screen; not compatible with the surfpack executable

Most global surrogates can be exported in all four formats. These include:
• Gaussian process (keyword gaussian_process surfpack)

• Artificial neural network (keyword neural_network)

• Radial basis Functions (keyword radial_basis)

• Polynomial (keyword polynomial)

However, for Multivariate Adaptive Regression Spline (keyword mars) and moving least squares (keyword moving_least_squares) models, only text_archive and binary_archive formats may be used. Currently, no other surrogate models can be exported. In addition, Dakota cannot import models that have been exported. They are strictly for use with external tools.

**Default Behavior**
No export.

**Expected Output**
Output depends on selected format; see the formats specification.

**Additional Discussion**
The Dakota examples folder includes a demonstration of using the surfpack executable with an exported model file.

```
filename_prefix
```

• Keywords Area

• model

• surrogate

• global

• neural_network

• export_model

• filename_prefix

User-customizable portion of exported model filenames

**Topics**
This keyword is related to the topics:

• surrogate_models

**Specification**

Alias: none

Argument(s): STRING

Default: exported_surrogate
6.3. MODEL

Description

When a file-based export of a surrogate model is specified, Dakota writes one file per response, per requested format. The files are named using the pattern `{prefix}.{response_descriptor}.{extension}`.

The `response_descriptor` portion of the pattern is filled in using the response descriptors provided by the user (or, if none are specified, descriptors automatically generated by Dakota). Extension is a three or four letter string that depends on the format. The `filename_prefix` keyword is used to supply the prefix portion of the pattern.

Examples

This input snippet directs Dakota to write one algebraic format file and one binary archive file for each response. The names of the files will follow the patterns `my_surrogate.{response_descriptor}.alg` (for the algebraic files) and `my_surrogate.{response_descriptor}.bsps` (for the binary files).

```
surrogate global gaussian_process surfpack
export_model
  filename_prefix = 'my_surrogate'
formats
  algebraic_file
  binary_archive
```

Formats

- Keywords Area
- model
- surrogate
- global
- neural_network
- export_model
- formats

Formats for surrogate model export

Topics

This keyword is related to the topics:

- surrogate_models

Specification

Alias: none

Argument(s): none

<p>| Required/- | Description of | Dakota Keyword | Dakota Keyword |</p>
<table>
<thead>
<tr>
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<th>Group</th>
<th></th>
<th>Description</th>
</tr>
</thead>
</table>
CHAPTER 6. KEYWORDS AREA

<table>
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<tr>
<th>Optional</th>
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<th>Export surrogate model to a plain-text archive file</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>binary_archive</td>
<td>Export surrogate model to a binary archive file</td>
</tr>
<tr>
<td>Optional</td>
<td>algebraic_file</td>
<td>Export surrogate model in algebraic format to a file</td>
</tr>
<tr>
<td>Optional</td>
<td>algebraic_console</td>
<td>Export surrogate model in algebraic format to the console</td>
</tr>
</tbody>
</table>

**Description**

Select from among the 2-4 available export formats available for this surrogate. Multiple selections are permitted. See export_model and the entries for the format selection keywords for further information.

**text_archive**

- Keywords Area
- model
- surrogate
- global
- neural_network
- export_model
- formats
- text_archive

Export surrogate model to a plain-text archive file

**Topics**

This keyword is related to the topics:

- surrogate_models

**Specification**

Alias: none

Argument(s): none
6.3. MODEL

Description

After the surrogate model has been built, Dakota will export it to a plain-text archival file suitable only for use with the surfpack executable (bin/surfpack). The file is named using the pattern `{prefix}.{response_descriptor}.sps`, in which 'sps' stands for Surfpack Surrogate. See `filename_prefix` for further information about exported surrogate file naming.

The Dakota examples folder includes a demonstration of using the surfpack executable with an exported model file.

---

binary_archive

- Keywords Area
- model
- surrogate
- global
- neural_network
- export_model
- formats
- binary_archive

Export surrogate model to a binary archive file

---

Topics

This keyword is related to the topics:

- surrogate_models

---

Specification

Alias: none

Argument(s): none

---

Description

After the surrogate model has been built, Dakota will export it to a binary archival file suitable only for use with the surfpack executable (bin/surfpack). The file is named using the pattern `{prefix}.{response_descriptor}.bsps`, in which 'bsps' stands for Binary Surfpack Surrogate. See `filename_prefix` for further information about exported surrogate file naming.

The Dakota examples folder includes a demonstration of using the surfpack executable with an exported model file.
algebraic_file

- Keywords Area
- model
- surrogate
- global
- neural_network
- export_model
- formats
- algebraic_file

Export surrogate model in algebraic format to a file

Topics

This keyword is related to the topics:

- surrogate_models

Specification

Alias: none

Argument(s): none

Description

After the surrogate model has been built, Dakota will export it to a file in a human-readable "algebraic" format. The file is named using the pattern \{prefix\}.{response_descriptor}.alg. See filename_prefix for further information about exported surrogate file naming. The file contains sufficient information for the user to (re)construct and evaluate the model outside of Dakota.

Expected Output

The format depends on the type of surrogate model, but in general will include a LaTeX-like representation of the analytic form of the model to aid tool development, all needed model hyperparameters, and headers describing the shape or dimension of the provided data.

The output written to the file matches exactly the output written to the console when algebraic_console is specified.
6.3. MODEL

- export_model
- formats
- algebraic_console

Export surrogate model in algebraic format to the console

Topics

This keyword is related to the topics:
- surrogate_models

Specification

Alias: none
Argument(s): none

Description

After the surrogate model has been built, Dakota will export it to the console (screen, or output file if Dakota was run using the -o option) in a human-readable “algebraic” format. The output contains sufficient information for the user to (re)construct and evaluate the model outside of Dakota.

Expected Output

The format depends on the type of surrogate model, but in general will include a LaTeX-like representation of the analytic form of the model to aid tool development, all needed model hyperparameters, and headers describing the shape or dimension of the provided data.

The output written to the screen for the exported model matches exactly the output written to file when algebraic_file is specified. Use of algebraic_file is preferred over algebraic_console, which exists largely to provide a measure of backward compatibility.

radial_basis

- Keywords Area
- model
- surrogate
- global
- radial_basis

Radial basis function (RBF) model

Specification

Alias: none
Argument(s): none
### Description

Radial basis functions $\phi$ are functions whose value typically depends on the distance from a center point, called the centroid, $c$.

The surrogate model approximation comprises a sum of $K$ weighted radial basis functions:

$$\hat{f}(x) = \sum_{k=1}^{K} w_k \phi(\|x - c_k\|)$$

These basis functions take many forms, but Gaussian kernels or splines are most common. The Dakota implementation uses a Gaussian radial basis function. The weights are determined via a linear least squares solution approach. See[67] for more details.

**Known Issue**: When using discrete variables, there have been sometimes significant differences in surrogate behavior observed across computing platforms in some cases. The cause has not yet been fully diagnosed and is currently under investigation. In addition, guidance on appropriate construction and use of surrogates with discrete variables is under development. In the meantime, users should therefore be aware that there is a risk of inaccurate results when using surrogates with discrete variables.

### Dakota Keyword Description

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
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</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>bases</td>
<td>bases</td>
<td>Initial number of radial basis functions</td>
</tr>
<tr>
<td>Optional</td>
<td>max_pts</td>
<td>max</td>
<td>Maximum number of RBF CVT points</td>
</tr>
<tr>
<td>Optional</td>
<td>min_partition</td>
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<td>(Inactive) Minimum RBF partition</td>
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<tr>
<td>Optional</td>
<td>max_subsets</td>
<td>max_subsets</td>
<td>Number of trial RBF subsets</td>
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<tr>
<td>Optional</td>
<td>export_model</td>
<td>export_model</td>
<td>Exports surrogate model in user-selected format</td>
</tr>
</tbody>
</table>

---

**bases**
- **Keywords Area**
- **model**
- **surrogate**
- **global**
- **radial_basis**
6.3. MODEL

- bases

Initial number of radial basis functions

Topics
This keyword is related to the topics:
- surrogate_models

Specification
Alias: none
Argument(s): INTEGER

Description
Initial number of radial basis functions. The default value is the smaller of the number of training points and 100.

max_pts
- Keywords Area
- model
- surrogate
- global
- radial_basis
- max_pts

Maximum number of RBF CVT points

Topics
This keyword is related to the topics:
- surrogate_models

Specification
Alias: none
Argument(s): INTEGER

Description
Maximum number of CVT points to use in generating each RBF center. Basis computing centroid of each. Defaults to $10 \times \text{(bases)}$. Reducing this will reduce model build time.
min_partition

- Keywords Area
- model
- surrogate
- global
- radial_basis
- min_partition

(Inactive) Minimum RBF partition

Topics
This keyword is related to the topics:

- surrogate_models

Specification
Alias: none
Argument(s): INTEGER

Description
This option currently has no effect and will likely be removed.

max_subsets

- Keywords Area
- model
- surrogate
- global
- radial_basis
- max_subsets

Number of trial RBF subsets

Topics
This keyword is related to the topics:

- surrogate_models
6.3. MODEL

Specification

Alias: none
Argument(s): INTEGER

Description

Number of passes to take to identify the best subset of basis functions to use. Defaults to the smaller of $3 \times (\text{bases})$ and 100.

```
export_model
```

- Keywords Area
- model
- surrogate
- global
- radial_basis
- export_model

Exports surrogate model in user-selected format

Topics

This keyword is related to the topics:

- surrogate_models

Specification

Alias: none
Argument(s): none

<table>
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<tr>
<th>Required/-</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<tr>
<td>Optional</td>
<td>filename_prefix</td>
<td>formats</td>
<td>User-customizable portion of exported model filenames</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td></td>
<td>Formats for surrogate model export</td>
</tr>
<tr>
<td>Required</td>
<td></td>
<td></td>
<td>Return value of export_model</td>
</tr>
</tbody>
</table>

Description

Export the surrogate for later evaluation using the surfpack executable ($\text{bin/surfpack}$) or a user-developed tool. Export format is controlled using the \text{formats} specification. Four formats are available in Dakota; however, not all have been enabled for all surrogates.

The four formats are:

- text_archive - Plain-text, machine-readable archive for use with the surfpack executable
CHAPTER 6. KEYWORDS AREA

- **binary_archive** - Binary, machine-readable archive for use with the surfpack executable

- **algebraic_file** - Plain-text, human-readable file intended for use with user-created tools; not compatible with the surfpack executable

- **algebraic_console** - Print the model in algebraic format to the screen; not compatible with the surfpack executable

Most global surrogates can be exported in all four formats. These include:

- Gaussian process (keyword `gaussian_process` surfpack)

- Artificial neural network (keyword `neural_network`)

- Radial basis Functions (keyword `radial_basis`)

- Polynomial (keyword `polynomial`)

However, for Multivariate Adaptive Regression Spline (keyword `mars`) and moving least squares (keyword `moving_least_squares`) models, only text_archive and binary_archive formats may be used. Currently, no other surrogate models can be exported. In addition, Dakota cannot import models that have been exported. They are strictly for use with external tools.

**Default Behavior**
No export.

**Expected Output**
Output depends on selected format; see the formats specification.

**Additional Discussion**
The Dakota examples folder includes a demonstration of using the surfpack executable with an exported model file.

**filename_prefix**

- Keywords Area
- model
- surrogate
- global
- radial_basis
- export_model
- filename_prefix

User-customizable portion of exported model filenames

**Topics**
This keyword is related to the topics:

- surrogate_models
6.3. MODEL

Specification

Alias: none

Argument(s): STRING

Default: exported_surrogate

Description

When a file-based export of a surrogate model is specified, Dakota writes one file per response, per requested format. The files are named using the pattern \{prefix\}.\{response_descriptor\}.\{extension\}.

The response_descriptor portion of the pattern is filled in using the response descriptors provided by the user (or, if none are specified, descriptors automatically generated by Dakota). Extension is a three or four letter string that depends on the format. The filename_prefix keyword is used to supply the prefix portion of the pattern.

Examples

This input snippet directs Dakota to write one algebraic format file and one binary archive file for each response. The names of the files will follow the patterns my_surrogate.\{response Descriptor\}.alg (for the algebraic files) and my_surrogate.\{response Descriptor\}.bsps (for the binary files).

```
surrogate global gaussian_process surfpack
  export_model
    filename_prefix = 'my_surrogate'
    formats
      algebraic_file
      binary_archive

    formats
      • Keywords Area
      • model
      • surrogate
      • global
      • radial_basis
      • export_model
      • formats

    Formats for surrogate model export
```

Topics

This keyword is related to the topics:

• surrogate_models

Specification

Alias: none

Argument(s): none
### Description

Select from among the 2-4 available export formats available for this surrogate. Multiple selections are permitted. See `export_model` and the entries for the format selection keywords for further information.

- **text_archive**
  - Keywords Area
  - model
  - surrogate
  - global
  - radial_basis
  - export_model
  - formats
  - text_archive

Export surrogate model to a plain-text archive file

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<tbody>
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<td>text_archive</td>
<td>Export surrogate model to a plain-text archive file</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>binary_archive</td>
<td>Export surrogate model to a binary archive file</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>algebraic_file</td>
<td>Export surrogate model in algebraic format to a file</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>algebraic_console</td>
<td>Export surrogate model in algebraic format to the console</td>
</tr>
</tbody>
</table>

### Topics

This keyword is related to the topics:

- surrogate_models

### Specification

**Alias:** none

**Argument(s):** none
6.3. **MODEL**

**Description**

After the surrogate model has been built, Dakota will export it to a plain-text archival file suitable only for use with the surfpack executable (bin/surfpack). The file is named using the pattern `{prefix}.{response_descriptor}.sps`, in which 'sps' stands for Surfpack Surrogate. See `filename_prefix` for further information about exported surrogate file naming.

The Dakota examples folder includes a demonstration of using the surfpack executable with an exported model file.

```plaintext
binary_archive

- Keywords Area
- model
- surrogate
- global
- radial_basis
- export_model
- formats
- binary_archive
```

Export surrogate model to a binary archive file

**Topics**

This keyword is related to the topics:

- surrogate_models

**Specification**

*Alias:* none

*Argument(s):* none

**Description**

After the surrogate model has been built, Dakota will export it to a binary archival file suitable only for use with the surfpack executable (bin/surfpack). The file is named using the pattern `{prefix}.{response_descriptor}.bsps`, in which 'bsps' stands for Binary Surfpack Surrogate. See `filename_prefix` for further information about exported surrogate file naming.

The Dakota examples folder includes a demonstration of using the surfpack executable with an exported model file.
algebraic_file

- Keywords Area
- model
- surrogate
- global
- radial_basis
- export_model
- formats
- algebraic_file

Export surrogate model in algebraic format to a file

**Topics**

This keyword is related to the topics:

- surrogate_models

**Specification**

**Alias:** none  
**Argument(s):** none

**Description**

After the surrogate model has been built, Dakota will export it to a file in a human-readable "algebraic" format. The file is named using the pattern `{prefix}.{response_descriptor}.alg`. See `filename_prefix` for further information about exported surrogate file naming. The file contains sufficient information for the user to (re)construct and evaluate the model outside of Dakota.

**Expected Output**

The format depends on the type of surrogate model, but in general will include a LaTeX-like representation of the analytic form of the model to aid tool development, all needed model hyperparameters, and headers describing the shape or dimension of the provided data.

The output written to the file matches exactly the output written to the console when `algebraic_console` is specified.
6.3. MODEL

- export_model
- formats
- algebraic_console

Export surrogate model in algebraic format to the console

Topics
This keyword is related to the topics:
- surrogate_models

Specification
Alias: none
Argument(s): none

Description
After the surrogate model has been built, Dakota will export it to the console (screen, or output file if Dakota was run using the -o option) in a human-readable "algebraic" format. The output contains sufficient information for the user to (re)construct and evaluate the model outside of Dakota.

Expected Output
The format depends on the type of surrogate model, but in general will include a LaTeX-like representation of the analytic form of the model to aid tool development, all needed model hyperparameters, and headers describing the shape or dimension of the provided data.

The output written to the screen for the exported model matches exactly the output written to file when algebraic_file is specified. Use of algebraic_file is preferred over algebraic_console, which exists largely to provide a measure of backward compatibility.

polynomial
- Keywords Area
- model
- surrogate
- global
- polynomial

Polynomial surrogate model

Specification
Alias: none
Argument(s): none
### Description

Linear, quadratic, and cubic polynomial surrogate models are available in Dakota. The utility of the simple polynomial models stems from two sources:

- over a small portion of the parameter space, a low-order polynomial model is often an accurate approximation to the true data trends
- the least-squares procedure provides a surface fit that smooths out noise in the data.

Local surrogate-based optimization methods (surrogate_based_local) are often successful when using polynomial models, particularly quadratic models. However, a polynomial surface fit may not be the best choice for modeling data trends globally over the entire parameter space, unless it is known a priori that the true data trends are close to linear, quadratic, or cubic. See[63] for more information on polynomial models.

**Known Issue:** *When using discrete variables, there have been sometimes significant differences in surrogate behavior observed across computing platforms in some cases. The cause has not yet been fully diagnosed and is currently under investigation. In addition, guidance on appropriate construction and use of surrogates with discrete variables is under development. In the meantime, users should therefore be aware that there is a risk of inaccurate results when using surrogates with discrete variables.*

### Theory

The form of the linear polynomial model is

\[
\hat{f}(\mathbf{x}) \approx c_0 + \sum_{i=1}^{n} c_i x_i
\]

the form of the quadratic polynomial model is:

\[
\hat{f}(\mathbf{x}) \approx c_0 + \sum_{i=1}^{n} c_i x_i + \sum_{i=1}^{n} \sum_{j \geq i}^{n} c_{ij} x_i x_j
\]
and the form of the cubic polynomial model is:

\[ \hat{f}(x) \approx c_0 + \sum_{i=1}^{n} c_i x_i + \sum_{i=1}^{n} \sum_{j \geq i}^{n} c_{ij} x_i x_j + \sum_{i=1}^{n} \sum_{j \geq i}^{n} \sum_{k \geq j}^{n} c_{ijk} x_i x_j x_k \]

In all of the polynomial models, \( \hat{f}(x) \) is the response of the polynomial model; the \( x_i, x_j, x_k \) terms are the components of the \( n \)-dimensional design parameter values; the \( c_0, c_i, c_{ij}, c_{ijk} \) terms are the polynomial coefficients, and \( n \) is the number of design parameters. The number of coefficients, \( n_c \), depends on the order of polynomial model and the number of design parameters. For the linear polynomial:

\[ n_{c_{\text{linear}}} = n + 1 \]

for the quadratic polynomial:

\[ n_{c_{\text{quad}}} = \frac{(n + 1)(n + 2)}{2} \]

and for the cubic polynomial:

\[ n_{c_{\text{cubic}}} = \frac{(n^3 + 6n^2 + 11n + 6)}{6} \]

There must be at least \( n_c \) data samples in order to form a fully determined linear system and solve for the polynomial coefficients. In Dakota, a least-squares approach involving a singular value decomposition numerical method is applied to solve the linear system.

**basis_order**

- Keywords Area
- model
- surrogate
- global
- polynomial
  - basis_order

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Description**

The polynomial order for the polynomial regression model (default = 2).
linear

- Keywords Area
- model
- surrogate
- global
- polynomial
- linear

Use a linear polynomial or trend function

**Specification**

Alias: none

Argument(s): none

**Description**

See parent page

quadratic

- Keywords Area
- model
- surrogate
- global
- polynomial
- quadratic

Use a quadratic polynomial or trend function

**Specification**

Alias: none

Argument(s): none

**Description**

See parent page
cubic

- Keywords Area
- model
- surrogate
- global
- polynomial
- cubic

Use a cubic polynomial

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

See parent page

**export_model**

- Keywords Area
- model
- surrogate
- global
- polynomial
- export_model

Exports surrogate model in user-selected format

**Topics**

This keyword is related to the topics:

- surrogate_models

**Specification**

**Alias:** none

**Argument(s):** none
### Description

Export the surrogate for later evaluation using the surfpack executable (bin/surfpack) or a user-developed tool. Export format is controlled using the `formats` specification. Four formats are available in Dakota; however, not all have been enabled for all surrogates.

The four formats are:

- **text_archive**: Plain-text, machine-readable archive for use with the surfpack executable
- **binary_archive**: Binary, machine-readable archive for use with the surfpack executable
- **algebraic_file**: Plain-text, human-readable file intended for use with user-created tools; not compatible with the surfpack executable
- **algebraic_console**: Print the model in algebraic format to the screen; not compatible with the surfpack executable

Most global surrogates can be exported in all four formats. These include:

- Gaussian process (keyword `gaussian_process surfpack`)
- Artificial neural network (keyword `neural_network`)
- Radial basis Funtions (keyword `radial_basis`)
- Polynomial (keyword `polynomial`)

However, for Multivariate Adaptive Regression Spline (keyword `mars`) and moving least squares (keyword `moving_least_squares`) models, only `text_archive` and `binary_archive` formats may be used.

Currently, no other surrogate models can be exported. In addition, Dakota cannot import models that have been exported. They are strictly for use with external tools.

#### Default Behavior
No export.

#### Expected Output
Output depends on selected format; see the `formats` specification.

#### Additional Discussion
The Dakota examples folder includes a demonstration of using the surfpack executable with an exported model file.
filename_prefix

- Keywords Area
- model
- surrogate
- global
- polynomial
- export_model
- filename_prefix

User-customizable portion of exported model filenames

**Topics**

This keyword is related to the topics:

- surrogate_models

**Specification**

*Alias:* none

*Argument(s):* STRING

*Default:* exported_surrogate

**Description**

When a file-based export of a surrogate model is specified, Dakota writes one file per response, per requested format. The files are named using the pattern `{prefix}.{response_descriptor}.{extension}`.

The `response_descriptor` portion of the pattern is filled in using the response descriptors provided by the user (or, if none are specified, descriptors automatically generated by Dakota). Extension is a three or four letter string that depends on the format. The `filename_prefix` keyword is used to supply the prefix portion of the pattern.

**Examples**

This input snippet directs Dakota to write one algebraic format file and one binary archive file for each response. The names of the files will follow the patterns `my_surrogate.{response_descriptor}.alg` (for the algebraic files) and `my_surrogate.{response_descriptor}.bsps` (for the binary files).

```plaintext
surrogate global gaussian_process surfpack
export_model
    filename_prefix = 'my_surrogate'
    formats
        algebraic_file
        binary_archive
```
Keywords Area

Model

Surrogate

Global

Polynomial

Export Model

Formats

Formats for surrogate model export

Topics

This keyword is related to the topics:

- surrogate_models

Specification

Alias: none

Argument(s): none

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
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<td>text_archive</td>
<td>Export surrogate</td>
</tr>
<tr>
<td>Optional</td>
<td>binary_archive</td>
<td>binary_archive</td>
<td>model to a plain-text</td>
</tr>
<tr>
<td>Optional</td>
<td>algebraic_file</td>
<td>algebraic_file</td>
<td>archive file</td>
</tr>
<tr>
<td>Optional</td>
<td>algebraic_console</td>
<td>algebraic_console</td>
<td>Export surrogate</td>
</tr>
</tbody>
</table>

Description

Select from among the 2-4 available export formats available for this surrogate. Multiple selections are permitted. See export_model and the entries for the format selection keywords for further information.
text_archive

- Keywords Area
- model
- surrogate
- global
- polynomial
- export_model
- formats
- text_archive

Export surrogate model to a plain-text archive file

**Topics**

This keyword is related to the topics:

- surrogate_models

**Specification**

*Alias*: none

*Argument(s)*: none

**Description**

After the surrogate model has been built, Dakota will export it to a plain-text archival file suitable only for use with the surfpack executable (bin/surfpack). The file is named using the pattern `{prefix}.{response_descriptor}.sps`, in which `sps` stands for Surfpack Surrogate. See filename_prefix for further information about exported surrogate file naming.

The Dakota examples folder includes a demonstration of using the surfpack executable with an exported model file.

binary_archive

- Keywords Area
- model
- surrogate
- global
- polynomial
- export_model
- formats
- binary_archive

Export surrogate model to a binary archive file
Topics
This keyword is related to the topics:

- surrogate_models

Specification
Alias: none
Argument(s): none

Description
After the surrogate model has been built, Dakota will export it to a binary archival file suitable only for use with the surfpack executable (bin/surfpack). The file is named using the pattern \{prefix\}.\{response_descriptor\}.bsps, in which 'bsps' stands for Binary Surfpack Surrogate. See filename.prefix for further information about exported surrogate file naming.

The Dakota examples folder includes a demonstration of using the surfpack executable with an exported model file.

- algebraic_file
  - Keywords Area
  - model
  - surrogate
  - global
  - polynomial
  - export_model
  - formats
  - algebraic_file

Export surrogate model in algebraic format to a file

Topics
This keyword is related to the topics:

- surrogate_models

Specification
Alias: none
Argument(s): none
6.3. MODEL

Description

After the surrogate model has been built, Dakota will export it to a file in a human-readable "algebraic" format. The file is named using the pattern `{prefix}.{response_descriptor}.alg`. See filename_prefix for further information about exported surrogate file naming. The file contains sufficient information for the user to (re)construct and evaluate the model outside of Dakota.

Expected Output

The format depends on the type of surrogate model, but in general will include a LaTeX-like representation of the analytic form of the model to aid tool development, all needed model hyperparameters, and headers describing the shape or dimension of the provided data.

The output written to the file matches exactly the output written to the console when algebraic_console is specified.

```
algebraic_console
• Keywords Area
• model
• surrogate
• global
• polynomial
• export_model
• formats
• algebraic_console
```

Export surrogate model in algebraic format to the console

Topics

This keyword is related to the topics:

• surrogate_models

Specification

Alias: none

Argument(s): none

Description

After the surrogate model has been built, Dakota will export it to the console (screen, or output file if Dakota was run using the -o option) in a human-readable "algebraic" format. The output contains sufficient information for the user to (re)construct and evaluate the model outside of Dakota.

Expected Output

The format depends on the type of surrogate model, but in general will include a LaTeX-like representation of the analytic form of the model to aid tool development, all needed model hyperparameters, and headers describing the shape or dimension of the provided data.

The output written to the screen for the exported model matches exactly the output written to file when algebraic_file is specified. Use of algebraic_file is preferred over algebraic_console, which exists largely to provide a measure of backward compatibility.
### Domain Decomposition

- **Keywords Area**
- **model**
- **surrogate**
- **global**
- **domain_decomposition**

Piecewise Domain Decomposition for Global Surrogate Models

### Specification

**Alias:** none

**Argument(s):** none

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<tr>
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<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<td>Type of the Geometric Cells Used for the Piecewise Decomposition Option of Global Surrogates</td>
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<td>support_layers</td>
<td>Optional Number of Support Layers for the Piecewise Decomposition Option of Global Surrogates</td>
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<tr>
<td>Optional</td>
<td></td>
<td>discontinuity_detection</td>
<td>Optional Discontinuity Detection Capability for the Piecewise Decomposition Option of Global Surrogates</td>
</tr>
</tbody>
</table>

### Description

Typical regression techniques use all available sample points to build continuous approximations of the underlying function.

An alternative option is to use piecewise decomposition to locally approximate the function at some point using a few sample points from its neighborhood only. This option currently supports Polynomial Regression, Gaussian Process (GP) Interpolation, and Radial Basis Functions (RBF) Regression. It requires a decomposition
cell type (currently set to be Voronoi cells). Optional parameters are: the number of layers of neighbors used to solve the regression problem (default is one layer), and an optional discontinuity detection capability (identified by a user-input jump or gradient threshold).

The method can also make use of the gradient and Hessian information, if available. The user needs to specify the keyword user_derivatives.

**cell_type**

- **Keywords Area**
- **model**
- **surrogate**
- **global**
- **domain_decomposition**
- **cell_type**

Type of the Geometric Cells Used for the Piecewise Decomposition Option of Global Surrogates

**Specification**

**Alias:** none

**Argument(s):** STRING

**Description**

The piecewise decomposition option for global surrogates is used to locally approximate a function at some point using a few sample points from its neighborhood.

This option requires a decomposition cell type that can vary from structured grid boxes, to polygonal Voronoi cells. Currently, this option only supports Voronoi cells.

**support_layers**

- **Keywords Area**
- **model**
- **surrogate**
- **global**
- **domain_decomposition**
- **support_layers**

Optional Number of Support Layers for the Piecewise Decomposition Option of Global Surrogates

**Specification**

**Alias:** none

**Argument(s):** INTEGER
CHAPTER 6. KEYWORDS AREA

Description
The piecewise decomposition option for global surrogates is used to locally approximate a function at some point using a few sample points from its neighborhood.

The neighborhood of a cell is parameterized via a number of (support layers). The default value is set to one layer of neighbors (cells that share direct edges with the cell under study). One more support layer would include the neighbors of that cells neighbors, and so on.

discontinuity_detection

• Keywords Area
• model
• surrogate
• global
• domain_decomposition
• discontinuity_detection

Optional Discontinuity Detection Capability for the Piecewise Decomposition Option of Global Surrogates

Specification
Alias: none
Argument(s): none

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<tr>
<th>Required/-Optional Required (Choose One)</th>
<th>Description of Group Threshold Mode (Group 1)</th>
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<th>Dakota Keyword Description</th>
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</thead>
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<tr>
<td>jump_threshold</td>
<td>Gradient Threshold Parameter of the Optional Discontinuity Detection Capability for the Piecewise Decomposition Option of Global Surrogates</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Description

The piecewise decomposition option for global surrogates is used to locally approximate a function at some point using a few sample points from its neighborhood.

The domain decomposition algorithm supports an optional discontinuity detection capability where seeds across a user-input discontinuity threshold are not considered neighbors when building the approximate connectivity Delaunay graph. Alternatively, the domain is split into patches that trap discontinuities between them. This capability can be specified using a jump or gradient threshold values in the input spec.

**jump_threshold**

- Keywords Area
- model
- surrogate
- global
- domain_decomposition
- discontinuity_detection
- jump_threshold

Gradient Threshold Parameter of the Optional Discontinuity Detection Capability for the Piecewise Decomposition Option of Global Surrogates

**Specification**

*Alias:* none

*Argument(s):* REAL

**Description**

The piecewise decomposition option for global surrogates is used to locally approximate a function at some point using a few sample points from its neighborhood.

The domain decomposition algorithm supports an optional discontinuity detection capability where seeds across a user-input discontinuity threshold are not considered neighbors when building the approximate connectivity Delaunay graph. Alternatively, the domain is split into patches that trap discontinuities between them. This capability can be specified using a jump threshold value in the input spec.
gradient_threshold

• Keywords Area

• model

• surrogate

• global

• domain_decomposition

• discontinuity_detection

• gradient_threshold

Gradient Threshold Parameter of the Optional Discontinuity Detection Capability for the Piecewise Decomposition Option of Global Surrogates

**Specification**

Alias: none

Argument(s): REAL

**Description**

The piecewise decomposition option for global surrogates is used to locally approximate a function at some point using a few sample points from its neighborhood.

The domain decomposition algorithm supports an optional discontinuity detection capability where seeds across a user-input discontinuity threshold are not considered neighbors when building the approximate connectivity Delaunay graph. Alternatively, the domain is split into patches that trap discontinuities between them. This capability can be specified using a gradient threshold value in the input spec.

total_points

• Keywords Area

• model

• surrogate

• global

• total_points

Specified number of training points

**Specification**

Alias: none

Argument(s): INTEGER

Default: recommended_points
6.3. MODEL

Description
See parent page.

minimum_points
- Keywords Area
- model
- surrogate
- global
- minimum_points

Construct surrogate with minimum number of points

Specification
Alias: none
Argument(s): none

Description
The minimum is d+1, for d input dimensions, except for polynomials. See parent page.

recommended_points
- Keywords Area
- model
- surrogate
- global
- recommended_points

Construct surrogate with recommended number of points

Specification
Alias: none
Argument(s): none

Description
This is the default option. It requires 5*d build points for d input dimensions, except for polynomial models. See parent page.
**dace_method_pointer**

- **Keywords Area**
- **model**
- **surrogate**
- **global**
- **dace_method_pointer**

Specify a method to gather training data

**Topics**

This keyword is related to the topics:

- **block_pointer**

**Specification**

**Alias:** none

**Argument(s):** STRING

**Default:** no design of experiments data

<table>
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<tr>
<th><strong>Required/-Optional</strong></th>
<th><strong>Description of Group</strong></th>
<th><strong>Dakota Keyword</strong></th>
<th><strong>Dakota Keyword Description</strong></th>
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</thead>
<tbody>
<tr>
<td><strong>Optional</strong></td>
<td></td>
<td><strong>auto_refinement</strong></td>
<td>Experimental auto-refinement of surrogate model</td>
</tr>
</tbody>
</table>

**Description**

The number of training points and the sources are specified on **global**, as well as the number of new training points required.

New training points are gathered by running the “truth” model using the method specified by **dace_method_pointer**. The DACE method will only be invoked if it has new samples to perform, and if new samples are required and no DACE iterator has been provided, an error will result.

The **dace_method_pointer** points to design of experiments method block used to generate truth model data.

Permissible methods include: Monte Carlo (random) sampling, Latin hypercube sampling, orthogonal array sampling, central composite design sampling, and Box-Behnken sampling.

Note that the number of samples specified in the method block may be overwritten, if the requested number of samples is less than **minimum_points**.

**auto_refinement**

- **Keywords Area**
- **model**
- **surrogate**
6.3. **MODEL**

- global
- dace\_method\_pointer
- auto\_refinement

Experimental auto-refinement of surrogate model

**Topics**

This keyword is related to the topics:

- surrogate\_models

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** no refinement

<table>
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<tr>
<th>Required/-</th>
<th>Description of</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>Group</td>
<td>max_iterations</td>
<td>Number of iterations allowed for optimizers and adaptive UQ methods</td>
</tr>
<tr>
<td></td>
<td></td>
<td>max_function_evaluations</td>
<td>Number of function evaluations allowed for optimizers</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>convergence_tolerance</td>
<td>Cross-validation threshold for surrogate convergence</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>soft_convergence_limit</td>
<td>Maximum number of iterations without improvement in cross-validation</td>
</tr>
</tbody>
</table>
CHAPTER 6. KEYWORDS AREA

<table>
<thead>
<tr>
<th>Optional</th>
<th>cross_validation_metric</th>
<th>Choice of error metric to satisfy</th>
</tr>
</thead>
</table>

**Description**

(Experimental option) Automatically refine the surrogate model until desired cross-validation quality is achieved. Refinement is accomplished by iteratively adding more data to the training set until the cross-validation convergence_tolerance is achieved, or max_function_evaluations or max_iterations is exceeded.

The amount of new training data that is incorporated each iteration is specified in the DACE method that is referred to by the model's dace_method_pointer. See refinement_samples for more information.

**max_iterations**

- Keywords Area
- model
- surrogate
- global
- dace_method_pointer
- auto_refinement
- max_iterations

Number of iterations allowed for optimizers and adaptive UQ methods

**Topics**

This keyword is related to the topics:

- method_independent_controls

**Specification**

Alias: none

Argument(s): INTEGER

Default: 100

**Description**

The maximum number of iterations is used as a stopping criterion for optimizers and some adaptive UQ methods. If it has not reached any other stopping criteria first, the method will stop after it has performed max_iterations iterations. See also max_function_evaluations.

Default Behavior

Default value is 100.
max_function_evaluations

- Keywords Area
- model
- surrogate
- global
- dace_method_pointer
- auto_refinement
- max_function_evaluations

Number of function evaluations allowed for optimizers

Topics
This keyword is related to the topics:

- method_independent_controls

Specification
Alias: none
Argument(s): INTEGER
Default: 1000

Description
The maximum number of function evaluations is used as a stopping criterion for optimizers. If it has not reached any other stopping criteria first, the optimizer will stop after it has performed max_function_evaluations evaluations. See also max_iterations.

Default Behavior
Default value is 1000.

convergence_tolerance

- Keywords Area
- model
- surrogate
- global
- dace_method_pointer
- auto_refinement
- convergence_tolerance

Cross-validation threshold for surrogate convergence
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): REAL
Default: 1.0e-4

Description

The surrogate model will be refined until the selected cross_validation_metric falls below this convergence tolerance.

Default Behavior

The default is 1e-4.

soft_convergence_limit

- Keywords Area
- model
- surrogate
- global
- dace_method_pointer
- auto_refinement
- soft_convergence_limit

Maximum number of iterations without improvement in cross-validation

Specification

Alias: none

Argument(s): INTEGER
Default: 0

Description

The purpose of this control is to cease auto-refinement when improvement in the cross-validation score appears to have stalled or occurs too slowly.

A rolling average of improvement in the cross-validation score is computed over soft_convergence_limit iterations. Auto-refinement is halted if the average becomes smaller than the convergence_tolerance. The average is computed but ignored until the number of iterations has exceeded soft_convergence_limit. The default setting of 0 disables soft convergence.

cross_validation_metric

- Keywords Area
- model
- surrogate
- global
• `dace_method_pointer`
• `auto_refinement`
• `cross_validation_metric`

Choice of error metric to satisfy

**Specification**

*Alias*: none  
*Argument(s)*: STRING  
*Default*: root-mean-squared error

<table>
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<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<tbody>
<tr>
<td>Optional</td>
<td></td>
<td><code>folds</code></td>
<td>Number of cross validation folds</td>
</tr>
</tbody>
</table>

**Description**

The cross-validation score that the auto-refinement routine seeks to satisfy is based on an error metric. Any of the surrogate diagnostic metrics may be used. These include:

• `root_mean_squared`
• `mean_abs`
• `rsquared`
• `sum_squared`
• `mean_squared`
• `sum_abs`
• `max_abs`

**Default Behavior** The default metric is the root mean squared error (`'root_mean_squared'`).

**folds**

• **Keywords Area**
• `model`
• `surrogate`
• `global`
• `dace_method_pointer`
• `auto_refinement`
• `cross_validation_metric`
• `folds`

Number of cross validation folds
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): INTEGER

Default: 10

Description

Number of folds (partitions) of the training data to use in cross validation (default 10).

actual_model_pointer

- Keywords Area
- model
- surrogate
- global
- actual_model_pointer

A surrogate model pointer that guides a method to whether it should use a surrogate model or compute truth function evaluations

Specification

Alias: none

Argument(s): STRING

Description

Dakota methods use global surrogate models to compute surrogate function approximations. They also need to know the true function evaluations. A global surrogate model now must have an actual_model_pointer keyword to decide for the method whether to evaluate the global surrogate model, or compute the true function evaluations if actual_model_pointer = TRUTH.

reuse_points

- Keywords Area
- model
- surrogate
- global
- reuse_points

Surrogate model training data reuse control

Topics

This keyword is related to the topics:

- surrogate_models
6.3. MODEL

**Specification**

**Alias:** reuse_samples  
**Argument(s):** none  
**Default:** all for import; none otherwise

<table>
<thead>
<tr>
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<th>Dakota Keyword</th>
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<td>all</td>
<td>Option for reuse_points</td>
</tr>
<tr>
<td>Required (Choose One)</td>
<td>(Group 1)</td>
<td>region</td>
<td>Option for reuse_points</td>
</tr>
<tr>
<td>none</td>
<td>none</td>
<td>Option for reuse_points</td>
<td></td>
</tr>
</tbody>
</table>

**Description**

Dakota’s global surrogate methods rely on training data, which can either come from evaluation of a “truth” model, which is generated by the method specified with `dace_method_pointer`, from a file of existing training data, identified by `import_build_points_file`, or both.

The `reuse_points` keyword controls the amount of training data used in building a surrogate model, either initially, or during iterative rebuild, as in surrogate-based optimization. If `import_build_points_file` is specified, `reuse_points` controls how the file contents are used. If used during iterative rebuild, it controls what data from previous surrogate builds is reused in building the current model.

- **all** (default for file import) - use all points in the file or available from previous builds
- **region** - use only the points falling in the current trust region (see `surrogate_based_local`)
- **none** (default when no import) - ignore the contents of the file or previous build points, and gather new training data using the specified DACE method

**all**

- Keywords Area
- model
- surrogate
- global
- `reuse_points`
- all

Option for `reuse_points`

**Specification**

**Alias:** none  
**Argument(s):** none
CHAPTER 6. KEYWORDS AREA

Description
This is described on the parent page.

region
• Keywords Area
• model
• surrogate
• global
• reuse_points
• region
Option for reuse_points

Specification
Alias: none
Argument(s): none

Description
This is described on the parent page.

none
• Keywords Area
• model
• surrogate
• global
• reuse_points
• none
Option for reuse_points

Specification
Alias: none
Argument(s): none

Description
This is described on the parent page.
import_build_points_file

- Keywords Area
- model
- surrogate
- global
- import_build_points_file

File containing points you wish to use to build a surrogate

Specification

**Alias:** import_points_file samples_file

**Argument(s):** STRING

**Default:** no point import from a file

<table>
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<tr>
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<th>Dakota Keyword Description</th>
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<td>Selects annotated tabular file format</td>
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<td></td>
<td></td>
<td>custom_annotated</td>
<td>Selects custom-annotated tabular file format</td>
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<tr>
<td></td>
<td></td>
<td>freeform</td>
<td>Selects freeform file format</td>
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<table>
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<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>active_only</td>
<td>Import only active variables from tabular data file</td>
</tr>
</tbody>
</table>

**Description**

The `import_build_points_file` allows the user to specify a file that contains a list of points and truth model responses used to construct a surrogate model. These can be used by all methods that (explicitly, e.g. surrogate-based optimization, or implicitly, e.g. efficient global optimization) operate on a surrogate. In particular, these points and responses are used in place of truth model evaluations to construct the initial surrogate. When used to construct surrogate models or emulators these are often called build points or training data.

**Default Behavior**

By default, methods do not import points from a file.

**Usage Tips**

Dakota parses input files without regard to whitespace, but the `import_build_points_file` must be in one of three formats:

- annotated (default)
- custom_annotated
- freeform
Examples

method
  polynomial_chaos
  expansion_order = 4
  import_build_points_file = 'dakota_uq_rosenbrock_pce_import.annot.pts.dat'

annotated
• Keywords Area
• model
• surrogate
• global
• import_build_points_file
• annotated

Selects annotated tabular file format

Topics

This keyword is related to the topics:
• file_formats

Specification

Alias: none
  Argument(s): none
  Default: annotated

Description

An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

  Default Behavior
  By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

  Usage Tips
• To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify custom_annotated header eval_id
• Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
• When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
• Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.
Examples

Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```python
environment
tabular_data
  tabular_data_file = 'dakota_summary.dat'
  annotated
```

Resulting tabular file:

```
%eval_id interface  x1  x2  obj_fn  nln_ineq_con_1  nln_ineq_con_2
1  NO_ID     0.9  1.1  0.0002  0.26       0.76
2  NO_ID     0.90009 1.1  0.0001996404857  0.2601620081  0.759955
3  NO_ID     0.89991 1.1  0.0002003604863  0.2598380081  0.760045
...```

- **custom_annotated**
  - **Keywords Area**
    - **model**
    - **surrogate**
    - **global**
    - **import_build_points_file**
    - **custom_annotated**

  Selects custom-annotated tabular file format

Topics

This keyword is related to the topics:

- **file_formats**

Specification

**Alias:** none

**Argument(s):** none

<p>| Required/- | Description of Group | Dakota Keyword Description |</p>
<table>
<thead>
<tr>
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<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>header</td>
<td>Enable header row in custom-annotated tabular file</td>
</tr>
</tbody>
</table>
CHAPTER 6. KEYWORDS AREA

**Description**

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging **freeform** and (fully) **annotated**.

**Default Behavior**

The **annotated** format is the default for tabular export/import. To control which header row and columns are in the input/output, specify **custom_annotated**, followed by options, in the relevant export/import context.

**Usage Tips**

- Prior to October 2011, calibration and surrogate data files were in **freeform** format. They now default to **annotated** format, though **freeform** remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the **freeform** option.

**Examples**

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
custom_annotated header eval_id
```

Resulting tabular file:

```
%eval_id   x1     x2    obj_fn  nln_ineq_con_1  nln_ineq_con_2
1          0.9    1.1   0.0002  0.26        0.76
2          0.90009 1.1  0.0001996404857 0.2601620081 0.759955
3          0.89991 1.1  0.0002003604863 0.2598380081 0.760045
...
```

**header**

- **Keywords Area**
- **model**
- **surrogate**
6.3. MODEL

- global
- import_build_points_file
- custom_annotated
- header

Enable header row in custom-annotated tabular file

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

See description of parent custom_annotated

**eval_id**

- Keywords Area

- model

- surrogate

- global

- import_build_points_file

- custom_annotated

- eval_id

Enable evaluation ID column in custom-annotated tabular file

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

See description of parent custom_annotated
interface_id

- Keywords Area
- model
- surrogate
- global
- import_build_points_file
- custom.annotated
- interface_id

Enable interface ID column in custom-annotated tabular file

**Specification**

*Alias:* none

*Argument(s):* none

**Description**

See description of parent *custom.annotated*

**freeform**

- Keywords Area
- model
- surrogate
- global
- import_build_points_file
- freeform

Selects freeform file format

**Topics**

This keyword is related to the topics:

- *file_formats*

**Specification**

*Alias:* none

*Argument(s):* none

*Default:* annotated
6.3. **MODEL**

**Description**

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

**Default Behavior**

The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

**Usage Tips**

- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

**Examples**

Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
freeform
```

Resulting tabular file:

```
0.9  1.1  0.0002  0.26  0.76
0.90009 1.1 0.0001996404857  0.2601620081 0.759955
0.89991 1.1 0.0002003604863  0.2598380081 0.760045
...```

**active_only**

- **Keywords Area**
- **model**
- **surrogate**
- **global**
- **import_build_points_file**
- **active_only**

Import only active variables from tabular data file

**Topics**

This keyword is related to the topics:

- **file_formats**
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none
  Argument(s): none

Description

By default, files for tabular data imports are expected to contain columns for all variables, active and inactive. The keyword `active_only` indicates that the file to import contains only the active variables.

This option should only be used in contexts where the inactive variables have no influence, for example, building a surrogate over active variables, with the state variables held at nominal. It should not be used in more complex nested contexts, where the values of inactive variables are relevant to the function evaluations used to build the surrogate.

export_approx_points_file

- Keywords Area
- model
- surrogate
- global
- export_approx_points_file

Output file for evaluations of a surrogate model

Specification

Alias: export_points_file
  Argument(s): STRING
  Default: no point export to a file

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
</table>
| Optional
  (Choose One)     | Tabular Format (Group 1) | annotated                   |
|                    |                        | custom_annotated            |
|                    |                        | Selects custom-annotated tabular file format |
|                    |                        | freeform                    |
|                    |                        | Selects freeform file format |

Description

The `export_approx_points_file` keyword allows the user to specify a file in which the points (input variable values) at which the surrogate model is evaluated and corresponding response values computed by the surrogate model will be written. The response values are the surrogate’s predicted approximation to the truth model responses at those points.
Usage Tips
Dakota exports tabular data in one of three formats:

- annotated (default)
- custom_annotated
- freeform

annotated
- Keywords Area
- model
- surrogate
- global
- export_approx_points_file
- annotated

Selects annotated tabular file format

Topics
This keyword is related to the topics:

- file_formats

Specification
Alias: none

Argument(s): none

Default: annotated

Description
An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior
By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips
- To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify custom_annotated header eval_id
- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.
**Examples**

Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns, and data for variables and responses. Input file fragment:

```plaintext
environment
tabular_data
  tabular_data_file = 'dakota_summary.dat'
annotated

Resulting tabular file:

<table>
<thead>
<tr>
<th>eval_id</th>
<th>interface</th>
<th>x1</th>
<th>x2</th>
<th>obj_fn</th>
<th>nln_ineq_con_1</th>
<th>nln_ineq_con_2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>NO_ID</td>
<td>0.9</td>
<td>1.1</td>
<td>0.0002</td>
<td>0.26</td>
<td>0.76</td>
</tr>
<tr>
<td>2</td>
<td>NO_ID</td>
<td>0.9009</td>
<td>1.1</td>
<td>0.0001996404857</td>
<td>0.2601620081</td>
<td>0.759955</td>
</tr>
<tr>
<td>3</td>
<td>NO_ID</td>
<td>0.89991</td>
<td>1.1</td>
<td>0.0002003604863</td>
<td>0.2598380081</td>
<td>0.760045</td>
</tr>
<tr>
<td>...</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
```

**custom_annotated**

- Keywords Area
- model
- surrogate
- global
- export_approx_points_file
- custom_annotated

Selects custom-annotated tabular file format

**Topics**

This keyword is related to the topics:

- file_formats

**Specification**

Alias: none

<p>| Required/- | Description of | Dakota Keyword | Dakota Keyword |</p>
<table>
<thead>
<tr>
<th>Optional</th>
<th>Group</th>
<th>header</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td></td>
<td>Enable header row in custom-annotated tabular file</td>
</tr>
</tbody>
</table>
6.3. MODEL

<table>
<thead>
<tr>
<th>Optional</th>
<th>eval_id</th>
<th>Optional</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>interface_id</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Enable evaluation ID column in custom-annotated tabular file</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Enable interface ID column in custom-annotated tabular file</td>
</tr>
</tbody>
</table>

### Description

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

### Default Behavior

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom_annotated, followed by options, in the relevant export/import context.

### Usage Tips

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

### Examples

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:

```environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
custom_annotated header eval_id
```

Resulting tabular file:

```
%eval_id x1 x2 obj_fn nln_ineq_con_1 nln_ineq_con_2
1 0.9 1.1 0.0002 0.26 0.76
2 0.90009 1.1 0.001996404857 0.2601620081 0.759955
3 0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...
```

### header

- Keywords Area
- model
- surrogate
• global

• export_approx_points_file

• custom.annotated

• header

Enable header row in custom-annotated tabular file

**Specification**

**Alias:** none  
**Argument(s):** none

**Description**

See description of parent `custom.annotated`

`eval_id`

• Keywords Area

• model

• surrogate

• global

• export_approx_points_file

• custom.annotated

• `eval_id`

Enable evaluation ID column in custom-annotated tabular file

**Specification**

**Alias:** none  
**Argument(s):** none

**Description**

See description of parent `custom.annotated`
interface_id

- Keywords Area
- model
- surrogate
- global
- export_approx_points_file
- custom_annotated
- interface_id

Enable interface ID column in custom-annotated tabular file

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

See description of parent [custom_annotated](#)

**freeform**

- Keywords Area
- model
- surrogate
- global
- export_approx_points_file
- freeform

Selects freeform file format

**Topics**

This keyword is related to the topics:

- fileFormats

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** annotated
CHAPTER 6. KEYWORDS AREA

Description
A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior
The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips
- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples
Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```
environment
  tabular_data
  tabular_data_file = 'dakota_summary.dat'
  freeform
```

Resulting tabular file:

```
0.9 1.1 0.0002 0.26 0.76
0.90009 1.1 0.0001996404857 0.2601620081 0.759955
0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...```

use_derivatives
- Keywords Area
- model
- surrogate
- global
- use_derivatives

Use derivative data to construct surrogate models

Specification
Alias: none
Argument(s): none
Default: use function values only
## Description

The `use_derivatives` flag specifies that any available derivative information should be used in global approximation builds, for those global surrogate types that support it (currently, polynomial regression and the Surfpack Gaussian process).

However, its use with Surfpack Gaussian process is not recommended.

### correction

- Keywords Area
- model
- surrogate
- global
- correction

Correction approaches for surrogate models

## Specification

**Alias:** none  
**Argument(s):** none  
**Default:** no surrogate correction

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Choose One</td>
<td>Correction Order</td>
<td>zeroth_order</td>
<td>Specify that truth values must be matched.</td>
</tr>
<tr>
<td></td>
<td>(Group 1)</td>
<td></td>
<td>first_order</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>second_order</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Required/Choose One</th>
<th>Correction Type</th>
<th>additive</th>
<th>Additive correction factor for local surrogate accuracy</th>
</tr>
</thead>
</table>
Description

Some of the surrogate model types support the use of correction factors that improve the local accuracy of the surrogate models.

The correction specification specifies that the approximation will be corrected to match truth data, either matching truth values in the case of zeroth-order matching, matching truth values and gradients in the case of first-order matching, or matching truth values, gradients, and Hessians in the case of second-order matching. For additive and multiplicative corrections, the correction is local in that the truth data is matched at a single point, typically the center of the approximation region. The additive correction adds a scalar offset (zeroth order), a linear function (first order), or a quadratic function (second order) to the approximation to match the truth data at the point, and the multiplicative correction multiplies the approximation by a scalar (zeroth order), a linear function (first order), or a quadratic function (second order) to match the truth data at the point. The additive first-order case is due to [57] and the multiplicative first-order case is commonly known as beta correction [40]. For the combined correction, the use of both additive and multiplicative corrections allows the satisfaction of an additional matching condition, typically the truth function values at the previous correction point (e.g., the center of the previous trust region). The combined correction is then a multipoint correction, as opposed to the local additive and multiplicative corrections. Each of these correction capabilities is described in detail in [24].

The correction factors force the surrogate models to match the true function values and possibly true function derivatives at the center point of each trust region. Currently, Dakota supports either zeroth-, first-, or second-order accurate correction methods, each of which can be applied using either an additive, multiplicative, or combined correction function. For each of these correction approaches, the correction is applied to the surrogate model and the corrected model is then interfaced with whatever algorithm is being employed. The default behavior is that no correction factor is applied.

The simplest correction approaches are those that enforce consistency in function values between the surrogate and original models at a single point in parameter space through use of a simple scalar offset or scaling applied to the surrogate model. First-order corrections such as the first-order multiplicative correction (also known as beta correction [15]) and the first-order additive correction [57] also enforce consistency in the gradients and provide a much more substantial correction capability that is sufficient for ensuring provable convergence in SBO algorithms. SBO convergence rates can be further accelerated through the use of second-order corrections which also enforce consistency in the Hessians [24], where the second-order information may involve analytic, finite-difference, or quasi-Newton Hessians.

Correcting surrogate models with additive corrections involves

\[ f_{\hat{h}_a}(x) = f_{l_a}(x) + \alpha(x) \]  \hspace{1cm} (6.1)

where multifidelity notation has been adopted for clarity. For multiplicative approaches, corrections take the form

\[ f_{\hat{h}_a}(x) = f_{l_0}(x)\beta(x) \]  \hspace{1cm} (6.2)

<table>
<thead>
<tr>
<th>Multiplicative</th>
<th>Corrective multiplicative factor for local surrogate accuracy.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Combined</td>
<td>Multipoint correction for a hierarchical surrogate</td>
</tr>
</tbody>
</table>
where, for local corrections, \( \alpha(x) \) and \( \beta(x) \) are first or second-order Taylor series approximations to the exact correction functions:

\[
\alpha(x) = A(x_c) + \nabla A(x_c)^T (x - x_c) + \frac{1}{2} (x - x_c)^T \nabla^2 A(x_c) (x - x_c)
\]

(6.3)

\[
\beta(x) = B(x_c) + \nabla B(x_c)^T (x - x_c) + \frac{1}{2} (x - x_c)^T \nabla^2 B(x_c) (x - x_c)
\]

(6.4)

where the exact correction functions are

\[
A(x) = f_{hi}(x) - f_{lo}(x)
\]

(6.5)

\[
B(x) = \frac{f_{hi}(x)}{f_{lo}(x)}
\]

(6.6)

Refer to[24] for additional details on the derivations.

A combination of additive and multiplicative corrections can provide for additional flexibility in minimizing the impact of the correction away from the trust region center. In other words, both additive and multiplicative corrections can satisfy local consistency, but through the combination, global accuracy can be addressed as well. This involves a convex combination of the additive and multiplicative corrections:

\[
\hat{f}_{hi,o}(x) = \gamma \hat{f}_{hi,o}(x) + (1 - \gamma) \hat{f}_{lo,o}(x)
\]

where \( \gamma \) is calculated to satisfy an additional matching condition, such as matching values at the previous design iterate.

It should be noted that in both first order correction methods, the function \( \hat{f}(x) \) matches the function value and gradients of \( f_t(x) \) at \( x = x_c \). This property is necessary in proving that the first order-corrected SBO algorithms are provably convergent to a local minimum of \( f_t(x) \). However, the first order correction methods are significantly more expensive than the zeroth order correction methods, since the first order methods require computing both \( \nabla f_t(x_c) \) and \( \nabla f_s(x_c) \). When the SBO strategy is used with either of the zeroth order correction methods, or with no correction method, convergence is not guaranteed to a local minimum of \( f_t(x) \). That is, the SBO strategy becomes a heuristic optimization algorithm. From a mathematical point of view this is undesirable, but as a practical matter, the heuristic variants of SBO are often effective in finding local minima.

Usage guidelines

- Both the additive zeroth order and multiplicative zeroth order correction methods are “free” since they use values of \( f_t(x_c) \) that are normally computed by the SBO strategy.

- The use of either the additive first order method or the multiplicative first order method does not necessarily improve the rate of convergence of the SBO algorithm.

- When using the first order correction methods, the gradient-related response keywords must be modified to allow either analytic or numerical gradients to be computed. This provides the gradient data needed to compute the correction function.

- For many computationally expensive engineering optimization problems, gradients often are too expensive to obtain or are discontinuous (or may not exist at all). In such cases the heuristic SBO algorithm has been an effective approach at identifying optimal designs[35].
zeroth_order

- Keywords Area
- model
- surrogate
- global
- correction
- zeroth_order

Specify that truth values must be matched.

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

The correction specification specifies that the approximation will be corrected to match truth data. The keyword `zeroth_order` matching ensures that truth values are matched.

first_order

- Keywords Area
- model
- surrogate
- global
- correction
- first_order

Specify that truth values and gradients must be matched.

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

This correction specification specifies that the approximation will be corrected to match truth data. The keyword `first_order` matching ensures that truth values and gradients are matched.
6.3. MODEL

second_order

- Keywords Area
- model
- surrogate
- global
- correction
- second_order

Specify that truth values, gradients and Hessians must be matched.

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

The correction specification specifies that the approximation will be corrected to match truth data. The keyword second_order matching ensures that truth values, gradients and Hessians are matched.

additive

- Keywords Area
- model
- surrogate
- global
- correction
- additive

Additive correction factor for local surrogate accuracy

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

Use an additive correction factor to improve the local accuracy of a surrogate.
CHAPTER 6. KEYWORDS AREA

multlicative

- Keywords Area
- model
- surrogate
- global
- correction
- multiplicative

Multiplicative correction factor for local surrogate accuracy.

**Specification**

Alias: none

**Argument(s):** none

**Description**

Use a multiplicative correction factor to improve the local accuracy of a surrogate.

combined

- Keywords Area
- model
- surrogate
- global
- correction
- combined

Multipoint correction for a hierarchical surrogate

**Specification**

Alias: none

**Argument(s):** none

**Description**

For the combined correction, the use of both additive and multiplicative corrections allows the satisfaction of an additional matching condition, typically the truth function values at the previous correction point (e.g., the center of the previous trust region). The combined correction is then a multipoint correction, as opposed to the local additive and multiplicative corrections.
6.3. MODEL

metrics

- Keywords Area
- model
- surrogate
- global
- metrics

Compute surrogate quality metrics

Topics

This keyword is related to the topics:

- surrogate_models

Specification

Alias: diagnostics
Argument(s): STRINGLIST
Default: No diagnostics

| Required/- | Description of Group | Dakota Keyword | Dakota Keyword Description |
| Optional/Optional | | cross_validation | press | Leave-one-out cross validation |
|------------------|----------------------|----------------|----------------------------|

Description

A variety of diagnostic metrics are available to assess the goodness of fit of a global surrogate to its training data. The default diagnostics are:

- root_mean_squared
- mean_abs
- rsquared

Additional available diagnostics include

- sum_squared
- mean_squared
- sum_abs
- max_abs

The keywords press and cross_validation further specify leave-one-out or k-fold cross validation, respectively, for all of the active metrics from above.
Theory

Most of these diagnostics refer to some operation on the residuals (the difference between the surrogate model and the truth model at the data points upon which the surrogate is built).

For example, \texttt{sum\_squared} refers to the sum of the squared residuals, and \texttt{mean\_abs} refers to the mean of the absolute value of the residuals. \texttt{rsquared} refers to the R-squared value typically used in regression analysis (the proportion of the variability in the response that can be accounted for by the surrogate model). Care should be taken when interpreting metrics, for example, errors may be near zero for interpolatory models or \texttt{rsquared} may not be applicable for non-polynomial models.

\texttt{cross\_validation}

- Keywords Area
- model
- surrogate
- global
- metrics
- cross\_validation

Perform \(k\)-fold cross validation

Topics

This keyword is related to the topics:

- \texttt{surrogate\_models}

Specification

\textbf{Alias:} none

\textbf{Argument(s):} none

\textbf{Default:} No cross validation

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group Partition Control (Group 1)</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>percent</td>
<td>\textit{percent}</td>
<td>\textit{percent}</td>
<td>Percent data per \textit{cross validation fold}</td>
</tr>
</tbody>
</table>
Description

General k-fold cross validation may be performed by specifying `cross_validation`. The cross-validation statistics will be calculated for all metrics. Cross validation may further specify:

- `folds`, the number of folds into which to divide the build data (between 2 and number of data points) or
- `percent`, the fraction of data (between 0 and 0.5) to use in each fold.

These will be adjusted as needed based on the number of available training points. The default number of folds $k = 10$, or 0.1

folds
- Keywords Area
- model
- surrogate
- global
- metrics
- cross_validation
- folds

Number of cross validation folds

Specification

Alias: none

Argument(s): INTEGER

Default: 10

Description

Number of folds (partitions) of the training data to use in cross validation (default 10).

percent
- Keywords Area
- model
- surrogate
- global
- metrics
- cross_validation
- percent

Percent data per cross validation fold
**Specification**

**Alias:** none  
**Argument(s):** REAL  
**Default:** 0.1  

**Description**

Percent of the training data to use in each cross validation fold (default 0.1).

- press
  - **Keywords Area**
  - **model**
  - **surrogate**
  - **global**
  - **metrics**
  - **press**

Leave-one-out cross validation

**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** No PRESS cross validation  

**Description**

Leave-one-out (PRESS) cross validation may be performed by specifying `press`. The cross-validation statistics will be calculated for all metrics.

**import_challenge_points_file**

- **Keywords Area**
- **model**
- **surrogate**
- **global**
- **import_challenge_points_file**

Datafile of points to assess surrogate quality

**Specification**

**Alias:** challenge_points_file  
**Argument(s):** STRING  
**Default:** no user challenge data
### Description

Specifies a data file containing variable and response (truth) values, in one of three formats:

- annotated (default)
- custom.annotated
- freeform

The surrogate is evaluated at the points in the file, and the surrogate (approximate) responses are compared against the truth results from the file. All metrics specified with `metrics` will be computed for the challenge data.

**annotated**

- Keywords Area
- model
- surrogate
- global
- import_challenge_points_file
- annotated

Selects annotated tabular file format

### Topics

This keyword is related to the topics:

- file_formats
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): none

Default: annotated

Description

An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. Each subsequent row contains an evaluation ID and interface ID, followed by data for variables, or variables followed by responses, depending on context.

Default Behavior

By default, Dakota imports and exports tabular files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips

- To specify pre-Dakota 6.1 tabular format, which did not include interface_id, specify custom_annotated
  header eval_id
- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to
  annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but
  extra is found and an error generated when there is insufficient data.
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export an annotated top-level tabular data file containing a header row, leading eval_id and interface_id columns,
and data for variables and responses. Input file fragment:

```
environment
  tabular_data
    tabular_data_file = 'dakota_summary.dat'
    annotated
```

Resulting tabular file:

```
%eval_id interface  x1  x2  obj_fn  nln_ineq_con_1  nln_ineq_con_2
1  NO_ID  0.9  1.1  0.0002  0.26  0.76
2  NO_ID  0.90009  1.1  0.0001996404857  0.2601620081  0.759955
3  NO_ID  0.89991  1.1  0.0002003604863  0.2598380081  0.760045
...
```

**custom_annotated**

- **Keywords Area**
- model
- surrogate
- global
- import_challenge_points_file
  - **custom_annotated**
  
  Selects custom-annotated tabular file format
6.3. MODEL

Topics
This keyword is related to the topics:

- file_formats

Specification

Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>header</td>
<td>Enable header row in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>eval_id</td>
<td>Enable evaluation ID column in custom-annotated tabular file</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>interface_id</td>
<td>Enable interface ID column in custom-annotated tabular file</td>
</tr>
</tbody>
</table>

Description

A custom-annotated tabular file is a whitespace-separated text file typically containing row data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well. Custom-annotated allows user options for whether header row, eval_id column, and interface_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

Default Behavior

The annotated format is the default for tabular export/import. To control which header row and columns are in the input/output, specify custom.annotated, followed by options, in the relevant export/import context.

Usage Tips

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export a custom-annotated tabular file in Dakota 6.0 format, which contained only header and eval_id (no interface_id), and data for variables and responses. Input file fragment:
CHAPTER 6. KEYWORDS AREA

environment
  tabular_data
    tabular_data_file = 'dakota_summary.dat'
    custom_annotated header eval_id

Resulting tabular file:

<table>
<thead>
<tr>
<th>%eval_id</th>
<th>x1</th>
<th>x2</th>
<th>obj_fn</th>
<th>nln_ineq_con_1</th>
<th>nln_ineq_con_2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.9</td>
<td>1.1</td>
<td>0.0002</td>
<td>0.26</td>
<td>0.76</td>
</tr>
<tr>
<td>2</td>
<td>0.90009</td>
<td>1.1</td>
<td>0.0001996404857</td>
<td>0.2601620081</td>
<td>0.759955</td>
</tr>
<tr>
<td>3</td>
<td>0.89991</td>
<td>1.1</td>
<td>0.0002003604863</td>
<td>0.2598380081</td>
<td>0.760045</td>
</tr>
<tr>
<td>...</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

header

- Keywords Area
- model
- surrogate
- global
- import_challenge_points_file
- custom_annotated
- header

Enable header row in custom-annotated tabular file

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

See description of parent custom_annotated

**eval_id**

- Keywords Area
- model
- surrogate
- global
- import_challenge_points_file
- custom_annotated
- eval_id

Enable evaluation ID column in custom-annotated tabular file
6.3. MODEL

Specification
Alias: none
Argument(s): none

Description
See description of parent custom_annotated

interface_id
- Keywords Area
- model
- surrogate
- global
- import_challenge_points_file
- custom_annotated
- interface_id
Enable interface ID column in custom-annotated tabular file

Specification
Alias: none
Argument(s): none

Description
See description of parent custom_annotated

freeform
- Keywords Area
- model
- surrogate
- global
- import_challenge_points_file
- freeform
Selects freeform file format

Topics
This keyword is related to the topics:
- file_formats
Specification

Alias: none

Argument(s): none

Default: annotated

Description

A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. Most commonly, each row contains data for variables, or variables followed by responses, though the format is used for other tabular exports/imports as well.

Default Behavior

The annotated format is the default for tabular export/import. To change this behavior, specify freeform in the relevant export/import context.

Usage Tips

- Prior to October 2011, calibration and surrogate data files were free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.
- In freeform, the num_rows x num_cols total data entries may be separated with any whitespace including spaces, tabs, and newlines. In this format, vectors may therefore appear as a single row or single column (or mixture; entries will populate the vector in order).
- Some TPLs like SCOLIB and JEGA manage their own file I/O and only support the freeform option.

Examples

Export a freeform tabular file containing only data for variables and responses. Input file fragment:

```
environment
tabular_data
tabular_data_file = 'dakota_summary.dat'
freeform
```

Resulting tabular file:

```
0.9 1.1 0.0002 0.26 0.76
0.90009 1.1 0.0001996404857 0.2601620081 0.759955
0.89991 1.1 0.0002003604863 0.2598380081 0.760045
...```

active_only

- Keywords Area
- model
- surrogate
- global
- import_challenge_points_file
- active_only

Import only active variables from tabular data file
Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none

Argument(s): none

Description

By default, files for tabular data imports are expected to contain columns for all variables, active and inactive. The keyword `active_only` indicates that the file to import contains only the active variables.

This option should only be used in contexts where the inactive variables have no influence, for example, building a surrogate over active variables, with the state variables held at nominal. It should not be used in more complex nested contexts, where the values of inactive variables are relevant to the function evaluations used to build the surrogate.

multipoint

- **Keywords Area**
- model
- surrogate
- multipoint

Construct a surrogate from multiple existing training points

Specification

Alias: none

Argument(s): none

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Required</strong></td>
<td>tana</td>
<td>actual_model_pointer</td>
<td>Local multi-point model via two-point nonlinear approximation Pointer to specify a ”truth” model, from which to construct a surrogate</td>
</tr>
</tbody>
</table>
Description

Multipoint approximations use data from previous design points to improve the accuracy of local approximations. The data often comes from the current and previous iterates of a minimization algorithm.

Currently, only the Two-point Adaptive Nonlinearity Approximation (TANA-3) method of [92] is supported with the \texttt{tana} keyword.

The truth model to be used to generate the value/gradient data used in the approximation is identified through the required \texttt{actual\_model\_pointer} specification.

See Also

These keywords may also be of interest:

- \texttt{local}
- \texttt{global}
- \texttt{hierarchical}

\texttt{tana}

- \texttt{Keywords Area}
- \texttt{model}
- \texttt{surrogate}
- \texttt{multipoint}
- \texttt{tana}

Local multi-point model via two-point nonlinear approximation

Specification

Alias: none

\textbf{Argument(s):} none

Description

\textbf{TANA} stands for Two Point Adaptive Nonlinearity Approximation.

The TANA-3 method[92] is a multipoint approximation method based on the two point exponential approximation[25]. This approach involves a Taylor series approximation in intermediate variables where the powers used for the intermediate variables are selected to match information at the current and previous expansion points.

\textit{Known Issue}: \textit{When using discrete variables, there have been sometimes significant differences in surrogate behavior observed across computing platforms in some cases. The cause has not yet been fully diagnosed and is currently under investigation. In addition, guidance on appropriate construction and use of surrogates with discrete variables is under development. In the meantime, users should therefore be aware that there is a risk of inaccurate results when using surrogates with discrete variables.}
6.3. MODEL

Theory

The form of the TANA model is:

\[ \hat{f}(x) \approx f(x_2) + \sum_{i=1}^{n} \frac{\partial f}{\partial x_i}(x_2) \frac{x_{i,2}^{1-p_i}}{p_i} (x_i^{p_i} - x_{i,2}^{p_i}) + \frac{1}{2} \epsilon(x) \sum_{i=1}^{n} (x_i^{p_i} - x_{i,2}^{p_i})^2 \]

where \( n \) is the number of variables and:

\[ p_i = 1 + \ln \left[ \frac{\partial f}{\partial x_i}(x_1) \right] / \ln \left[ \frac{x_{i,1}}{x_{i,2}} \right] \]

\[ \epsilon(x) = \frac{H}{\sum_{i=1}^{n} \left( x_i^{p_i} - x_{i,1}^{p_i} \right)^2 + \sum_{i=1}^{n} \left( x_i^{p_i} - x_{i,2}^{p_i} \right)^2} H = 2 \left[ f(x_1) - f(x_2) - \sum_{i=1}^{n} \frac{\partial f}{\partial x_i}(x_2) \frac{x_{i,2}^{1-p_i}}{p_i} \right] \]

and \( x_2 \) and \( x_1 \) are the current and previous expansion points. Prior to the availability of two expansion points, a first-order Taylor series is used.

actual_model_pointer

- Keywords Area
- model
- surrogate
- multipoint
- actual_model_pointer

Pointer to specify a "truth" model, from which to construct a surrogate

Topics

This keyword is related to the topics:

- block_pointer

Specification

Alias: none

Argument(s): STRING

Description

This must point to a model block, identified by id_model. That model will be run to generate training data, from which a surrogate model will be constructed.

See block_pointer for details about pointers.

local

- Keywords Area
- model
- surrogate
- local

Build a locally accurate surrogate from data at a single point
Specification

Alias: none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required</td>
<td></td>
<td>taylor_series</td>
<td>Construct a Taylor Series expansion around a point</td>
</tr>
<tr>
<td></td>
<td></td>
<td>actual_model_pointer</td>
<td>Pointer to specify a &quot;truth&quot; model, from which to construct a surrogate</td>
</tr>
</tbody>
</table>

Description

Local approximations use value, gradient, and possibly Hessian data from a single point to form a series expansion for approximating data in the vicinity of this point.

The currently available local approximation is the taylor_series selection.

The truth model to be used to generate the value/gradient/Hessian data used in the series expansion is identified through the required actual_model_pointer specification. The use of a model pointer (as opposed to an interface pointer) allows additional flexibility in defining the approximation. In particular, the derivative specification for the truth model may differ from the derivative specification for the approximation, and the truth model results being approximated may involve a model recursion (e.g., the values/gradients from a nested model).

See Also

These keywords may also be of interest:

- global
- hierarchical
- multipoint


taylor_series

- Keywords Area
- model
- surrogate
- local
- taylor_series

Construct a Taylor Series expansion around a point

Specification

Alias: none

Argument(s): none
6.3. MODEL

Description

The Taylor series model is purely a local approximation method. That is, it provides local trends in the vicinity of a single point in parameter space.

The order of the Taylor series may be either first-order or second-order, which is automatically determined from the gradient and Hessian specifications in the responses specification (see responses for info on how to specify gradients and Hessians) for the truth model.

Known Issue: When using discrete variables, there have been sometimes significant differences in surrogate behavior observed across computing platforms in some cases. The cause has not yet been fully diagnosed and is currently under investigation. In addition, guidance on appropriate construction and use of surrogates with discrete variables is under development. In the meantime, users should therefore be aware that there is a risk of inaccurate results when using surrogates with discrete variables.

Theory

The first-order Taylor series expansion is:

\[
\hat{f}(x) \approx f(x_0) + \nabla_x f(x_0)^T (x - x_0)
\]

and the second-order expansion is:

\[
\hat{f}(x) \approx f(x_0) + \nabla_x f(x_0)^T (x - x_0) + \frac{1}{2} (x - x_0)^T \nabla^2_x f(x_0) (x - x_0)
\]

where \(x_0\) is the expansion point in n-dimensional parameter space and \(f(x_0), \nabla_x f(x_0), \text{ and } \nabla^2_x f(x_0)\) are the computed response value, gradient, and Hessian at the expansion point, respectively.

As dictated by the responses specification used in building the local surrogate, the gradient may be analytic or numerical and the Hessian may be analytic, numerical, or based on quasi-Newton secant updates.

In general, the Taylor series model is accurate only in the region of parameter space that is close to \(x_0\). While the accuracy is limited, the first-order Taylor series model reproduces the correct value and gradient at the point \(x_0\), and the second-order Taylor series model reproduces the correct value, gradient, and Hessian. This consistency is useful in provably-convergent surrogate-based optimization. The other surface fitting methods do not use gradient information directly in their models, and these methods rely on an external correction procedure in order to satisfy the consistency requirements of provably-convergent SBO.

actual_model_pointer

- Keywords Area
- model
- surrogate
- local
- actual_model_pointer

Pointer to specify a "truth" model, from which to construct a surrogate

Topics

This keyword is related to the topics:

- block_pointer
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none
Argument(s): STRING

Description

This must point to a model block, identified by id_model. That model will be run to generate training data, from which a surrogate model will be constructed.

See block_pointer for details about pointers.

Hierarchical approximations use corrected results from a low fidelity model as an approximation to the results of a high fidelity “truth” model.

Specification

Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/- Optional Required</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>ordered_model_fidelities</td>
<td>Specification of an hierarchy of model fidelities, ordered from low to high.</td>
</tr>
<tr>
<td></td>
<td>correction</td>
<td>correction</td>
<td>Correction approaches for surrogate models</td>
</tr>
</tbody>
</table>

Description

Hierarchical approximations use corrected results from a low fidelity model as an approximation to the results of a high fidelity “truth” model. These approximations are also known as model hierarchy, multifidelity, variable fidelity, and variable complexity approximations. The required ordered_model_fidelities specification points to a sequence of model specifications of varying fidelity, ordered from lowest to highest fidelity. The highest fidelity model provides the truth model, and each of the lower fidelity alternatives provides different levels of approximation at different levels of cost.

In multifidelity optimization, the search algorithm relies primarily on the lower fidelity models, which are corrected for consistency with higher fidelity models. The higher fidelity models are used primarily for verifying candidate steps based on solution of low fidelity approximate subproblems and updating for low fidelity corrections. In multifidelity uncertainty quantification, resolution levels are tailored across the ordered model hierarchy with fine resolution of the lowest fidelity and then decreasing resolution for each level of model discrepancy.
The correction specification specifies which correction technique will be applied to the low fidelity results in order to match the high fidelity results at one or more points. In the hierarchical case (as compared to the global case), the correction specification is required, since the omission of a correction technique would effectively eliminate the purpose of the high fidelity model. If it is desired to use a low fidelity model without corrections, then a hierarchical approximation is not needed and a single model should be used. Refer to global for additional information on available correction approaches.

Theory

Multifidelity Surrogates: Multifidelity modeling involves the use of a low-fidelity physics-based model as a surrogate for the original high-fidelity model. The low-fidelity model typically involves a coarser mesh, looser convergence tolerances, reduced element order, or omitted physics. It is a separate model in its own right and does not require data from the high-fidelity model for construction. Rather, the primary need for high-fidelity evaluations is for defining correction functions that are applied to the low-fidelity results.

Multifidelity Surrogate Models

A second type of surrogate is the \{model hierarchy\} type (also called multifidelity, variable fidelity, variable complexity, etc.). In this case, a model that is still physics-based but is of lower fidelity (e.g., coarser discretization, reduced element order, looser convergence tolerances, omitted physics) is used as the surrogate in place of the high-fidelity model. For example, an inviscid, incompressible Euler CFD model on a coarse discretization could be used as a low-fidelity surrogate for a high-fidelity Navier-Stokes model on a fine discretization.

See Also

These keywords may also be of interest:

- global
- local
- multipoint
- multilevel_sampling
- polynomial_chaos
- stoch_collocation
- surrogate_based_local

ordered_model_fidelities

- Keywords Area
- model
- surrogate
- hierarchical
- ordered_model_fidelities

Specification of an hierarchy of model fidelities, ordered from low to high.
CHAPTER 6. KEYWORDS AREA

Specification

Alias: model_fidelity_sequence
Argument(s): STRINGLIST

Description

A hierarchical surrogate model manages an ordered set of model fidelities, each of which may in turn involve multiple discretization levels (in the case of a simulation model) or additional model recursions.

The ordering is assumed to be from lowest fidelity to highest fidelity, as dictated by an accuracy versus cost trade-off. Corresponding sequence specifications within methods (e.g., quadrature_order_sequence, sparse_grid_level_sequence, expansion_order_sequence, etc. within stochastic expansion methods) should be synchronized with this model order.

Additional Discussion

Internal to the model, only one low fidelity model instance and one high fidelity model instance are active at any given time, although various optimization and UQ algorithms can be used to traverse deep multilevel and multifidelity hierarchies by activating different model combinations and different response modes within the hierarchical model infrastructure.

Examples

```python
model,
  id_model = 'HIERARCH'
  surrogate hierarchical
    ordered_model_fidelities = 'LF' 'MF' 'HF'
    correction additive zeroth_order

model,
  id_model = 'LF'
  simulation
    interface_pointer = 'LF_DRIVER'

model,
  id_model = 'MF'
  simulation
    interface_pointer = 'MF_DRIVER'

model,
  id_model = 'HF'
  simulation
    interface_pointer = 'HF_DRIVER'
```

See Also

These keywords may also be of interest:

- multilevel_sampling
- polynomial_chaos
- stoch_collocation
- surrogate_based_local
correction

- Keywords Area
- model
- surrogate
- hierarchical
- correction

Correction approaches for surrogate models

**Specification**

**Alias:** none
**Argument(s):** none
**Default:** no surrogate correction

| Required/-| Description of Group | Dakota Keyword | Dakota Keyword Description |
| Optional (Choose One) | Correction Order (Group 1) | zeroth_order | Specify that truth values must be matched. |
| first_order | Specify that truth values and gradients must be matched. |
| second_order | Specify that truth values, gradients and Hessians must be matched. |

| Required (Choose One) | Correction Type (Group 2) | additive | Additive correction factor for local surrogate accuracy |
| multiplicative | Multiplicative correction factor for local surrogate accuracy. |
Description

Some of the surrogate model types support the use of correction factors that improve the local accuracy of the surrogate models.

The correction specification specifies that the approximation will be corrected to match truth data, either matching truth values in the case of zeroth-order matching, matching truth values and gradients in the case of first-order matching, or matching truth values, gradients, and Hessians in the case of second-order matching. For additive and multiplicative corrections, the correction is local in that the truth data is matched at a single point, typically the center of the approximation region. The additive correction adds a scalar offset (zeroth-order), a linear function (first-order), or a quadratic function (second-order) to the approximation to match the truth data at the point, and the multiplicative correction multiplies the approximation by a scalar (zeroth-order), a linear function (first-order), or a quadratic function (second-order) to match the truth data at the point. The additive first-order case is due to[57] and the multiplicative first-order case is commonly known as beta correction[40]. For the combined correction, the use of both additive and multiplicative corrections allows the satisfaction of an additional matching condition, typically the truth function values at the previous correction point (e.g., the center of the previous trust region). The combined correction is then a multipoint correction, as opposed to the local additive and multiplicative corrections. Each of these correction capabilities is described in detail in[24].

The correction factors force the surrogate models to match the true function values and possibly true function derivatives at the center point of each trust region. Currently, Dakota supports either zeroth-, first-, or second-order accurate correction methods, each of which can be applied using either an additive, multiplicative, or combined correction function. For each of these correction approaches, the correction is applied to the surrogate model and the corrected model is then interfaced with whatever algorithm is being employed. The default behavior is that no correction factor is applied.

The simplest correction approaches are those that enforce consistency in function values between the surrogate and original models at a single point in parameter space through use of a simple scalar offset or scaling applied to the surrogate model. First-order corrections such as the first-order multiplicative correction (also known as beta correction[15]) and the first-order additive correction[57] also enforce consistency in the gradients and provide a much more substantial correction capability that is sufficient for ensuring provable convergence in SBO algorithms. SBO convergence rates can be further accelerated through the use of second-order corrections which also enforce consistency in the Hessians[24], where the second-order information may involve analytic, finite-difference, or quasi-Newton Hessians.

Correcting surrogate models with additive corrections involves

\[ \hat{f}_{hi_a}(\mathbf{x}) = f_{lo}(\mathbf{x}) + \alpha(\mathbf{x}) \]  \hspace{1cm} (6.9)

where multifidelity notation has been adopted for clarity. For multiplicative approaches, corrections take the form

\[ \hat{f}_{hi_s}(\mathbf{x}) = f_{lo}(\mathbf{x}) \beta(\mathbf{x}) \]  \hspace{1cm} (6.10)

where, for local corrections, \( \alpha(\mathbf{x}) \) and \( \beta(\mathbf{x}) \) are first or second-order Taylor series approximations to the exact correction functions:
\[ \alpha(x) = A(x_c) + \nabla A(x_c)^T (x - x_c) + \frac{1}{2} (x - x_c)^T \nabla^2 A(x_c)(x - x_c) \] (6.11)

\[ \beta(x) = B(x_c) + \nabla B(x_c)^T (x - x_c) + \frac{1}{2} (x - x_c)^T \nabla^2 B(x_c)(x - x_c) \] (6.12)

where the exact correction functions are

\[ A(x) = f_{hi}(x) - f_{lo}(x) \] (6.13)

\[ B(x) = \frac{f_{hi}(x)}{f_{lo}(x)} \] (6.14)

Refer to [24] for additional details on the derivations.

A combination of additive and multiplicative corrections can provide for additional flexibility in minimizing the impact of the correction away from the trust region center. In other words, both additive and multiplicative corrections can satisfy local consistency, but through the combination, global accuracy can be addressed as well. This involves a convex combination of the additive and multiplicative corrections:

\[ \tilde{f}_{hi}(x) = \gamma \tilde{f}_{hi}(x) + (1 - \gamma) \tilde{f}_{hi,lo}(x) \]

where \( \gamma \) is calculated to satisfy an additional matching condition, such as matching values at the previous design iterate.

It should be noted that in both first order correction methods, the function \( \tilde{f}(x) \) matches the function value and gradients of \( f_t(x) \) at \( x = x_c \). This property is necessary in proving that the first order-corrected SBO algorithms are provably convergent to a local minimum of \( f_t(x) \). However, the first order correction methods are significantly more expensive than the zeroth order correction methods, since the first order methods require computing both \( \nabla f_t(x_c) \) and \( \nabla f_s(x_c) \). When the SBO strategy is used with either of the zeroth order correction methods, or with no correction method, convergence is not guaranteed to a local minimum of \( f_t(x) \). That is, the SBO strategy becomes a heuristic optimization algorithm. From a mathematical point of view this is undesirable, but as a practical matter, the heuristic variants of SBO are often effective in finding local minima.

Usage guidelines

- Both the additive zeroth_order and multiplicative zeroth_order correction methods are “free” since they use values of \( f_t(x_c) \) that are normally computed by the SBO strategy.
- The use of either the additive first_order method or the multiplicative first_order method does not necessarily improve the rate of convergence of the SBO algorithm.
- When using the first order correction methods, the gradient-related response keywords must be modified to allow either analytic or numerical gradients to be computed. This provides the gradient data needed to compute the correction function.
- For many computationally expensive engineering optimization problems, gradients often are too expensive to obtain or are discontinuous (or may not exist at all). In such cases the heuristic SBO algorithm has been an effective approach at identifying optimal designs [35].

zeroth_order

- Keywords Area
- model
CHAPTER 6. KEYWORDS AREA

- surrogate
- hierarchical
- correction
- zeroth_order

Specify that truth values must be matched.

**Specification**

**Alias:** none  
**Argument(s):** none

**Description**

The correction specification specifies that the approximation will be corrected to match truth data. The keyword `zeroth_order` matching ensures that truth values are matched.

**first_order**

- Keywords Area
- model
- surrogate
- hierarchical
- correction
- first_order

Specify that truth values and gradients must be matched.

**Specification**

**Alias:** none  
**Argument(s):** none

**Description**

This correction specification specifies that the approximation will be corrected to match truth data. The keyword `first_order` matching ensures that truth values and gradients are matched.
6.3. MODEL

**second_order**

- Keywords Area
- model
- surrogate
- hierarchical
- correction
- second_order

Specify that truth values, gradients and Hessians must be matched.

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

The correction specification specifies that the approximation will be corrected to match truth data. The keyword `second_order` matching ensures that truth values, gradients and Hessians are matched.

**additive**

- Keywords Area
- model
- surrogate
- hierarchical
- correction
- additive

Additive correction factor for local surrogate accuracy

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

Use an additive correction factor to improve the local accuracy of a surrogate.
**multiplicative**
- Keywords Area
- model
- surrogate
- hierarchical
- correction
- multiplicative

Multiplicative correction factor for local surrogate accuracy.

**Specification**

Alias: none
Argument(s): none

**Description**

Use a multiplicative correction factor to improve the local accuracy of a surrogate.

**combined**
- Keywords Area
- model
- surrogate
- hierarchical
- correction
- combined

Multipoint correction for a hierarchical surrogate

**Specification**

Alias: none
Argument(s): none

**Description**

For the combined correction, the use of both additive and multiplicative corrections allows the satisfaction of an additional matching condition, typically the truth function values at the previous correction point (e.g., the center of the previous trust region). The combined correction is then a multipoint correction, as opposed to the local additive and multiplicative corrections.
6.3.4 nested

- Keywords Area
- model
- nested

A model whose responses are computed through the use of a sub-iterator

**Specification**

**Alias:** none

**Argument(s):** none

<table>
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<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<td><strong>Required</strong></td>
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<td>optional_interface_pointer</td>
<td>Pointer to interface that provides non-nested responses</td>
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<tr>
<td></td>
<td></td>
<td>sub_method_pointer</td>
<td>The sub_method_pointer specifies the method block for the sub-iterator</td>
</tr>
</tbody>
</table>

**Description**

Instead of appealing directly to a primary interface, a nested model maps variables to responses by executing a secondary iterator, or a "sub-iterator". In other words, a function evaluation of the primary study consists of a solution of an entire secondary study - potentially many secondary function evaluations.

The sub-iterator in turn operates on a sub-model. The sub-iterator responses may be combined with non-nested contributions from an optional interface specification.

A **sub_method_pointer** must be provided in order to specify the method block describing the sub-iterator. The remainder of the model is specified under that keyword.

A **optional_interface_pointer points** to the interface specification and optional_interface_responses_pointer points to a responses specification describing the data to be returned by this interface. This interface is used to provide non-nested data, which is then combined with data from the nested iterator using the primary_response_mapping. (See the discussions for the sub_method_pointer and optional_interface_pointer keywords.)

**See Also**

These keywords may also be of interest:

- single
- surrogate
### optional_interface_pointer

- **Keywords Area**
- **model**
- **nested**
- **optional_interface_pointer**

Pointer to interface that provides non-nested responses

### Topics

This keyword is related to the topics:

- **block_pointer**

### Specification

**Alias:** none  
**Argument(s):** STRING  
**Default:** no optional interface

<p>| Required/- | Description of | Dakota Keyword | Dakota Keyword |</p>
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<td>Optional</td>
<td></td>
<td>optional_interface-</td>
<td>Pointer to responses block that defines non-nested responses</td>
</tr>
<tr>
<td>Optional</td>
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<td>_responses_pointer</td>
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</table>

### Description

`optional_interface_pointer` is used to specify an optional interface (using that interface block’s `id_interface` label) to provide non-nested responses to the nested model.

To generate the complete set of primary responses (response functions, objective functions, and calibration terms) expected by the nested model, primary responses from the optional interface may be combined (by addition) with responses derived from sub-iterator results, or they may be presented unchanged to the nested model. The way that Dakota treats primary responses from these two sources depends on the number of rows of and entries in the `primary_response_mapping` matrix.

To understand how, it is helpful to consider the following expression. Nested model primary responses $r$ are computed from the column vector of optional interface responses $f$, the `primary_response_mapping` matrix $W$, and the column vector of results from the sub-iterator $s$.

$$\{r\} = \left\{ \frac{f}{0} \right\} + \left\{ \frac{[W]\{s\}}{0} \right\}$$

The number of rows in $f$ is equal to the number of primary responses returned by the optional interface, and in $r$, the number of primary responses expected by the nested model. In this expression, 0 represents ”padding” that may be needed by either the optional interface vector or the sub-iterator vector to make them the same dimension as $r$. One or the other of these quantities may be padded, but not both. In terms of the Dakota input, this means that the number of nested model primary responses must equal the larger of these two quantities: the number of optional interface responses or the number of rows in the `primary_response_mapping`. 


The nested model’s secondary responses (nonlinear constraints) are the secondary responses from the optional interface augmented by the secondary responses constructed from sub-iterator results. Unlike primary responses from these two sources, which may be combined by adding, it is not possible presently to combine secondary responses. For this reason, the number of nested model’s secondary responses must equal the number of secondary responses provided by the optional interface, plus the number provided by the sub-iterator (i.e. the number of rows in the secondary_response_mapping). Secondary responses from the optional interface are inserted first into the nested model’s nonlinear constraints; those from the sub-iterator come after. If the nested model has secondary responses and an optional interface is used, it is necessary to specify a separate response block for the optional interface using the optional_interface_response_pointer. Targets and upper and lower bounds for the nonlinear constraints are taken from the nested model’s response block.

Examples

The first example illustrates the use of an optional interface and primary response mapping. No secondary responses are present. Assume that the inner method returns two results (suppose its the mean and standard deviation of a single response), so that the dimensions of primary_response_mapping will be interpreted by Dakota as 1x2, just as they are written here.

The nested model (nested) expects two primary responses (outer_resp block), and the optional interface returns two (opt_resp block).

model
  id_model 'nested'
  nested
    optional_interface_pointer 'opt_intf'
    optional_interface_response_pointer 'opt_resp'
    sub_method_pointer 'inner_method'
    primary_response_mapping 1.0 2.0

  responses_pointer 'outer_resp'
  variables_pointer 'outer_vars'

responses
  id_responses 'opt_resp'
  response_functions 2
    descriptors 'opt1' 'opt2'
    no_gradients
    no_hessians

responses
  id_responses 'outer_resp'
  response_functions 2
    descriptors 'out1' 'out2'
    no_gradients
    no_hessians

The first nested model response, out1 will be computed \(out1 = opt1 + 1.0 \cdot mean + 2.0 \cdot stddev\), and the second response out2 will be equal to simply opt2. In the matrix form introduced above, including the implicit padding:

\[
\begin{bmatrix}
  out1 \\
  out2
\end{bmatrix} =
\begin{bmatrix}
  opt1 \\
  opt2
\end{bmatrix} +
\begin{bmatrix}
  1.0 \cdot mean + 2.0 \cdot stddev \\
  0
\end{bmatrix}
\]

The optional_interface_response_pointer was not strictly needed. Because the number of responses returned by the optional interface and expected by the nested model is the same (and no secondary responses are present), the nested model’s response specification alone would have sufficed.
If it were desired to combine \textit{opt2} with the sub-iterator’s results and set \textit{out1} to \textit{opt1} with no combination, then the primary\_response\_mapping matrix could be changed to:

\begin{verbatim}
primary_response_mapping  0.0  0.0
1.0  2.0
\end{verbatim}

Secondary responses will be demonstrated in the second example.

```plaintext
model
id_model 'nested'

optional_interface_pointer 'opt\_intf'
  optional_interface_response_pointer 'opt\_resp'
sub_method_pointer 'inner\_method'
  primary_response_mapping 1.0 2.0
secondary_response_mapping 1.0 0.0
  responses_pointer 'outer\_resp'
variables_pointer 'outer\_vars'

responses
id_responses 'opt\_resp'
objective_functions 2
  descriptors 'opt1' 'opt2'
nonlinear_inequality_constraints 1
  descriptors 'optc'
no_gradients
no_hessians

responses
id_responses 'outer\_resp'
objective_functions 2
  descriptors 'out1' 'out2'
nonlinear_inequality_constraints 2
  descriptors 'outc1' 'outc2'
no_gradients
no_hessians
```

The nested model expects a total of two constraints. Because the secondary\_response\_mapping has one row, one of these constraints will be supplied from the sub-iterator. The other is provided by the optional interface. Secondary responses from the optional iterator come first, and so \textit{optc} is placed in \textit{outc1}. \textit{outc2} takes the value computed from the sub-iterator results.

\textbf{optional\_interface\_responses\_pointer}

- **Keywords Area**
- **model**
- **nested**
- **optional\_interface\_pointer**
- **optional\_interface\_responses\_pointer**

Pointer to responses block that defines non-nested responses

\textbf{Topics}

This keyword is related to the topics:

- **block\_pointer**
6.3. MODEL

Specification

Alias: none
Argument(s): STRING
Default: reuse of top-level responses specification

Description

optional_interface_responses_pointer points to the responses block (specifically, its id_responses label) that defines the non-nested response to return to the nested model. The primary_response_mapping keywords control how these non-nested responses are combined with responses from the nested sub-iterator. See the entry for optional_interface_pointer for a full description. If optional_interface_pointer is not provided, the top-level responses specification is reused.

sub_method_pointer

• Keywords Area
• model
• nested
• sub_method_pointer

The sub_method_pointer specifies the method block for the sub-iterator

Topics

This keyword is related to the topics:

• block_pointer

Specification

Alias: none
Argument(s): STRING

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<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<td></td>
<td>Specify the number of iterator servers when Dakota is run in parallel</td>
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<td></td>
<td>iterator_scheduling</td>
<td></td>
<td>Specify the scheduling of concurrent iterators when Dakota is run in parallel</td>
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<td>Specify the number of processors per iterator server when Dakota is run in parallel. Primary mapping of top-level variables to sub-model variables.</td>
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<tr>
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<td>Secondary mapping of top-level variables to sub-model variables.</td>
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<tr>
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<td>secondary_variable_mapping</td>
<td>Secondary mapping of top-level variables to sub-model variables.</td>
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<td>primary_response_mapping</td>
<td>Primary mapping of sub-model responses to top-level responses.</td>
<td></td>
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<tr>
<td>Optional</td>
<td>secondary_response_mapping</td>
<td>Secondary mapping of sub-model responses to top-level responses.</td>
<td></td>
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</tr>
</tbody>
</table>

### Description

The `sub_method_pointer` specifies the method block for the sub-iterator.

See `block_pointer` for details about pointers.

A nested model performs an evaluation (variables-to-responses mapping) by running a complete sub-iterator (i.e., method) to completion. The sub-iterator, which is specified using the `sub_method_pointer`, has its own model. This model, referred to here as the sub-model, possesses its own variables and responses. Prior to every execution of the sub-iterator, information about the nested model’s variables is injected into the sub-model’s variables. After the sub-iterator has completed, its results are passed back up to the nested model as responses.

Communication of variables information from a nested model to its sub-iterator, and in the opposite direction of sub-iterator results to nested model responses, is called mapping. (This mapping must not be confused with the variables-to-responses mapping that constitutes an evaluation.) Dakota allows considerable power and flexibility in how nested model mappings are performed. They are specified using four keywords: for the variables, `primary_variable_mapping` and `secondary_variable_mapping`; and for the responses, `primary_response_mapping` and `secondary_response_mapping`. They are described below.

### Variable Mappings

In the variable mapping case, primary and secondary variable mapping specifications are used to map from the top-level variables into the sub-model variables. These mappings support three possibilities in any combination: (1) insertion of an active top-level variable value into an identified sub-model distribution parameter for an identified active sub-model variable, (2) insertion of an active top-level variable value into an identified active sub-model variable value, and (3) addition of an active top-level variable value as an inactive sub-model variable, augmenting the active sub-model variables.

For the variable mappings, the primary and secondary specifications are lists of strings that are used to target specific sub-model variables and their sub-parameters, respectively. The primary strings are matched to sub-
model variable descriptors such as ‘cdv_1’ (either user-supplied or default labels). The secondary strings are matched to random variable distribution parameters such as ‘mean’ or ‘num_trials’ or design/state variable sub-parameters such as ‘lower_bound’ or ‘upper_bound’.

An important limitation is that real-valued top-level variables must map to real-valued sub-model variables or real-valued sub-parameters, and integer-valued top-level variables must map to either integer-valued sub-model variables or integer-valued sub-parameters. However, as long as these real versus integer constraints are satisfied, mappings are free to cross variable types (design, aleatory uncertain, epistemic uncertain, state) and domain types (continuous, discrete).

Both primary_variable_mapping and secondary_variable_mapping specifications are optional, which is designed to support the following three possibilities:

1. If both primary and secondary variable mappings are specified, then an active top-level variable value will be inserted into the identified sub-parameter (the secondary mapping) for the identified sub-model variable (the primary mapping).

2. If a primary mapping is specified but a secondary mapping is not, then an active top-level variable value will be inserted into the identified sub-model variable value (the primary mapping).

3. If a primary mapping is not specified (corresponding secondary mappings, if specified, are ignored), then an active top-level variable value will be inserted into a corresponding sub-model variable, based on matching of variable types (e.g., top-level and sub-model variable specifications both allocate a set of ‘continuous_design’ variables which are active at the top level). Multiple sub-model variable types may be updated in this manner, provided that they are all active in the top-level variables. Since there is a direct variable correspondence for these default insertions, sub-model bounds and descriptors are also updated from the top-level bounds and labels in order to eliminate the need for redundant input file specifications. Thus, it is typical for the sub-model variables specification to only contain the minimal required information, such as the number of variables of each type, for these insertion targets. The sub-model must allocate enough space for each of the types that will accept default insertions, and the leading set of matching sub-model variables are updated (i.e., the sub-model may allocate more than needed and the trailing set will be unmodified).

These different variable mapping possibilities may be used in any combination by employing empty strings ("") for particular omitted mappings (the number of strings in user-supplied primary and secondary variable mapping specifications must equal the total number of active top-level variables, including both continuous and discrete types). The ordering of the active variables is the same as shown in dakota.input.summary on Input Spec Summary and as presented in the variables section of this manual.

Inactive nested model variables are treated differently from those in the active view. If inactive variables are present at the outer level, then the default type 3 mapping is used for these variables; that is, outer loop inactive variables are inserted into inner loop variables (active or inactive) based on matching of variable types, top-level bounds and labels are also propagated, the inner loop must allocate sufficient space to receive the outer loop values, and the leading subset within this inner loop allocation is updated. This capability is important for allowing nesting beyond two levels, since an active variable at the outer-most loop may become inactive at the next lower level, but still needs to be further propagated down to lower levels in the recursion.

Response Mappings

For the response mappings, the primary and secondary specifications determine how results from the completed sub-iterator are mapped into nested model responses. The response mapping defines a matrix which scales and combines the results from the inner loop into outer loop responses. Each row of the mapping corresponds to one outer loop response, and each column of the mapping corresponds to a result from the inner loop. The results returned from the sub-model are best thought of as forming a column vector; the nested model responses are then the dot-product of the mapping matrix and results vector. The number and type of results that are available and must be accounted for in the response mapping depends on the sub-iterator type:

- optimization: the final objective function(s) and nonlinear constraints
nonlinear least squares: the final least squares terms and nonlinear constraints

daleatory uncertainty quantification (UQ): for each response function, a mean statistic, a standard deviation statistic, and all probability/reliability/generic reliability/response level results for any user-specified response_levels, probability_levels, reliability_levels, and/or gen_reliability_levels, in that order.

epistemic and mixed aleatory/epistemic UQ using interval estimation methods: lower and upper interval bounds for each response function.

epistemic and mixed aleatory/epistemic UQ using evidence methods: for each response function, lower and upper interval bounds (belief and plausibility) for all probability/reliability/generic reliability/response level results computed from any user-specified response_levels, probability_levels, reliability_levels, and/or gen_reliability_levels, in that order. Parameter studies and design of experiments: for optimization and least squares response data sets, the best solution found (lowest constraint violation if infeasible, lowest composite objective function if feasible). For generic response data sets, a best solution metric is not defined, so the sub-iterator response vector is empty in this case.

The primary_response_mapping matrix maps sub-iterator results into top-level objective functions, least squares terms, or generic response functions, depending on the declared top-level response set. The secondary_response_mapping matrix maps sub-iterator results into top-level nonlinear inequality and equality constraints.

Summary
The nested model constructs admit a wide variety of multi-iterator, multi-model solution approaches. For example, optimization within optimization (for hierarchical multidisciplinary optimization), uncertainty quantification within uncertainty quantification (for second-order probability), uncertainty quantification within optimization (for optimization under uncertainty), and optimization within uncertainty quantification (for uncertainty of optima) are all supported, with and without surrogate model indirection. Several examples of nested model usage are provided in the Users Manual, most notably mixed epistemic-aleatory UQ, optimization under uncertainty (OUU), and surrogate-based UQ.

Examples
Two examples are provided to illustrate nested models. The first is a relatively simple case. Although it is somewhat contrived, it demonstrates several features of nested models. A step-by-step explanation is provided below.

environment
  method_pointer 'opt'

method
  id_method 'opt'
  asynch_pattern_search
  model_pointer 'outer_model'
  output verbose

model
  id_model 'outer_model'
  variables_pointer 'outer_vars'
  responses_pointer 'outer_resps'
  nested
    sub_method_pointer 'UQ_method'
    primary_variable_mapping 'x1' 'x2'
    secondary_variable_mapping 'mean' 'mean'
    primary_response_mapping 0 0 0.3 0 0 0 0.7

variables
  id_variables 'outer_vars'
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```
continuous_design 2
  descriptors 'x1_mean' 'x2_mean'
  lower_bounds -2.0 -2.0
  upper_bounds 2.0 2.0

responses
  id_responses 'outer_resps'
  objective_functions 1
  descriptors 'sum_p'
  no_gradients
  no_hessians

method
  id_method 'UQ_method'
  sampling samples 30
  seed 1234
  model_pointer 'UQ_model'
  probability_levels 0.9 0.9

model
  id_model 'UQ_model'
  single
  variables_pointer 'inner_vars'
  responses_pointer 'inner_resps'
  interface_pointer 'inf'

variables
  id_variables 'inner_vars'
  normal_uncertain 2
  descriptors 'x1' 'x2'
  means 0.0 0.0
  std_deviations 1.0 1.0

responses
  id_responses 'inner_resps'
  response_functions 2
  descriptors 'f1' 'f2'
  no_gradients
  no_hessians

interface
  id_interface 'inf'
  direct
  analysis_drivers 'text_book'
```

The example input is an ‘optimization under uncertainty’ or OUU. In an OUU, some statistic of the simulation response is optimized. In this case, a weighted sum of the 90th percentiles of two simulation responses from the text_book driver is being minimized. The uncertainty in these responses is driven by uncertainty in the input variables, which are normally distributed. The means of the uncertain variables are the design variables in the optimization.

In Dakota, this is accomplished by nesting an uncertainty quantification method (sampling), which computes the 90th percentiles, within an optimizer (method-asynch_pattern_search), which iteratively adjusts the variable means to minimize the objective. For every evaluation requested by the optimizer, the design variables (x1_mean and x2_mean in the example) are inserted into the means of the uncertain variables (x1 and x2), then the sampling study is run to completion, and finally the resulting statistics for the responses f1 and f2 are mapped into the responses sum_p.

It may be helpful to sketch out the relationships between blocks as indicated by their various pointers in order to understand the nested structure of the study. The top-level or outer method, ‘opt’, has a model named ‘outer_model’. This model refers to variables and responses blocks (‘outer_vars’ and ‘outer-
that are used by the optimizer. The 'outer_model' block also refers to a sub-method, 'UQ-method' which defines the UQ study and has its own model, which in turn possess variables, an interface, and responses.

Next, note the primary and secondary variable mappings in 'outer_model', which specify that the values of the active design variables $x_1$ and $x_2$ are to be inserted into the means of the uncertain variables $x_1$ and $x_2$.

The response mapping in 'outer_model' is a matrix with a single row and six columns. The single row corresponds to the number of responses in the outer method. As described above, for each of our two sub-model responses, the sampling method returns a mean, a standard deviation, and a single probability level in that order to the nested model. There are a total of six results and accordingly six columns in the mapping matrix. The coefficients 0.3 and 0.7 in the matrix result in a weighted sum of the 90th percentiles:

$$\text{sum}_p = 0.3 \times (90\text{th percentile of } f_1) + 0.7 \times (90\text{th percentile of } f_2)$$

The next example is a fragment of an input file, showing only the nested model itself. It illustrates more complex variable and response mappings.

```
primary_variable_mapping = '' 'X' 'Y'
secondary_variable_mapping = '' '' 'mean' 'mean'
primary_response_mapping = 1. 0. 0. 0. 0. 0. 0. 0. 0.
secondary_response_mapping = 0. 0. 0. 1. 3. 0. 0. 0. 0.
          0. 0. 0. 0. 0. 1. 3. 0.
```

The variable mappings correspond to 4 top-level variables, the first two of which employ the default mappings from active top-level variables to sub-model variables of the same type (option 3 above) and the latter two of which are inserted into the mean distribution parameters of sub-model variables 'X' and 'Y' (option 1 above).

The response mappings define a 3 by 9 matrix corresponding to 9 inner loop results and 3 outer loop response functions (one primary response function and 2 secondary functions, such as one objective and two constraints). Each row of the response mapping is a vector which is multiplied (i.e., with a dot-product) against the 9 sub-iterator results to determine the outer loop function.

Consider again a UQ example with 3 response functions, each providing a mean, a standard deviation, and one level mapping (if no level mappings are specified, the responses would only have a mean and standard deviation). The primary response mapping can be seen to extract the first result from the inner loop, which would correspond to the mean of the first response function. This mapped sub-iterator response becomes a single objective function, least squares term, or generic response function at the outer level, as dictated by the top-level response specification. The secondary response mapping maps the fourth sub-iterator result plus 3 times the fifth sub-iterator result (mean plus 3 standard deviations) into one top-level nonlinear constraint and the seventh sub-iterator result plus 3 times the eighth sub-iterator result (mean plus 3 standard deviations) into another top-level nonlinear constraint, where these top-level nonlinear constraints may be inequality or equality, as dictated by the top-level response specification.

Note that a common case is for each sub-iterator result to be mapped to a unique outer loop response (for example, in the nested UQ case where one wants to determine an interval on each inner loop statistic). In these simple cases, the response mapping would define an identity matrix.
6.3. MODEL

- iterator_servers

Specify the number of iterator servers when Dakota is run in parallel

Topics
This keyword is related to the topics:

- concurrency_and_parallelism

Specification
Alias: none
Argument(s): INTEGER

Description
An important feature for component-based iterators is that execution of sub-iterator runs may be performed concurrently. The optional iterator_servers specification supports user override of the automatic parallel configuration for the number of iterator servers. That is, if the automatic configuration is undesirable for some reason, the user can enforce a desired number of partitions at the iterator parallelism level. Currently, hybrid, multi_start, and pareto_set component-based iterators support concurrency in their sub-iterators. Refer to ParallelLibrary and the Parallel Computing chapter of the Users Manual [4] for additional information.

iterator_scheduling

- Keywords Area
- model
- nested
- sub_method_pointer
- iterator_scheduling

Specify the scheduling of concurrent iterators when Dakota is run in parallel

Topics
This keyword is related to the topics:

- concurrency_and_parallelism

Specification
Alias: none
Argument(s): none

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<th>Required/-</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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CHAPTER 6. KEYWORDS AREA

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<td>Choose One</td>
<td>master</td>
<td>Specify a dedicated master partition for parallel iterator scheduling</td>
<td></td>
</tr>
<tr>
<td>peer</td>
<td>Specify a peer partition for parallel iterator scheduling</td>
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</table>

Description

An important feature for component-based iterators is that execution of sub-iterator runs may be performed concurrently. The optional `iterator_scheduling` specification supports user override of the automatic parallel configuration for the number of iterator servers. That is, if the automatic configuration is undesirable for some reason, the user can enforce a desired number of partitions at the iterator parallelism level. Currently, `hybrid`, `multi_start`, and `pareto_set` component-based iterators support concurrency in their sub-iterators. Refer to ParallelLibrary and the Parallel Computing chapter of the Users Manual [4] for additional information.

**master**

- **Keywords Area**
- **model**
- **nested**
- **sub_method_pointer**
- **iterator_scheduling**
- **master**

Specify a dedicated master partition for parallel iterator scheduling

**Topics**

This keyword is related to the topics:

- **concurrency_and_parallelism**

**Specification**

**Alias:** none  
**Argument(s):** none

**Description**

This option overrides the Dakota parallel automatic configuration, forcing the use of a dedicated master partition. In a dedicated master partition, one processor (the "master") dynamically schedules work on the iterator servers. This reduces the number of processors available to create servers by 1.
6.3. MODEL

peer

- Keywords Area
- model
- nested
- sub_method_pointer
- iterator_scheduling
- peer

Specify a peer partition for parallel iterator scheduling

Topics

This keyword is related to the topics:

- concurrency_and_parallelism

Specification

Alias: none

Argument(s): none

Description

This option overrides the Dakota parallel automatic configuration, forcing the use of a peer partition. In a peer partition, all processors are available to be assigned to iterator servers. Note that unlike the case of evaluation_scheduling, it is not possible to specify static or dynamic.

processors_per_iterator

- Keywords Area
- model
- nested
- sub_method_pointer
- processors_per_iterator

Specify the number of processors per iterator server when Dakota is run in parallel

Topics

This keyword is related to the topics:

- concurrency_and_parallelism
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): INTEGER

Description

An important feature for component-based iterators is that execution of sub-iterator runs may be performed concurrently. The optional processors_per_iterator specification supports user override of the automatic parallel configuration for the number of processors in each iterator server. That is, if the automatic configuration is undesirable for some reason, the user can enforce a desired server size at the iterator parallelism level. Currently, hybrid, multi_start, and pareto_set component-based iterators support concurrency in their sub-iterators. Refer to ParallelLibrary and the Parallel Computing chapter of the Users Manual[4] for additional information.

primary_variable_mapping

- Keywords Area
- model
- nested
- sub_method_pointer
- primary_variable_mapping

Primary mapping of top-level variables to sub-model variables

Specification

Alias: none

Argument(s): STRINGLIST

Default: default variable insertions based on variable type

Description

The primary_variable_mapping, secondary_variable_mapping, primary_response_mapping, and secondary_response_mapping keywords control how top-level variables and responses are mapped to variables and responses in the sub-model. Their usage is explained on the parent keyword (sub_method_pointer) page.

secondary_variable_mapping

- Keywords Area
- model
- nested
- sub_method_pointer
- secondary_variable_mapping

Secondary mapping of top-level variables to sub-model variables
6.3. MODEL

**Specification**

**Alias:** none

**Argument(s):** STRINGLIST

**Default:** primary mappings into sub-model variables are value-based

**Description**

The `primary_variable_mapping, secondary_variable_mapping, primary_response_mapping,` and `secondary_response_mapping` keywords control how top-level variables and responses are mapped to variables and responses in the sub-model. Their usage is explained on the parent keyword (`sub_method_pointer`) page.

**primary_response_mapping**

- **Keywords Area**
- model
- nested
- `sub_method_pointer`
- `primary_response_mapping`

Primary mapping of sub-model responses to top-level responses

**Specification**

**Alias:** none

**Argument(s):** REALLIST

**Default:** no sub-iterator contribution to primary functions

**Description**

The `primary_variable_mapping, secondary_variable_mapping, primary_response_mapping,` and `secondary_response_mapping` keywords control how top-level variables and responses are mapped to variables and responses in the sub-model. Their usage is explained on the parent keyword (`sub_method_pointer`) page.

**secondary_response_mapping**

- **Keywords Area**
- model
- nested
- `sub_method_pointer`
- `secondary_response_mapping`

Secondary mapping of sub-model responses to top-level responses
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): REALLIST

Default: no sub-iterator contribution to secondary functions

Description

The `primary_variable_mapping`, `secondary_variable_mapping`, `primary_response_mapping`, and `secondary_response_mapping` keywords control how top-level variables and responses are mapped to variables and responses in the sub-model. Their usage is explained on the parent keyword (sub_method_pointer) page.

Input Spec Summary

This file is derived automatically from dakota.xml, which is used in the generation of parser system files that are compiled into the Dakota executable. Therefore, these files are the definitive source for input syntax, capability options, and associated data inputs. Refer to the Developers Manual information on how to modify the input specification and propagate the changes through the parsing system.

Key features of the input specification and the associated user input files include:

- In the input specification, required individual specifications simply appear, optional individual and group specifications are enclosed in [], required group specifications are enclosed in (), and either-or relationships are denoted by the | symbol. These symbols only appear in dakota.input.summary; they must not appear in actual user input files.

- Keyword specifications (i.e., `environment`, `method`, `model`, `variables`, `interface`, and `responses`) begin with the keyword possibly preceded by white space (blanks, tabs, and newlines) both in the input specifications and in user input files. For readability, keyword specifications may be spread across several lines. Earlier versions of Dakota (prior to 4.1) required a backslash character (\) at the ends of intermediate lines of a keyword. While such backslashes are still accepted, they are no longer required.

- Some of the keyword components within the input specification indicate that the user must supply INTEGER, REAL, STRING, INTEGERLIST, REALLIST, or STRINGLIST data as part of the specification. In a user input file, the "=" is optional, data in a LIST can be separated by commas or whitespace, and the STRING data are enclosed in single or double quotes (e.g., 'text book' or "text book").

- In user input files, input is largely order-independent (except for entries in lists of data), case insensitive, and white-space insensitive. Although the order of input shown in the Sample Input Files generally follows the order of options in the input specification, this is not required.

- In user input files, specifications may be abbreviated so long as the abbreviation is unique. For example, the npsol_sqp specification within the method keyword could be abbreviated as npsol, but dot_sqp should not be abbreviated as dot since this would be ambiguous with other DOT method specifications.

- In both the input specification and user input files, comments are preceded by #.

- ALIAS refers to synonymous keywords, which often exist for backwards compatibility. Users are encouraged to use the most current keyword.

dakota.input.summary:
6.3. MODEL

KEYWORD01 environment
  [ tabular_data ALIAS tabular_graphics_data
    [ tabular_data_file ALIAS tabular_graphics_file STRING ]
    [ annotated ]
    [ custom_annotated
      [ header ]
      [ eval_id ]
      [ interface_id ]
    ]
    [ freeform ]
  ]
  [ output_file STRING ]
  [ error_file STRING ]
  [ read_restart STRING
    [ stop_restart INTEGER >= 0 ]
  ]
  [ write_restart STRING ]
  [ output_precision INTEGER >= 0 ]
  [ results_output
    [ results_output_file STRING ]
  ]
  [ graphics ]
  [ check ]
  [ pre_run
    [ input STRING ]
    [ output STRING
      [ annotated ]
      [ custom_annotated
        [ header ]
        [ eval_id ]
        [ interface_id ]
      ]
      [ freeform ]
    ]
  ]
  [ run
    [ input STRING ]
    [ output STRING ]
  ]
  [ post_run
    [ input STRING
      [ annotated ]
      [ custom_annotated
        [ header ]
        [ eval_id ]
        [ interface_id ]
      ]
      [ freeform ]
    ]
    [ output STRING ]
  ]
  [ top_method_pointer ALIAS method_pointer STRING ]

KEYWORD12 method
  [ id_method STRING ]
  [ output}
debug
| verbose
| normal
| quiet
| silent

{ final_solutions INTEGER >= 0 }
{ hybrid
  ( sequential ALIAS uncoupled
    { method_name_list STRINGLIST
      [ model_pointer_list STRING ]
    } method_pointer_list STRINGLIST
  )

  ( embedded ALIAS coupled
    { method_name_list STRINGLIST
      [ model_pointer_list STRING ]
    } method_pointer_list STRINGLIST
  )

  { method_name_list STRINGLIST
    [ model_pointer_list STRING ]
  } method_pointer_list STRINGLIST

  ( collaborative
    { method_name_list STRINGLIST
      [ model_pointer_list STRING ]
    } method_pointer_list STRINGLIST
  )

  [ iterator_servers INTEGER > 0 ]
  [ iterator_scheduling master | peer ]
  [ processors_per_iterator INTEGER > 0 ]

  ( multi_start
    ( method_name STRING
      [ model_pointer STRING ]
    )
    [ method_pointer STRING
      [ random_starts INTEGER
        [ seed INTEGER ]
      ]
    ]
    [ starting_points REALLIST ]
    [ iterator_servers INTEGER > 0 ]
    [ iterator_scheduling master | peer ]
    [ processors_per_iterator INTEGER > 0 ]
  )

  ( pareto_set
    ( method_name ALIAS opt_method_name STRING
      [ model_pointer ALIAS opt_model_pointer STRING ]
    )
  )
6.3. MODEL

| method_pointer ALIAS opt_method_pointer STRING |
| random_weight_sets INTEGER |
| { seed INTEGER } |
| weight_sets ALIAS multi_objective_weight_sets REALLIST |
| iterator_servers INTEGER > 0 |
| iterator_scheduling |
| master |
| peer |
| { processors_per_iterator INTEGER > 0 } |
|
| ( branch_and_bound |
| method_pointer STRING |
| { method_name STRING |
| { model_pointer STRING } |
| { scaling } |
| ) |
|
| ( surrogate_based_local |
| method_pointer ALIAS approx_method_pointer STRING |
| method_name ALIAS approx_method_name STRING |
| model_pointer ALIAS approx_model_pointer STRING |
| soft_convergence_limit INTEGER |
| truth_surrogate_bypass |
| approx_subproblem |
| original_primary |
| single_objective |
| augmented_lagrangian_objective |
| lagrangian_objective |
| original_constraints |
| linearized_constraints |
| no_constraints |
| } |
| merit_function |
| penalty_merit |
| adaptive_penalty_merit |
| lagrangian_merit |
| augmented_lagrangian_merit |
| acceptance_logic |
| tr_ratio |
| filter |
| } |
| constraint_relax |
| homotopy |
| } |
| trust_region |
| { initial_size REALLIST } |
| { minimum_size REAL } |
| contract_threshold REAL |
| expand_threshold REAL |
| contraction_factor REAL |
| expansion_factor REAL |
| } |
| { max_iterations INTEGER >= 0 } |
| { convergence_tolerance REAL } |
| { constraint_tolerance REAL } |
| ) |
\{( surrogate_based_global
  method_pointer ALIAS approx_method_pointer STRING
  method_name ALIAS approx_method_name STRING
  model_pointer ALIAS approx_model_pointer STRING
  \[ replace_points \]
  \[ max_iterations INTEGER >= 0 \]
)\}
\{( dot_frcg
  \[ max_iterations INTEGER >= 0 \]
  \[ convergence_tolerance REAL \]
  \[ constraint_tolerance REAL \]
  \[ speculative \]
  \[ max_function_evaluations INTEGER >= 0 \]
  \[ scaling \]
  \[ model_pointer STRING \]
)\}
\{( dot_mmfd
  \{ dot_frcg
  \{ dot_mmfd
  \{ dot_bfgs
  \{ dot_slp
  \{ dot_sqp
  \} dot
  \{ frcg
  \{ mmfd
  \{ bfgs
  \{ slp
  \{ sqp
  \} max_iterations INTEGER >= 0 \]
  \} convergence_tolerance REAL \]
  \} constraint_tolerance REAL \]
  \} speculative \]
  \} max_function_evaluations INTEGER >= 0 \]
  \} scaling \]
  \} model_pointer STRING \]
)\}
\{( conmin_frcg
  \{ max_iterations INTEGER >= 0 \]
  \{ convergence_tolerance REAL \]
  \{ constraint_tolerance REAL \]
  \{ speculative \]
  \{ max_function_evaluations INTEGER >= 0 \]
  \} scaling \]
  \} model_pointer STRING \]
)\}
\{( conmin_mmfd
  \{ conmin_frcg
  \{ conmin_mmfd
  \{ conmin_bfgs
  \{ conmin_slp
  \{ conmin_sqp
  \} conmin
  \{ frcg
  \{ mmfd
  \{ bfgs
  \{ slp
  \{ sqp
  \} max_iterations INTEGER >= 0 \]
  \} convergence_tolerance REAL \]
  \} constraint_tolerance REAL \]
  \} speculative \]
  \} max_function_evaluations INTEGER >= 0 \]
  \} scaling \]
  \} model_pointer STRING \]
)\}
\{( dl_solver STRING
  \{ conmin
  \{ frcg
  \{ mmfd
  \{ bfgs
  \{ slp
  \{ sqp
  \} max_iterations INTEGER >= 0 \]
  \} convergence_tolerance REAL \]
  \} constraint_tolerance REAL \]
  \} speculative \]
  \} max_function_evaluations INTEGER >= 0 \]
  \} scaling \]
  \} model_pointer STRING \]
)\}
6.3. MODEL

```plaintext
max_function_evaluations INTEGER >= 0
scaling
model_pointer STRING

| npsol_sqp |
| verify_level INTEGER |
| function_precision REAL |
| linesearch_tolerance REAL |
| convergence_tolerance REAL |
| max_iterations INTEGER == 0 |
| constraint_tolerance REAL |
| speculative |
| max_function_evaluations INTEGER >= 0 |
| scaling |
| model_pointer STRING |

| nlssol_sqp |
| stanford |
| npsol |
| nlssol |
| verify_level INTEGER |
| function_precision REAL |
| linesearch_tolerance REAL |
| convergence_tolerance REAL |
| max_iterations INTEGER == 0 |
| constraint_tolerance REAL |
| speculative |
| max_function_evaluations INTEGER >= 0 |
| scaling |
| model_pointer STRING |

| nlpsol_sqp |
| max_iterations INTEGER >= 0 |
| convergence_tolerance REAL |
| max_function_evaluations INTEGER >= 0 |
| scaling |
| model_pointer STRING |

| optpp_cg |
| max_step REAL |
| gradient_tolerance REAL |
| max_iterations INTEGER >= 0 |
| convergence_tolerance REAL |
| speculative |
| max_function_evaluations INTEGER >= 0 |
| scaling |
| model_pointer STRING |

| optpp_q_newton |
| optpp_fd_newton |
| optpp_g_newton |
| optpp_newton |
| search_method |
value_based_line_search
| gradient_based_line_search |
| trust_region |
| tr_pds |
```
| merit_function
| el_bakry
| argaez_tapia
| van_shanno
|
| steplength_to_boundary REAL |
| centering_parameter REAL |
| max_step REAL |
| gradient_tolerance REAL |
| max_iterations INTEGER >= 0 |
| convergence_tolerance REAL |
| speculative |
| max_function_evaluations INTEGER >= 0 |
| scaling |
| model_pointer STRING |
|
| optpp_pds |
| search_scheme_size INTEGER |
| max_iterations INTEGER >= 0 |
| convergence_tolerance REAL |
| max_function_evaluations INTEGER >= 0 |
| scaling |
| model_pointer STRING |
|
| asynch_pattern_search ALIAS coliny_apps |
| initial_delta REAL |
| contraction_factor REAL |
| threshold_delta REAL |
| solution_target ALIAS solution_accuracy REAL |
| synchronization
| blocking
| nonblocking |
| merit_function
| merit_max |
| merit_max_smooth |
| merit1 |
| merit1_smooth |
| merit2 |
| merit2_smooth |
| merit2_squared |
| constraint_penalty REAL |
| smoothing_factor REAL |
| constraint_tolerance REAL |
| max_function_evaluations INTEGER >= 0 |
| scaling |
| model_pointer STRING |
|
| mesh_adaptive_search |
| initial_delta REAL |
| threshold_delta REAL |
| function_precision REAL |
| seed INTEGER > 0 |
| history_file STRING |
| display_format STRING |
| variable_neighborhood_search REAL |
| neighbor_order INTEGER > 0 |
[ display_all_evaluations ]
[ use_surrogate
  inform_search
  | optimize ]
[ max_iterations INTEGER >= 0 ]
[ max_function_evaluations INTEGER >= 0 ]
[ scaling ]
[ model_pointer STRING ]
}
|
owpac
[ trust_region
  [ initial_size REALIST ]
  [ minimum_size REAL ]
  [ contract_threshold REAL ]
  [ expand_threshold REAL ]
  [ contraction_factor REAL ]
  [ expansion_factor REAL ]
]
[ max_iterations INTEGER >= 0 ]
[ max_function_evaluations INTEGER >= 0 ]
[ scaling ]
[ model_pointer STRING ]
}
|
snowpac
[ seed INTEGER > 0 ]
[ trust_region
  [ initial_size REALIST ]
  [ minimum_size REAL ]
  [ contract_threshold REAL ]
  [ expand_threshold REAL ]
  [ contraction_factor REAL ]
  [ expansion_factor REAL ]
]
[ max_iterations INTEGER >= 0 ]
[ max_function_evaluations INTEGER >= 0 ]
[ scaling ]
[ model_pointer STRING ]
}
|
moqa
[ fitness_type
  layer_rank
  | domination_count ]
| replacement_type
  elitist
  | roulette_wheel
  | unique_roulette_wheel
  | ( below_limit REAL
    [ shrinkage_fraction ALIAS shrinkage_percentage REAL ]
  )
|
[ niching_type
  radial REALIST
  | distance REALIST ]
|
[ max_designs REALIST
  [ num_designs INTEGER >= 2 ]}
[ convergence_type
metric_tracker
  [ percent_change REAL ]
  [ num_generations INTEGER >= 0 ]
]

[ postprocessor_type
orthogonal_distance REALLIST
]

[ max_iterations INTEGER >= 0 ]
[ max_function_evaluations INTEGER >= 0 ]
[ scaling ]
[ population_size INTEGER >= 0 ]
[ log_file STRING ]
[ print_each_pop ]
[ initialization_type
  simple_random
  | unique_random
  | flat_file STRING
]

[ crossover_type
multi_point_binary INTEGER
  | multi_point_parameterized_binary INTEGER
  | multi_point_real INTEGER
  |
  shuffle_random
  [ num_parents INTEGER > 0 ]
  [ num_offspring INTEGER > 0 ]
]
[ crossover_rate REAL ]
]

[ mutation_type
bit_random
  | replace_uniform
  |
  { offset_normal
    | offset_cauchy
    | offset_uniform
    [ mutation_scale REAL ]
  }
[ mutation_rate REAL ]
]
[ seed INTEGER > 0 ]
[ convergence_tolerance REAL ]
[ model_pointer STRING ]
]

[ soga
  [ fitness_type
    merit_function
    [ constraint_penalty REAL ]
  ]

[ replacement_type
elitist
  | favor_feasible
  | roulette_wheel
  | unique_roulette_wheel
  |
[ convergence_type
  { best_fitness_tracker
    [ percent_change REAL ]
  ]
6.3. MODEL

[ num_generations INTEGER \geq 0 ]
)

[ average_fitness_tracker
[ percent_change REAL ]
[ num_generations INTEGER \geq 0 ]
)

[ max_iterations INTEGER \geq 0 ]
[ max_function_evaluations INTEGER \geq 0 ]
[ scaling ]
[ population_size INTEGER \geq 0 ]
[ log_file STRING ]
[ print_each_pop ]
[ initialization_type
  simple_random
  | unique_random
  | flat_file STRING
]
[ crossover_type
  multi_point_binary INTEGER
  | multi_point_parameterized_binary INTEGER
  | multi_point_real INTEGER

[ shuffle_random
  [ num_parents INTEGER \geq 0 ]
  [ num_offspring INTEGER > 0 ]
]
[ crossover_rate REAL ]
]
[ mutation_type
  bit_random
  | replace_uniform

[ offset_normal
  | offset_cauchy
  | offset_uniform
  [ mutation_scale REAL ]
]
[ mutation_rate REAL ]
]
[ seed INTEGER > 0 ]
[ convergence_tolerance REAL ]
[ model_pointer STRING ]
)

[ coliny_pattern_search
[ constant_penalty ]
[ no_expansion ]
[ expand_after_success INTEGER ]
[ pattern_basis
  coordinate
  | simplex

| stochastic
| total_pattern_size INTEGER ]
[ exploratory_moves
  multi_step
  | adaptive_pattern
  | basic_pattern

[ synchronization

}
blocking
| nonblocking |
| [ contraction_factor REAL ]
| [ constraint_penalty REAL ]
| [ initial_delta REAL ]
| [ threshold_delta REAL ]
| [ solution_target ALIAS solution_accuracy REAL ]
| [ seed INTEGER > 0 ]
| [ show_misg_options ]
| [ misc_options STRINGLIST ]
| [ max_iterations INTEGER >= 0 ]
| [ convergence_tolerance REAL ]
| [ max_function_evaluations INTEGER >= 0 ]
| [ scaling ]
| [ model_pointer STRING ]
|
| { coliny_solis_wets }
| [ contract_after_failure INTEGER ]
| [ no_expansion ]
| [ expand_after_success INTEGER ]
| [ constant_penalty ]
| [ contraction_factor REAL ]
| [ constraint_penalty REAL ]
| [ initial_delta REAL ]
| [ threshold_delta REAL ]
| [ solution_target ALIAS solution_accuracy REAL ]
| [ seed INTEGER > 0 ]
| [ show_misg_options ]
| [ misc_options STRINGLIST ]
| [ max_iterations INTEGER >= 0 ]
| [ convergence_tolerance REAL ]
| [ max_function_evaluations INTEGER >= 0 ]
| [ scaling ]
| [ model_pointer STRING ]
|
| { coliny_cobyla }
| [ initial_delta REAL ]
| [ threshold_delta REAL ]
| [ solution_target ALIAS solution_accuracy REAL ]
| [ seed INTEGER > 0 ]
| [ show_misg_options ]
| [ misc_options STRINGLIST ]
| [ max_iterations INTEGER >= 0 ]
| [ convergence_tolerance REAL ]
| [ max_function_evaluations INTEGER >= 0 ]
| [ scaling ]
| [ model_pointer STRING ]
|
| { coliny_direct }
| [ division
| major_dimension |
| all_dimensions |
| [ global_balance_parameter REAL ]
| [ local_balance_parameter REAL ]
| [ max_boxsize_limit REAL ]
| [ min_boxsize_limit REAL ]
| [ constraint_penalty REAL ]
|
6.3. MODEL

[ solution_target ALIAS solution_accuracy REAL ]
[ seed INTEGER > 0 ]
[ show_m misc_options ]
[ misc_options STRINGLIST ]
[ max_iterations INTEGER >= 0 ]
[ convergence_tolerance REAL ]
[ max_function_evaluations INTEGER >= 0 ]
[ scaling ]
[ model_pointer STRING ]
)
|
| ( coliny_ea
[ population_size INTEGER > 0 ]
[ initialization_type
  simple_random
  | unique_random
  | flat_file STRING
  ]
[ fitness_type
  linear_rank
  | merit_function
  ]
[ replacement_type
  random INTEGER
  | chc INTEGER
  | elitist INTEGER
  [ new_solutions_generated INTEGER ]
  ]
[ crossover_rate REAL ]
[ crossover_type
  two_point
  | blend
  | uniform
  ]
[ mutation_rate REAL ]
[ mutation_type
  replace_uniform
  ]
[ offset_normal
  | offset_cauchy
  | offset_uniform
  [ mutation_scale REAL ]
  [ mutation_range INTEGER ]
  ]
[ non_adaptive ]
|
[ constraint_penalty REAL ]
[ solution_target ALIAS solution_accuracy REAL ]
[ seed INTEGER > 0 ]
[ show_m misc_options ]
[ misc_options STRINGLIST ]
[ max_iterations INTEGER >= 0 ]
[ convergence_tolerance REAL ]
[ max_function_evaluations INTEGER >= 0 ]
[ scaling ]
[ model_pointer STRING ]
)
|
| ( coliny_beta
  beta_solver_name STRING
  [ solution_target ALIAS solution_accuracy REAL ]
  [ seed INTEGER > 0 ]
CHAPTER 6. KEYWORDS AREA

| show_misc_options |
| misc_options STRINGLIST |
| max_iterations INTEGER >= 0 |
| convergence_tolerance REAL |
| max_function_evaluations INTEGER >= 0 |
| scaling |
| model_pointer STRING |
|
| nl2sol |
| function_precision REAL |
| absolute_conv_tol REAL |
| x_conv_tol REAL |
| singular_conv_tol REAL |
| singular_radius REAL |
| false_conv_tol REAL |
| initial_trust_radius REAL |
| covariance INTEGER |
| regression_diagnostics |
| convergence_tolerance REAL |
| max_iterations INTEGER >= 0 |
| speculative |
| max_function_evaluations INTEGER >= 0 |
| scaling |
| model_pointer STRING |
|
| nonlinear_cg |
| misc_options STRINGLIST |
| convergence_tolerance REAL |
| max_iterations INTEGER >= 0 |
| scaling |
| model_pointer STRING |
|
| ncsu_direct |
| solution_target ALIAS solution_accuracy REAL |
| min_boxsize_limit REAL |
| volume_boxsize_limit REAL |
| convergence_tolerance REAL |
| max_iterations INTEGER >= 0 |
| max_function_evaluations INTEGER >= 0 |
| scaling |
| model_pointer STRING |
|
| genie_opt_darts |
| genie_direct |
| seed INTEGER > 0 |
| max_function_evaluations INTEGER >= 0 |
| scaling |
| model_pointer STRING |
|
| efficient_global |
| initial_samples INTEGER |
| seed INTEGER > 0 |
| max_iterations INTEGER >= 0 |
| gaussian_process ALIAS kriging |
| surfpack |
| dakota |
6.3. MODEL

[ use_derivatives ]
[ import_build_points_file ALIAS import_points_file STRING
  [ annotated
  |
  [ custom_annotated
    [ header ]
    [ eval_id ]
    [ interface_id ]
  ]
  |
  [ freeform
    [ active_only ]
  ]
]
[ export_approx_points_file ALIAS export_points_file STRING
  [ annotated
  |
  [ custom_annotated
    [ header ]
    [ eval_id ]
    [ interface_id ]
  ]
  |
  [ freeform
  ]
  [ model_pointer STRING ]
]

[ polynomial_chaos ALIAS nond_polynomial_chaos
  [ samples_on_emulator ALIAS samples INTEGER ]
  [ seed INTEGER > 0 ]
  [ fixed_seed ]
  [ max_refinement_iterations INTEGER >= 0 ]
  [ convergence_tolerance REAL ]
  [ final_moments
    none
    | standard
    | central
  ]
  [ p_refinement
    uniform
    |
    [ dimension_adaptive
      sobol
      | decay
      | generalized
    ]
  ]
  [ askey
    wiener
  ]
  [ quadrature_order_sequence INTEGERLIST
    [ dimension_preference REALLIST ]
    [ nested
      | non_nested
    ]
  ]
]

[ sparse_grid_level_sequence INTEGERLIST
  [ restricted
    | unrestricted
  ]
  [ dimension_preference REALLIST ]
  [ nested
    | non_nested
  ]
]
| cubature_integrand INTEGER |
| ( expansion_order_sequence INTEGERLIST |
|   ( dimension_preference REALLIST |
|     [ basis_type |
|       tensor_product |
|       total_order |
|     [ adapted |
|     [ advancements INTEGER |
|     [ soft_convergence_limit INTEGER |
|   ) |
|   ) |
|   ) |
| collocation_points_sequence INTEGERLIST |
| collocation_ratio REAL |
| [ ratio_order REAL |
|   [ { least_squares |
|     [ svd |
|     [ equality_constrained |
|   ) |
|   ] |
| ( orthogonal_matching_pursuit ALIAS omp |
| [ noise_tolerance REALLIST |
| ] |
| [ basis_pursuit ALIAS bp |
| [ basis_pursuit_denoising ALIAS bpdn |
| [ noise_tolerance REALLIST |
| ] |
| [ least_angle_regression ALIAS lars |
| [ noise_tolerance REALLIST |
| ] |
| [ least_absolute_shrinkage ALIAS lasso |
| [ noise_tolerance REALLIST |
| [ l2_penalty REAL |
| ] |
| [ cross_validation |
| [ noise_only |
| ] |
| [ use_derivatives |
| [ tensor_grid |
| [ reuse_points ALIAS reuse_samples |
| [ max_iterations INTEGER >= 0 |
| [ max_solver_iterations INTEGER >= 0 |
| ) |
| ) |
| ( expansion_samples_sequence INTEGERLIST |
| [ reuse_points ALIAS reuse_samples |
| [ incremental_lhs |
| ) |
| [ import_build_points_file ALIAS import_points_file STRING |
| [ annotated |
| [ custom.annotated |
| [ header |
| [ eval_id |
| [ interface_id |
| ] |
| ) |
| ) |
| freeform |
6.3. MODEL

[ active_only ]
]
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]
]
[ export_expansion_file STRING ]
[ reliability_levels REALLIST
[ num_reliability_levels INTEGERLIST ]
]
[ response_levels REALLIST
[ num_response_levels INTEGERLIST ]
[ compute
  probabilities
  reliabilities
  gen_reliabilities
  system
  series
  parallel
]
]
[ distribution
cumulative
complementary
]
[ probability_levels REALLIST
[ num_probability_levels INTEGERLIST ]
]
[ gen_reliability_levels REALLIST
[ num_gen_reliability_levels INTEGERLIST ]
]
[ rng
  mt19937
  rnum2
]
[ model_pointer STRING ]
)

( stoch_collocation ALIAS nond_stoch_collocation
[ samples_on_emulator ALIAS samples INTEGER ]
[ seed INTEGER > 0 ]
[ fixed_seed ]
[ max_refinement_iterations INTEGER >= 0 ]
[ convergence_tolerance REAL ]
[ final_moments
  none
  standard
  central
]
[ { p_refinement
    uniform
    { dimension_adaptive
      sobol
      generalized
    }
  }
]
[ { h_refinement
    uniform
    { dimension_adaptive
      sobol
      generalized
    }
    { local_adaptive
    }
  ]
6.3. MODEL

[ piecewise
| askey
| wiener ]
quadrature_order_sequence INTEGERLIST
|
| sparse_grid_level_sequence INTEGERLIST
| restricted
| unrestricted ]
| nodal
| hierarchical ]
)
dimension_preference REALLIST ]
| use_derivatives ]
| nested
| non_nested ]
| variance_based_decomp
| interaction_order INTEGER > 0 ]
| drop_tolerance REAL ]
|
diagonal_covariance
| full_covariance ]
sample_type
| lhs
| random ]

probability_refinement ALIAS sample_refinement
| import
| adapt_import
| mm_adapt_import
| refinement_samples INTEGERLIST ]
|
import_approx_points_file STRING
| annotated
|
| custom_annotated
| header ]
| eval_id ]
| interface_id ]
|
| freeform
| active_only ]

export_approx_points_file ALIAS export_points_file STRING
| annotated
|
| custom_annotated
| header ]
| eval_id ]
| interface_id ]
|
| freeform

reliability_levels REALLIST
| num_reliability_levels INTEGERLIST ]
|
response_levels REALLIST
| num_response_levels INTEGERLIST ]
| compute
| probabilities
| reliabilities
CHAPTER 6. KEYWORDS AREA

| gen_reliabilities
|   [ system
|     series
|     [ parallel
|     ]
|   ]
| [ distribution
|   cumulative
|   [ complementary
|   ]
|   [ probability_levels REALLIST
|     [ num_probability_levels INTEGERLIST ]
|   ]
|   [ gen_reliability_levels REALLIST
|     [ num_gen_reliability_levels INTEGERLIST ]
|   ]
|   [ rng
|     mt19937
|     | rnum2
|   ]
|   [ model_pointer STRING ]
| )
| ( sampling ALIAS nond_sampling
|   [ samples ALIAS initial_samples INTEGER ]
|   [ seed INTEGER > 0 ]
|   [ fixed_seed ]
|   [ sample_type
|     lhs
|     | random
|     | incremental_lhs
|     | incremental_random
|   ]
|   [ refinement_samples INTEGERLIST ]
|   [ d_optimal
|     [ candidate_designs INTEGER > 0
|     | leja_oversample_ratio REAL ]
|   ]
|   [ variance_based_decomp
|     [ drop_tolerance REAL ]
|   ]
|   [ backfill ]
|   [ principal_components
|     [ percent_variance_explained REAL ]
|   ]
|   [ wilks
|     [ order INTEGER ]
|     [ confidence_level REAL ]
|     [ one_sided_lower ]
|     [ one_sided_upper ]
|     [ two_sided ]
|   ]
|   [ final_moments
|     none
|     | standard
|     | central
|   ]
|   [ reliability_levels REALLIST
|     [ num_reliability_levels INTEGERLIST ]
|   ]
|   [ response_levels REALLIST


6.3. MODEL

```
[ num_response_levels INTEGERLIST ]
[ compute
  probabilities |
  reliabilities |
  gen_reliabilities
[ system
  series |
  parallel ]
]

[ distribution
  cumulative |
  complementary ]

[ probability_levels REALLIST
  [ num_probability_levels INTEGERLIST ] ]

[ gen_reliability_levels REALLIST
  [ num_gen_reliability_levels INTEGERLIST ] ]

[ rng
  mt19937 |
  rnum2 ]

[ model_pointer STRING ]

[ multilevel_sampling ALIAS multilevel_mc
  [ seed INTEGER > 0 ]
  [ fixed_seed ]
  [ pilot_samples INTEGERLIST ]
  [ sample_type
    lhs |
    random ]

[ export_sample_sequence
  [ annotated ]
  [ custom_annotated
    [ header ]
    [ eval_id ]
    [ interface_id ] ]
  [ freeform ]

[ max_iterations INTEGER >= 0 ]
[ convergence_tolerance REAL ]
[ final_moments
  none |
  standard |
  central ]

[ distribution
  cumulative |
  complementary ]

[ probability_levels REALLIST
  [ num_probability_levels INTEGERLIST ] ]

[ gen_reliability_levels REALLIST ]
```
[ num_gen_reliability_levels INTEGERLIST ]
]
[rng
 mt19937
 | rnum2
 ]
[ model_pointer STRING ]
)
|
{ importance_sampling ALIAS nond_importance_sampling

 [ samples ALIAS initial_samples INTEGER ]
[ seed INTEGER > 0 ]
import
| adapt_import
| mm_adapt_import
[ refinement_samples INTEGERLIST ]
[ response_levels REALLIST
[ num_response_levels INTEGERLIST ]
[ compute
 probabilities
 [ gen_reliabilities
 [ system
 series
 | parallel
 ]
 ]
]
[ max_iterations INTEGER >= 0 ]
[ convergence_tolerance REAL ]
[ distribution
 cumulative
 | complementary
 ]
[ probability_levels REALLIST
[ num_probability_levels INTEGERLIST ]
]
[ gen_reliability_levels REALLIST
[ num_gen_reliability_levels INTEGERLIST ]
]
[rng
 mt19937
 | rnum2
 ]
[ model_pointer STRING ]
)
|
{ gpais ALIAS gaussian_process_adaptive_importance_sampling

 [ build_samples ALIAS samples INTEGER ]
[ seed INTEGER > 0 ]
[ samples_on_emulator INTEGER ]
[ import_build_points_file ALIAS import_points_file STRING
 [ annotated
 |
 { custom_annotated
 [ header ]
 [ eval_id ]
 [ interface_id ]
 |
 { freeform
 [ active_only ]
 ]
)}

6.3. MODEL

[ export_approx_points_file ALIAS export_points_file STRING
  [ annotated
    [ custom_annotated
      [ header ]
      [ eval_id ]
      [ interface_id ]
    ]
  ]
  [ freeform ]
]
[ response_levels REALLIST
  [ num_response_levels INTEGERLIST ]
  [ compute
    probabilities
    [ gen_reliabilities
      [ system
        series
        parallel
      ]
    ]
  ]
  [ max_iterations INTEGER >= 0 ]
][ distribution
  cumulative
  [ complementary ]
]
[ probability_levels REALLIST
  [ num_probability_levels INTEGERLIST ]
]
[ gen_reliability_levels REALLIST
  [ num_gen_reliability_levels INTEGERLIST ]
]
[ rng
  mt19937
  | rnum2
]
[ model_pointer STRING ]
]
[ adaptive_sampling ALIAS nond_adaptive_sampling
  [ initial_samples ALIAS samples INTEGER ]
  [ seed INTEGER > 0 ]
  [ samples_on_emulator INTEGER ]
  [ fitness_metric
    predicted_variance
    | distance
    | gradient
  ]
  [ batch_selection
    naive
    | distance_penalty
    | topology
    | constant_liar
  ]
  [ refinement_samples INTEGERLIST ]
]
[ import_build_points_file ALIAS import_points_file STRING
  [ annotated
    [ custom_annotated
      [ header ]
      [ eval_id ]
    ]
  ]
]
[ interface_id ]
|
| { freeform
| active_only }
|
[ export_approx_points_file ALIAS export_points_file STRING
| annotated
|
| { custom_annotated
| header ]
| eval_id ]
| interface_id ]
|
| { freeform
|
[ response_levels REALLIST
| num_response_levels INTEGERLIST ]
| compute
| probabilities
| gen_reliabilities
| system
| series
| parallel ]
|
| misc_options STRINGLIST ]
| max_iterations INTEGER >= 0 ]
| distribution
| cumulative
| complementary ]
|
[ probability_levels REALLIST
| num_probability_levels INTEGERLIST ]
|
[ gen_reliability_levels REALLIST
| num_gen_reliability_levels INTEGERLIST ]
|
| rng
| mt19937
| rnum2 ]
|
| model_pointer STRING ]
|
| pof_darts ALIAS nond_pof_darts
| build_samples ALIAS samples INTEGER
| seed INTEGER > 0 ]
| lipschitz
| local
| global ]
|
[ samples_on_emulator INTEGER ]
| response_levels REALLIST
| num_response_levels INTEGERLIST ]
| compute
| probabilities
| gen_reliabilities
| system
| series
6.3. MODEL

```plaintext
| parallel
|
|
| distribution
cumulative
| complementary
|
| probability_levels REALLIST
| num_probability_levels INTEGERLIST |
|
| gen_reliability_levels REALLIST
| num_gen_reliability_levels INTEGERLIST |
|
| rng
| mt19937
| rnum2
|
| model_pointer STRING |
|
| rkd_darts ALIAS nond_rkd_darts
build_samples ALIAS samples INTEGER
| seed INTEGER > 0 |
| lipschitz
local
| global |
| samples_on_emulator INTEGER |
| response_levels REALLIST
| num_response_levels INTEGERLIST |
| compute
probabilities
gen_reliabilities
| system
series
| parallel |
|
| distribution
cumulative
| complementary
|
| probability_levels REALLIST
| num_probability_levels INTEGERLIST |
|
| gen_reliability_levels REALLIST
| num_gen_reliability_levels INTEGERLIST |
|
| rng
| mt19937
| rnum2 |
| model_pointer STRING |
|
| global_evidence ALIAS nond_global_evidence
| samples INTEGER |
| seed INTEGER > 0 |
| sbo
| ego
```
[ gaussian_process ALIAS kriging
  surfpack
  | dakota
  ]
[ use_derivatives ]
[ import_build_points_file ALIAS import_points_file STRING
  [ annotated
  ]
  [ custom_annotated
    [ header ]
    [ eval_id ]
    [ interface_id ]
  ]
  ]
  [ freeform
    [ active_only ]
  ]
[ export_approx_points_file ALIAS export_points_file STRING
  [ annotated
  ]
  [ custom_annotated
    [ header ]
    [ eval_id ]
    [ interface_id ]
  ]
  ]
  [ freeform
  ]
]
| ea
| lhs |
[ response_levels REALLIST
  [ num_response_levels INTEGERLIST ]
  [ compute
    probabilities
    | gen_reliabilities
    [ system
      series
      | parallel
    ]
  ]
]
[ distribution
  cumulative
  | complementary
  ]
[ probability_levels REALLIST
  [ num_probability_levels INTEGERLIST ]
]
[ gen_reliability_levels REALLIST
  [ num_gen_reliability_levels INTEGERLIST ]
]
[ rng
  mt19937
  | rnum2
  ]
[ model_pointer STRING ]
]
| [ global_interval_est ALIAS nond_global_interval_est
  [ samples INTEGER ]
  [ seed INTEGER > 0 ]
]
6.3. MODEL

```plaintext
[ max_iterations INTEGER >= 0 ]
[ convergence_tolerance REAL ]
[ max_function_evaluations INTEGER >= 0 ]
[ sbo ]
  ego
  [ gaussian_process ALIAS kriging
    surfpack
    | dakota
  ]
[ use_derivatives ]
[ import_build_points_file ALIAS import_points_file STRING
  | annotated
  | ( custom_annotated
    | header ]
[ eval_id ]
[ interface_id ]
]
 |
( freeform
  | active_only ]
|
[ export_approx_points_file ALIAS export_points_file STRING
  | annotated
  | ( custom_annotated
    | header ]
[ eval_id ]
[ interface_id ]
]
 |
( freeform
  ]
|
 ea
| lhs ]
[ rng
 mt19937
 | rnum2
 ]
[ model_pointer STRING ]
)
 |
( bayes_calibration ALIAS nond_bayes_calibration
  | queso
  chain_samples ALIAS samples INTEGER
  | seed INTEGER > 0 ]
  | emulator
    ( gaussian_process ALIAS kriging
      surfpack
      | dakota
  | build_samples INTEGER ]
  | posterior_adaptive ]
[ import_build_points_file ALIAS import_points_file STRING
  | annotated
  | ( custom_annotated
    | header ]
[ eval_id ]
[ interface_id ]
]
|
|
```
{ freeform
  [ active_only ]
}

{ pce
  sparse_grid_level_sequence INTEGERLIST
  |
  { expansion_order_sequence INTEGERLIST
    collocation_points_sequence INTEGERLIST
    | collocation_ratio REAL
    | cross_validation ]
    { posterior_adaptive ]
    [ import_build_points_file ALIAS import_points_file STRING
      [ annotated
      |
      { custom_annotated
        [ header ]
        [ eval_id ]
        [ interface_id ]
      ]
      |
      { freeform
        [ active_only ]
      ]
    }
  }

{ orthogonal_least_interpolation
  collocation_points_sequence INTEGERLIST
  [ posterior_adaptive ]
  [ import_build_points_file ALIAS import_points_file STRING
    [ annotated
    |
    { custom_annotated
      [ header ]
      [ eval_id ]
      [ interface_id ]
    ]
    |
    { freeform
      [ active_only ]
    ]
  }
}

{ sc
  sparse_grid_level_sequence INTEGERLIST
  }
  [ use_derivatives ]
  |
  [ standardized_space ]
  [ logit_transform ]
  [ export_chain_points_file STRING
    [ annotated
    |
    { custom_annotated
      [ header ]
      [ eval_id ]
      [ interface_id ]
    ]
    |
    { freeform

[ dram
| delayed_rejection
| adaptive_metropolis
| metropolis_hastings
| multilevel ]
[
| rng
| mt19937
| rnum2
]
[
| pre_solve
| sqp
| nip
| none
]
[
| proposal_covariance
| ( derivatives
| proposal_updates INTEGER ]
| prior
| ( values REALIST
| diagonal
| matrix
| ( filename STRING
| diagonal
| matrix
)
| ( gpmsa
| chain_samples ALIAS samples INTEGER
| seed INTEGER > 0 ]
| build_samples INTEGER
| import_build_points_file ALIAS import_points_file STRING
| ( annotated
| ( custom_annotated
| header )
| ( eval_id )
| ( interface_id )
| ( freeform
| ( standardized_space )
| ( logit_transform )
| ( gpmsa_normalize )
| export_chain_points_file STRING
| ( annotated
| ( custom_annotated
| header )
| ( eval_id )
| ( interface_id )
| ( freeform
]
[ dram
| delayed_rejection
| adaptive_metropolis
| metropolis_hastings ]
[ rng
| mt19937
| rnum2
|]
[ proposal_covariance
| { derivatives
| { proposal_updates INTEGER }
| }
| prior
| { values REALLIST
diagonal
| matrix
| }
| { filename STRING
diagonal
| matrix
| }
|]
[ wasabi
| { seed INTEGER > 0 }
| emulator
| { gaussian_process ALIAS kriging
| surfpack
| dakota
| { build_samples INTEGER }
| posterior_adaptive
| { import_build_points_file ALIAS import_points_file STRING
| { annotated
| |
| { custom_annotated
| { header
| { eval_id
| { interface_id
| }
| { freeform
| { active_only
| }
| }
| }
|]
| pce
| sparse_grid_level_sequence INTEGERLIST
| { expansion_order_sequence INTEGERLIST
| collocation_points_sequence INTEGERLIST
| { collocation_ratio REAL
| cross_validation
| posterior_adaptive
| { import_build_points_file ALIAS import_points_file STRING
| { annotated
| |
| { custom_annotated
| { header }
| ]
6.3. MODEL

[ eval_id ]
[ interface_id ]
|
{ freeform
  [ active_only ]
}
|
{ orthogonal_least_interpolation
  collocation_points_sequence INTEGERLIST
  [ posterior_adaptive ]
  [ import_build_points_file ALIAS import_points_file STRING
    [ annotated
      |
      { custom_annotated
        [ header ]
        [ eval_id ]
        [ interface_id ]
      ]
      |
      { freeform
        [ active_only ]
      ]
    ]
  ]
  |
  ( sc
    sparse_grid_level_sequence INTEGERLIST
  )
  |
  [ use_derivatives ]
}
[ standardized_space ]
[ data_distribution
  [ gaussian
    means REALLIST
  ]
  |
  [ covariance REALLIST
    diagonal
    | matrix
  ]
]
[ obs_data_filename STRING ]
[ posterior_density_export_filename STRING ]
[ posterior_samples_export_filename STRING ]
[ posterior_samples_import_filename STRING ]
[ generate_posterior_samples
  evaluate_posterior_density
]
|
{ dream
  chain_samples ALIAS samples INTEGER
  [ seed INTEGER > 0 ]
  [ chains INTEGER >= 3 ]
  [ num_of INTEGER >= 1 ]
  [ crossover_chain_pairs INTEGER >= 0 ]
  [ gr_threshold REAL > 0.0 ]
  [ jump_step INTEGER >= 0 ]
  [ emulator
    ( gaussian_process ALIAS kriging
      surfpack
    )
  ]
}
CHAPTER 6. KEYWORDS AREA

| dakota |
| build_samples INTEGER |
| posterior_adaptive |
| import_build_points_file ALIAS import_points_file STRING |
| annotated |
| { custom_annotated |
| header |
| eval_id |
| interface_id |
| } |
| freeform |
| active_only |
| } |

| pce |
| sparse_grid_level_sequence INTEGERLIST |
| { expansion_order_sequence INTEGERLIST |
| collocation_points_sequence INTEGERLIST |
| collocation_ratio REAL |
| cross_validation |
| posterior_adaptive |
| import_build_points_file ALIAS import_points_file STRING |
| annotated |
| { custom_annotated |
| header |
| eval_id |
| interface_id |
| } |
| freeform |
| active_only |
| } |

| orthogonal_least_interpolation |
| collocation_points_sequence INTEGERLIST |
| posterior_adaptive |
| import_build_points_file ALIAS import_points_file STRING |
| annotated |
| { custom_annotated |
| header |
| eval_id |
| interface_id |
| } |
| freeform |
| active_only |
| } |

| ac |
| sparse_grid_level_sequence INTEGERLIST |
| } |
| use_derivatives |
6.3. MODEL

[ standardized_space ]

[ export_chain_points_file STRING
  [ annotated
    | ( custom_annotated
      [ header ]
      [ eval_id ]
      [ interface_id ]
    )
    | ( freeform
  )
]

[ experimental_design
  initial_samples ALIAS samples INTEGER
  num_candidates INTEGER > 0
  [ max_hifi_evaluations INTEGER >= 0 ]
  [ import_candidate_points_file STRING
    [ annotated
      | ( custom_annotated
        [ header ]
        [ eval_id ]
        [ interface_id ]
      )
      | ( freeform
    )
  ]
  | calibrate_error_multipliers
    one
    | per_experiment
    | per_response
    | both
    [ hyperprior_alphas REALIST
      hyperprior_betas REALIST
    ]
  ]

[ burn_in_samples INTEGER ]
[ posterior_stats
  [ kl_divergence ]
  [ mutual_info ]
]

[ model_discrepancy
  [ discrepancy_type
    gaussian_process ALIAS kriging
    | polynomial
    [ correction_order
      constant
      | linear
      | quadratic
    ]
  ]
  [ num_prediction_configs INTEGER >= 0 ]
  [ prediction_configs REALLIST
    [ annotated
      |
      ( custom_annotated
        [ header ]
        [ eval_id ]
        [ interface_id ]
      )
    ]
  ]


```
}]
| ( freeform |
[ export_discrepancy_file STRING |
| annotated |
| ( custom_annotated |
[ header ] |
[ eval_id ] |
[ interface_id ] |
| ( freeform |
[ export_corrected_model_file STRING |
| annotated |
| ( custom_annotated |
[ header ] |
[ eval_id ] |
[ interface_id ] |
| ( freeform |
[ export_corrected_variance_file STRING |
| annotated |
| ( custom_annotated |
[ header ] |
[ eval_id ] |
[ interface_id ] |
| ( freeform |
[ sub_sampling_period INTEGER ] |
[ probability_levels REALLIST ] |
| ( num_probability_levels INTEGERLIST ] |
| ( convergence_tolerance REAL ] |
| ( max_iterations INTEGER >= 0 ] |
| ( model_pointer STRING ] |
)
```

```
| ( dace grid |
| random |
| oas |
| lhs |
| oa_lhs |
| box_benhken |
| central_composite |
[ samples INTEGER ] |
| ( seed INTEGER > 0 ] |
| ( main_effects ] |
| ( quality_metrics ] |
| ( variance_based_decomp |
[ drop_tolerance REAL ] |
```
6.3. MODEL

[ fixed_seed ]
[ symbols INTEGER ]
[ model_pointer STRING ]
)
|
( fsu_cvt
[ samples INTEGER ]
[ seed INTEGER > 0 ]
[ latinize ]
[ quality_metrics ]
[ variance_based_decomp
  { drop_tolerance REAL ]
|
fixed_seed ]
[ trial_type
  grid
  | halton
  | random
|
[ num_trials INTEGER ]
[ max_iterations INTEGER >= 0 ]
[ model_pointer STRING ]
)
|
( psuade_moat
[ partitions INTEGERLIST ]
[ samples INTEGER ]
[ seed INTEGER > 0 ]
[ model_pointer STRING ]
)
|
( local_evidence ALIAS nond_local_evidence
  [ sqp
  | nip ]
  [ response_levels REALLIST
    { num_response_levels INTEGERLIST ]
    { compute
      probabilities
      | gen_reliabilities
    [ system
      series
      | parallel
    ]
  ]
|
[ probability_levels REALLIST
  { num_probability_levels INTEGERLIST ]
|
[ gen_reliability_levels REALLIST
  { num_gen_reliability_levels INTEGERLIST ]
]
[ distribution
  cumulative
  | complementary
|
[ model_pointer STRING ]
)
|
( local_interval_est ALIAS nond_local_interval_est
  [ sqp
  | nip ]
  [ convergence_tolerance REAL ]
CHAPTER 6. KEYWORDS AREA

[ model_pointer STRING ]
)

( local_reliability ALIAS nond_local_reliability
  [ mpp_search
    x_taylor_mean
    | u_taylor_mean
    | x_taylor_mpp
    | u_taylor_mpp
    | x_two_point
    | u_two_point
    | no_approx
    [ sqp
    | nip ]
  [ integration
    first_order
    | second_order
  [ probability_refinement ALIAS sample_refinement
    import
    | adapt_import
    | mm_adapt_import
    [ refinement_samples INTEGERLIST ]
    [ seed INTEGER > 0 ]
  ]
]
]

[ response_levels REALIST
  [ num_response_levels INTEGERLIST ]
  [ compute
    probabilities
    | reliabilities
    | gen_reliabilities
    [ system
      series
      | parallel
    ]
]
]

[ reliability_levels REALIST
  [ num_reliability_levels INTEGERLIST ]
]

[ max_iterations INTEGER >= 0 ]
[ convergence_tolerance REAL ]
[ final_moments
  none
  | standard
  | central
]
[ distribution
  cumulative
  | complementary
]

[ probability_levels REALIST
  [ num_probability_levels INTEGERLIST ]
]

[ gen_reliability_levels REALIST
  [ num_gen_reliability_levels INTEGERLIST ]
]

[ model_pointer STRING ]
)

( global_reliability ALIAS nond_global_reliability
6.3. MODEL

[ initial_samples INTEGER ]
x_gaussian_process ALIAS x_kriging
| u_gaussian_process ALIAS u_kriging
  surfpack
  dakota ]
[ import_build_points_file ALIAS import_points_file STRING
  [ annotated
    |
    [ custom_annotated
      [ header ]
      [ eval_id ]
      [ interface_id ]
    ]
    |
    [ freeform
      [ active_only ]
    ]
  ]
[ export_approx_points_file ALIAS export_points_file STRING
  [ annotated
    |
    [ custom_annotated
      [ header ]
      [ eval_id ]
      [ interface_id ]
    ]
    |
    [ freeform
      |
    [ use_derivatives ]
    [ seed INTEGER > 0 ]
  ]
rng
  mt19937
  | rnum2]
[ response_levels REALLIST
  [ num_response_levels INTEGERLIST ]
  [ compute
    probabilities
    | gen_reliabilities
    [ system
      series
      | parallel
    ]
  ]
[ max_iterations INTEGER >= 0 ]
[ convergence_tolerance REAL ]
[ distribution
cumulative
| complementary
]
[ probability_levels REALLIST
  [ num_probability_levels INTEGERLIST ]
]
[ gen_reliability_levels REALLIST
  [ num_gen_reliability_levels INTEGERLIST ]
]
[ model_pointer STRING ]
|
| fsu_quasi_mc
halton
| hammersley
| latinize |
| quality_metrics |
| variance_based_decomp
| drop_tolerance REAL |
| samples INTEGER |
| fixed_sequence |
| sequence_start INTEGERLIST |
| sequence_leap INTEGERLIST |
| prime_base INTEGERLIST |
| max_iterations INTEGER >= 0 |
| model_pointer STRING |
|
| ( vector_parameter_study
  final_point REALLIST
  | step_vector REALLIST
  num_steps INTEGER
  | model_pointer STRING |
|)
|
| ( list_parameter_study
  list_of_points REALLIST
  |
  | ( import_points_file STRING
    | annotated |
    | custom_annotated
    | header |
    | eval_id |
    | interface_id |
    |
    | ( freeform
      | active_only |
    |
    | model_pointer STRING |
  |)
|
| ( centered_parameter_study
  step_vector REALLIST
  steps_per_variable ALIAS deltas_per_variable INTEGERLIST
  | model_pointer STRING |
  |
| ( multidim_parameter_study
  partitions INTEGERLIST
  | model_pointer STRING |
  |
| ( richardson_extrap
  estimate_order
  | converge_order
  | converge_qoi
  | refinement_rate REAL |
  | convergence_tolerance REAL |
  | max_iterations INTEGER >= 0 |
  | model_pointer STRING |
  )

KEYWORD model
6.3. MODEL

[ id_model STRING ]
( single ALIAS simulation
  [ interface_pointer STRING ]
  [ solution_level_control STRING
    solution_level_cost REALLIST
  ]
)
)

| surrogate
[ id_surrogates INTEGERLIST ]
( global
  [ gaussian_process ALIAS kriging
    dakota
    [ point_selection ]
    [ trend
      constant
      | linear
      | reduced_quadratic
    ]
  ]
  [ surfpack
    trend
    constant
    | linear
    | reduced_quadratic
    | quadratic
  ]
  [ optimization_method STRING ]
  [ max_trials INTEGER > 0 ]
  [ nugget REAL > 0 ]
  [ find_nugget INTEGER ]
  [ correlation_lengths REALLIST ]
  [ export_model
    [ filename_prefix STRING ]
    ( formats
      [ text_archive ]
      [ binary_archive ]
      [ algebraic_file ]
      [ algebraic_console ]
    )
  ]
  )
)
)
)

| mars
[ max_bases INTEGER ]
( interpolation
  linear
  | cubic
  )
)

| moving_least_squares
[ basis_order ALIAS poly_order INTEGER >= 0 ]
[ weight_function INTEGER ]
  export_model
[ filename_prefix STRING ]
{ formats
  [ text_archive ]
  [ binary_archive ]
}

| neural_network
[ max_nodes ALIAS nodes INTEGER ]
[ range REAL ]
[ random_weight INTEGER ]
[ export_model
[ filename_prefix STRING ]
{ formats
  [ text_archive ]
  [ binary_archive ]
  [ algebraic_file ]
  [ algebraic_console ]
}

| radial_basis
[ bases INTEGER ]
[ max_pts INTEGER ]
[ min_partition INTEGER ]
[ max_subsets INTEGER ]
[ export_model
[ filename_prefix STRING ]
{ formats
  [ text_archive ]
  [ binary_archive ]
  [ algebraic_file ]
  [ algebraic_console ]
}

| polynomial
basis_order INTEGER \geq 0
| linear
| quadratic
| cubic
[ export_model
[ filename_prefix STRING ]
{ formats
  [ text_archive ]
  [ binary_archive ]
  [ algebraic_file ]
  [ algebraic_console ]
}

| domain_decomposition
[ cell_type STRING ]
[ support_layers INTEGER ]
[ discontinuity_detection
jump_threshold REAL
| gradient_threshold REAL
6.3. MODEL

| total_points INTEGER
| minimum_points
| recommended_points |
| ( dace_method_pointer STRING
| auto_refinement
| max_iterations INTEGER > 0 |
| max_function_evaluations INTEGER > 0 |
| convergence_tolerance REAL |
| soft_convergence_limit INTEGER >= 0 |
| cross_validation_metric STRING
| ( folds INTEGER > 0 |
|)
|)
| actual_model_pointer STRING |
| reuse_points ALIAS reuse_samples
| all |
| region |
| none |
|)
|)
| import_build_points_file ALIAS import_points_file ALIAS samples_file STRING
| annotated
| |
| ( custom_annotated
| header |
| eval_id |
| interface_id |
|)
|)
| ( freeform
| active_only |
|)
|)
| export_approx_points_file ALIAS export_points_file STRING
| annotated
| |
| ( custom_annotated
| header |
| eval_id |
| interface_id |
|)
|)
| ( freeform
|)
|)
| use_derivatives |
| correction
| zeroth_order
| first_order
| second_order
| additive
| multiplicative
| combined |
|)
| metrics ALIAS diagnostics STRINGLIST
| cross_validation
| ( folds INTEGER
| percent REAL |
|)
| press |
|)
| import_challenge_points_file ALIAS challenge_points_file STRING
[ annotated
| custom.annotated
| header ]
| eval_id ]
| interface_id ]
| freeform
| active_only ]
|
| multipoint
tana
actual_model_pointer STRING
|
local
taylor_series
actual_model_pointer STRING
|
hierarchical
ordered_model_fidelities ALIAS model_fidelity_sequence STRINGLIST
| correction
| zeroth_order
| first_order
| second_order
| additive
| multiplicative
| combined
|
| nested
| optional_interface_pointer STRING
| optional_interface_responses_pointer STRING ]
| sub_method_pointer STRING
| iterator_servers INTEGER > 0 ]
| iterator_scheduling
| master
| peer
| processors_per_iterator INTEGER > 0 ]
| primary_variable_mapping STRINGLIST ]
| secondary_variable_mapping STRINGLIST ]
| primary_response_mapping REALLIST ]
| secondary_response_mapping REALLIST ]
|
| active_subspace ALIAS subspace
actual_model_pointer STRING
| initial_samples INTEGER ]
| sample_type
| lhs
| random
|
| truncation_method
6.3. MODEL

[ bing_li ]
[ constantine ]
[ energy
  [ truncation_tolerance REAL ]
]
[ cross_validation
  [ minimum
    | relative
    | decrease ]
  [ relative_tolerance REAL ]
  [ decrease_tolerance REAL ]
  [ max_rank INTEGER ]
  [ exhaustive ]
]
[ dimension INTEGER ]
[ bootstrap_samples INTEGER ]
[ build_surrogate
  [ refinement_samples INTEGERLIST ]
]
[ normalization
  mean_value
  | mean_gradient
  | local_gradient
]

[ adapted_basis
  actual_model_pointer STRING
  sparse_grid_level INTEGER
  ( expansion_order INTEGER
    collocation_ratio REAL
  )
]

[ random_field
  build_source
    rf_data_file STRING
    dace_method_pointer STRING
  ( analytic_covariance
    squared_exponential
    | exponential
  )
]
[ expansion_form
  karhunen_loeve
  | principal_components
]
[ expansion_bases INTEGER ]
[ truncation_tolerance REAL ]
[ propagation_model_pointer STRING ]
[ variables_pointer STRING ]
[ responses_pointer STRING ]
[ hierarchical_tagging ]

KEYWORD12 variables
[ id_variables STRING ]
[ active
  all ]
<table>
<thead>
<tr>
<th>design</th>
<th>uncertain</th>
<th>aleatory</th>
<th>epistemic</th>
<th>state</th>
</tr>
</thead>
<tbody>
<tr>
<td>mixed</td>
<td>relaxed</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

[ continuous_design INTEGER > 0
  [ initial_point ALIAS cdv_initial_point REALLIST ]
  [ lower_bounds ALIAS cdv_lower_bounds REALLIST ]
  [ upper_bounds ALIAS cdv_upper_bounds REALLIST ]
  [ scale_types ALIAS cdv_scale_types STRINGLIST ]
  [ scales ALIAS cdv_scales REALLIST ]
  [ descriptors ALIAS cdv_descriptors STRINGLIST ] ]

[ discrete_design_range INTEGER > 0
  [ initial_point ALIAS ddv_initial_point INTEGERLIST ]
  [ lower_bounds ALIAS ddv_lower_bounds INTEGERLIST ]
  [ upper_bounds ALIAS ddv_upper_bounds INTEGERLIST ]
  [ descriptors ALIAS ddv_descriptors STRINGLIST ] ]

[ discrete_design_set
  [ integer INTEGER > 0
    [ elements_per_variable ALIAS num_set_values INTEGERLIST ]
    [ elements ALIAS set_values INTEGERLIST ]
    [ categorical STRINGLIST ]
    [ adjacency_matrix INTEGERLIST ]
    [ initial_point INTEGERLIST ]
    [ descriptors STRINGLIST ] ]
  [ string INTEGER > 0
    [ elements_per_variable ALIAS num_set_values INTEGERLIST ]
    [ elements ALIAS set_values STRINGLIST ]
    [ adjacency_matrix INTEGERLIST ]
    [ initial_point STRINGLIST ]
    [ descriptors STRINGLIST ] ]
  [ real INTEGER > 0
    [ elements_per_variable ALIAS num_set_values INTEGERLIST ]
    [ elements ALIAS set_values REALLIST ]
    [ categorical STRINGLIST ]
    [ adjacency_matrix INTEGERLIST ]
    [ initial_point REALLIST ]
    [ descriptors STRINGLIST ] ] ]

[ normal_uncertain INTEGER > 0
  [ means ALIAS nuv_means REALLIST ]
  [ std_deviations ALIAS nuv_std_deviations REALLIST ]
  [ lower_bounds ALIAS nuv_lower_bounds REALLIST ]
  [ upper_bounds ALIAS nuv_upper_bounds REALLIST ]
  [ initial_point REALLIST ]
  [ descriptors ALIAS nuv_descriptors STRINGLIST ] ]

[ lognormal_uncertain INTEGER > 0
  [ lambdas ALIAS lnuv_lambdas REALLIST ]
  [ zetas ALIAS lnuv_zetas REALLIST ] ]
( | means ALIAS lnuv_means REALLIST
  std_deviations ALIAS lnuv_std_deviations REALLIST
  | error_factors ALIAS lnuv_error_factors REALLIST
  )
  | [ lower_bounds ALIAS lnuv_lower_bounds REALLIST ]
  | [ upper_bounds ALIAS lnuv_upper_bounds REALLIST ]
  | [ initial_point REALLIST ]
  | [ descriptors ALIAS lnuv_descriptors STRINGLIST ]
)

| uniform_uncertain INTEGER > 0
| lower_bounds ALIAS uuv_lower_bounds REALIST
| upper_bounds ALIAS uuv_upper_bounds REALIST
| [ initial_point REALLIST ]
| [ descriptors ALIAS uuv_descriptors STRINGLIST ]
| ]

| loguniform_uncertain INTEGER > 0
| lower_bounds ALIAS luuv_lower_bounds REALIST
| upper_bounds ALIAS luuv_upper_bounds REALIST
| [ initial_point REALLIST ]
| [ descriptors ALIAS luuv_descriptors STRINGLIST ]
| ]

| triangular_uncertain INTEGER > 0
| modes ALIAS tuv_modes REALLIST
| lower_bounds ALIAS tuv_lower_bounds REALIST
| upper_bounds ALIAS tuv_upper_bounds REALIST
| [ initial_point REALLIST ]
| [ descriptors ALIAS tuv_descriptors STRINGLIST ]
| ]

| exponential_uncertain INTEGER > 0
| betas ALIAS euv_betas REALIST
| [ initial_point REALLIST ]
| [ descriptors ALIAS euv_descriptors STRINGLIST ]
| ]

| beta_uncertain INTEGER > 0
| alphas ALIAS buv_alphas REALLIST
| betas ALIAS buv_betas REALIST
| lower_bounds ALIAS buv_lower_bounds REALIST
| upper_bounds ALIAS buv_upper_bounds REALIST
| [ initial_point REALLIST ]
| [ descriptors ALIAS buv_descriptors STRINGLIST ]
| ]

| gamma_uncertain INTEGER > 0
| alphas ALIAS gauv_alphas REALLIST
| betas ALIAS gauv_betas REALLIST
| [ initial_point REALLIST ]
| [ descriptors ALIAS gauv_descriptors STRINGLIST ]
| ]

| gumbel_uncertain INTEGER > 0
| alphas ALIAS guuv_alphas REALLIST
| betas ALIAS guuv_betas REALLIST
| [ initial_point REALLIST ]
| [ descriptors ALIAS guuv_descriptors STRINGLIST ]
| ]

| frechet_uncertain INTEGER > 0
| alphas ALIAS fuv_alphas REALLIST
| betas ALIAS fuv_betas REALLIST
| [ initial_point REALLIST ]
| [ descriptors ALIAS fuv_descriptors STRINGLIST ]
| ]

| weibull_uncertain INTEGER > 0
| alphas ALIAS wuv_alphas REALLIST
| betas ALIAS wuv_betas REALLIST
[ initial_point REALLIST ]
[ descriptors ALIAS wuv_descriptors STRINGLIST ]
]
[ histogram_bin_uncertain INTEGER > 0
[ pairs_per_variable ALIAS num_pairs INTEGERLIST ]
abscissas ALIAS huv_bin_abscissas REALLIST
ordinates ALIAS huv_bin_ordinates REALLIST
| counts ALIAS huv_bin_counts REALLIST
[ initial_point REALLIST ]
[ descriptors ALIAS huv_bin_descriptors STRINGLIST ]
]
[ poisson_uncertain INTEGER > 0
lambdas REALLIST
[ initial_point INTEGERLIST ]
[ descriptors STRINGLIST ]
]
[ binomial_uncertain INTEGER > 0
probability_per_trial ALIAS prob_per_trial REALLIST
num_trials INTEGERLIST
[ initial_point INTEGERLIST ]
[ descriptors STRINGLIST ]
]
[ negative_binomial_uncertain INTEGER > 0
probability_per_trial ALIAS prob_per_trial REALLIST
num_trials INTEGERLIST
[ initial_point INTEGERLIST ]
[ descriptors STRINGLIST ]
]
[ geometric_uncertain INTEGER > 0
probability_per_trial ALIAS prob_per_trial REALLIST
[ initial_point INTEGERLIST ]
[ descriptors STRINGLIST ]
]
[ hypergeometric_uncertain INTEGER > 0
total_population INTEGERLIST
selected_population INTEGERLIST
num_drawn INTEGERLIST
[ initial_point INTEGERLIST ]
[ descriptors STRINGLIST ]
]
[ histogram_point_uncertain
[ integer INTEGER > 0
[ pairs_per_variable ALIAS num_pairs INTEGERLIST ]
abscissas INTEGERLIST
counts REALLIST
[ initial_point INTEGERLIST ]
[ descriptors STRINGLIST ]
]
[ string INTEGER > 0
[ pairs_per_variable ALIAS num_pairs INTEGERLIST ]
abscissas STRINGLIST
counts REALLIST
[ initial_point STRINGLIST ]
[ descriptors STRINGLIST ]
]
[ real INTEGER > 0
[ pairs_per_variable ALIAS num_pairs INTEGERLIST ]
abscissas REALLIST
counts REALLIST
[ initial_point REALLIST ]
[ descriptors STRINGLIST ]
]
6.3. MODEL

[ uncertain_correlation_matrix REALIST ]
[ continuous_interval_uncertain ALIAS interval_uncertain INTEGER > 0
  [ num_intervals ALIAS iuv_num_intervals INTEGERLIST ]
  [ interval_probabilities ALIAS interval_probs ALIAS iuv_interval_probs REALIST ]
  lower_bounds REALLIST
  upper_bounds REALLIST
  [ initial_point REALLIST ]
  [ descriptors ALIAS iuv_descriptors STRINGLIST ] ]

[ discrete_interval_uncertain ALIAS discrete_uncertain_range INTEGER > 0
  [ num_intervals INTEGERLIST ]
  [ interval_probabilities ALIAS interval_probs ALIAS range_probabilities ALIAS range_probs REALIST ]
  lower_bounds INTEGERLIST
  upper_bounds INTEGERLIST
  [ initial_point INTEGERLIST ]
  [ descriptors STRINGLIST ] ]

[ discrete_uncertain_set
  [ integer INTEGER > 0
    [ elements_per_variable ALIAS num_set_values INTEGERLIST ]
    elements ALIAS set_values INTEGERLIST
    [ set_probabilities ALIAS set_probs REALIST ]
    [ categorical STRINGLIST ]
    [ initial_point INTEGERLIST ]
    [ descriptors STRINGLIST ] ]

[ string INTEGER > 0
  [ elements_per_variable ALIAS num_set_values INTEGERLIST ]
  elements ALIAS set_values STRINGLIST
  [ set_probabilities ALIAS set_probs REALIST ]
  [ initial_point STRINGLIST ]
  [ descriptors STRINGLIST ] ]

[ real INTEGER > 0
  [ elements_per_variable ALIAS num_set_values INTEGERLIST ]
  elements ALIAS set_values REALLIST
  [ set_probabilities ALIAS set_probs REALIST ]
  [ categorical STRINGLIST ]
  [ initial_point REALLIST ]
  [ descriptors STRINGLIST ] ]

[ continuous_state INTEGER > 0
  [ initial_state ALIAS csv_initial_state REALLIST ]
  [ lower_bounds ALIAS csv_lower_bounds REALLIST ]
  [ upper_bounds ALIAS csv_upper_bounds REALLIST ]
  [ descriptors ALIAS csv_descriptors STRINGLIST ] ]

[ discrete_state_range INTEGER > 0
  [ initial_state ALIAS dsv_initial_state INTEGERLIST ]
  [ lower_bounds ALIAS dsv_lower_bounds INTEGERLIST ]
  [ upper_bounds ALIAS dsv_upper_bounds INTEGERLIST ]
  [ descriptors ALIAS dsv_descriptors STRINGLIST ] ]

[ discrete_state_set
  [ integer INTEGER > 0
    [ elements_per_variable ALIAS num_set_values INTEGERLIST ]
    elements ALIAS set_values INTEGERLIST
    [ categorical STRINGLIST ]
    [ initial_state INTEGERLIST ]
    [ descriptors STRINGLIST ] ]
[ string INTEGER > 0
  [ elements_per_variable ALIAS num_set_values INTEGERLIST ]
  elements ALIAS set_values STRINGLIST
  [ initial_state STRINGLIST ]
  [ descriptors STRINGLIST ]
]
[ real INTEGER > 0
  [ elements_per_variable ALIAS num_set_values INTEGERLIST ]
  elements ALIAS set_values REALLIST
  [ categorical STRINGLIST ]
  [ initial_state REALLIST ]
  [ descriptors STRINGLIST ]
]
[ linear_inequality_constraint_matrix REALLIST ]
[ linear_inequality_lower_bounds REALLIST ]
[ linear_inequality_upper_bounds REALLIST ]
[ linear_inequality_scale_types STRINGLIST ]
[ linear_inequality_scales REALLIST ]
[ linear_equality_constraint_matrix REALLIST ]
[ linear_equality_target REALLIST ]
[ linear_equality_scale_types STRINGLIST ]
[ linear_equality_scales REALLIST ]

KEYWORD12 interface
  [ id_interface STRING ]
  [ analysis_drivers STRINGLIST ]
  [ input_filter STRING ]
  [ output_filter STRING ]
  [ system
    [ parameters_file STRING ]
    [ results_file STRING ]
    [ file_tag ]
    [ file_save ]
    [ labeled ]
    [ aprepro ALIAS dprepro ]
    [ work_directory
      [ named STRING ]
      [ directory_tag ALIAS dir_tag ]
      [ directory_save ALIAS dir_save ]
      [ link_files STRINGLIST ]
      [ copy_files STRINGLIST ]
      [ replace ]
    ]
    [ allow_existing_results ]
    [ verbatim ]
  ]

  [ fork
    [ parameters_file STRING ]
    [ results_file STRING ]
    [ file_tag ]
    [ file_save ]
    [ labeled ]
    [ aprepro ALIAS dprepro ]
    [ work_directory
      [ named STRING ]
      [ directory_tag ALIAS dir_tag ]
      [ directory_save ALIAS dir_save ]
      [ link_files STRINGLIST ]
      [ copy_files STRINGLIST ]
    ]
  ]
6.3. MODEL

```plaintext
[ replace ]

[ allow_existing_results ]
[ verbatim ]

[ direct
[ processors_per_analysis INTEGER > 0 ]
)
| matlab

| python
| numpy ]
)
| scilab
| grid
| analysis_components STRINGLIST ]
]
| algebraic_mappings STRING ]
| failure_capture
| abort
| retry INTEGER
| recover REALIST
| continuation ]

[ deactivate
[ active_set_vector ]
[ evaluation_cache ]
[ strict_cache_equality
| cache_tolerance REAL ]
]
| restart_file ]
]
| asynchronous
[ evaluation_concurrency INTEGER > 0 ]
| local_evaluation_scheduling
dynamic
| static ]
| analysis_concurrency INTEGER > 0 ]
]
| evaluation_servers INTEGER > 0 ]
| evaluation_scheduling
master ]
| peer
dynamic
| static ]
]
| processors_per_evaluation INTEGER > 0 ]
| analysis_servers INTEGER > 0 ]
| analysis_scheduling
master
| peer ]
]

KEYWORD12 responses
| id_responses STRING ]
| descriptors ALIAS response_descriptors STRINGLIST ]
| objective_functions ALIAS num_objective_functions INTEGER >= 0
| sense STRINGLIST ]
```
CHAPTER 6. KEYWORDS AREA

[ primary_scale_types ALIAS objective_function_scale_types STRINGLIST ]
[ primary_scales ALIAS objective_function_scales REALLIST ]
[ weights ALIAS multi_objective_weights REALLIST ]
[ nonlinear_inequality_constraints ALIAS num_nonlinear_inequality_constraints INTEGER >= 0
  [ lower_bounds ALIAS nonlinear_inequality_lower_bounds REALLIST ]
  [ upper_bounds ALIAS nonlinear_inequality_upper_bounds REALLIST ]
[ scale_types ALIAS nonlinear_inequality_scale_types STRINGLIST ]
[ scales ALIAS nonlinear_inequality_scales REALLIST ]
]
[ nonlinear_equality_constraints ALIAS num_nonlinear_equality_constraints INTEGER >= 0
  [ targets ALIAS nonlinear_equality_targets REALLIST ]
  [ scale_types ALIAS nonlinear_equality_scale_types STRINGLIST ]
  [ scales ALIAS nonlinear_equality_scales REALLIST ]
]
[ scalar_objectives ALIAS num_scalar_objectives INTEGER >= 0 ]
[ field_objectives ALIAS num_field_objectives INTEGER >= 0 lengths INTEGERLIST
  [ num_coordinates_per_field INTEGERLIST ]
  [ read_field_coordinates ]
]
)
|
| calibration_terms ALIAS least_squares_terms ALIAS num_least_squares_terms INTEGER >= 0
| [ scalar_calibration_terms INTEGER >= 0 ]
| [ field_calibration_terms INTEGER >= 0 lengths INTEGERLIST
  [ num_coordinates_per_field INTEGERLIST ]
  [ read_field_coordinates ]
|
| primary_scale_types ALIAS calibration_term_scale_types ALIAS least_squares_term_scale_types STRINGLIST ]
| [ primary_scales ALIAS calibration_term_scales ALIAS least_squares_term_scales REALLIST ]
| [ weights ALIAS calibration_weights ALIAS least_squares_weights REALLIST ]
|
| { calibration_data
  [ num_experiments INTEGER >= 0 ]
  [ num_config_variables INTEGER >= 0 ]
  [ variance_type STRINGLIST ]
  [ scalar_data_file STRING
    [ annotated ]
    | { custom_annotated
      [ header ]
      [ exp_id ]
    ]
    | { freeform ]
    | [ interpolate ]
  ]
|
| calibration_data_file ALIAS least_squares_data_file STRING
| [ annotated ]
| { custom_annotated
  [ header ]
  [ exp_id ]
|
| { freeform
  [ num_experiments INTEGER >= 0 ]
  [ num_config_variables INTEGER >= 0 ]
  [ variance_type STRINGLIST ]
]
6.3. MODEL

```
[ nonlinear_inequality_constraints ALIAS num_nonlinear_inequality_constraints INTEGER >= 0
  [ lower_bounds ALIAS nonlinear_inequality_lower_bounds REALLIST ]
  [ upper_bounds ALIAS nonlinear_inequality_upper_bounds REALLIST ]
  [ scale_types ALIAS nonlinear_inequality_scale_types STRINGLIST ]
  [ scales ALIAS nonlinear_inequality_scales REALLIST ]
]

[ nonlinear_equality_constraints ALIAS num_nonlinear_equality_constraints INTEGER >= 0
  [ targets ALIAS nonlinear_equality_targets REALLIST ]
  [ scale_types ALIAS nonlinear_equality_scale_types STRINGLIST ]
  [ scales ALIAS nonlinear_equality_scales REALLIST ]
]
)

(response_functions ALIAS num_response_functions INTEGER >= 0
  [ scalar_responses ALIAS num_scalar_responses INTEGER >= 0 ]
  [ field_responses ALIAS num_field_responses INTEGER >= 0
    lengths INTEGERLIST
    [ num_coordinates_per_field INTEGERLIST ]
    [ read_field_coordinates ]
  ]
)
)

no_gradients
| analytic_gradients
|
(mixed_gradients
  id_numerical_gradients INTEGERLIST
  id_analytic_gradients INTEGERLIST
  [ method_source ]
  [ { dakota
    [ ignore_bounds ]
    [ relative
    | absolute
    | bounds ]
  ]
  [ vendor ]
  [ interval_type ]
  [ forward
  | central ]
  [ fd_step_size ALIAS fd_gradient_step_size REALLIST ]
)
)

( numerical_gradients
  [ method_source ]
  [ { dakota
    [ ignore_bounds ]
    [ relative
    | absolute
    | bounds ]
  ]
  [ vendor ]
  [ interval_type ]
  [ forward
  | central ]
  [ fd_step_size ALIAS fd_gradient_step_size REALLIST ]
)
)

no_hessians
|
( numerical_hessians
  [ fd_step_size ALIAS fd_hessian_step_size REALLIST ]
  [ relative
  | absolute
  | bounds ]
```
[ forward
| central ]
)
|
| quasi_hessians
( bfgs
[ damped ]
)
| srl
|
| analytic_hessians
|
| mixed_hessians
[ id_numerical_hessians INTEGERLIST
  [ fd_step_size ALIAS fd_hessian_step_size REALLIST ]
] |
| relative
| absolute
| bounds |
| forward
| central |
[ id_quasi_hessians INTEGERLIST
  { bfgs
    [ damped ]
  }
| srl
[ id_analytic_hessians INTEGERLIST ]
)

6.3.5 active_subspace

- Keywords Area
- model
- active_subspace

Active (variable) subspace model

**Specification**

Alias: subspace

Argument(s): none

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional Required Group</td>
<td>actual_model-pointer</td>
<td>Description</td>
<td>Pointer to specify a full-space model, from which to construct a lower dimensional surrogate</td>
</tr>
</tbody>
</table>
### Description

A model that transforms the original model (given by `actual_model_pointer`) to one with a reduced set of variables. This reduced model is identified by iteratively sampling the gradient of the original model and performing a singular value decomposition of the gradient matrix.

**Expected Output**

A subspace model will perform an initial sampling design to identify an active subspace using one of the truncation methods.

**Usage Tips**

If the desired subspace size is not identified, consider using the explicit `dimension` truncation option or one of the other truncation methods.

**Examples**

Perform an initial 100 gradient samples and use the `bing_li` truncation method to identify an active subspace. The truncation method uses 150 bootstrap samples to compute the Bing Li truncation metric.

```plaintext
model
  subspace
  id_model = 'SUBSPACE'
  actual_model_pointer = 'FULLSPACE'
```
CHAPTER 6. KEYWORDS AREA

initial_samples 100
truncation_method bing_li
bootstrap_samples 150

Theory

The idea behind active subspaces is to find directions in the input variable space in which the quantity of interest is nearly constant. After rotation of the input variables, this method can allow significant dimension reduction. Below is a brief summary of the process.

1. Compute the gradient of the quantity of interest, \( q = f(x) \), at several locations sampled from the full input space,
   \[
   \nabla_x f_i = \nabla f(x_i).
   \]

2. Compute the eigendecomposition of the matrix \( \hat{C} \),
   \[
   \hat{C} = \frac{1}{M} \sum_{i=1}^{M} \nabla_x f_i \nabla_x f_i^T = \hat{W} \hat{\Lambda} \hat{W}^T,
   \]
   where \( \hat{W} \) has eigenvectors as columns, \( \hat{\Lambda} = \text{diag}(\hat{\lambda}_1, \ldots, \hat{\lambda}_N) \) contains eigenvalues, and \( N \) is the total number of parameters.

3. Using a truncation method or specifying a dimension to estimate the active subspace size, split the eigenvectors into active and inactive directions,
   \[
   \hat{W} = \begin{bmatrix} \hat{W}_1 & \hat{W}_2 \end{bmatrix}.
   \]
   These eigenvectors are used to rotate the input variables.

4. Next the input variables, \( x \), are expanded in terms of active and inactive variables,
   \[
   x = \hat{W}_1 y + \hat{W}_2 z.
   \]

5. A surrogate is then built as a function of the active variables,
   \[
   g(y) \approx f(x)
   \]

For additional information, see:


actual_model_pointer

- Keywords Area
- model
- active_subspace
- actual_model_pointer

Pointer to specify a full-space model, from which to construct a lower dimensional surrogate
6.3. MODEL

Topics
This keyword is related to the topics:

- block_pointer

Specification
Alias: none
Argument(s): STRING

Description
This must point to a model block, identified by id_model. That model will be run to generate gradient data, from which an active subspace model will be identified and built.

See block_pointer for details about pointers.

initial_samples

- Keywords Area
- model
- active_subspace
- initial_samples

Initial number of samples for sampling-based methods

Specification
Alias: none
Argument(s): INTEGER
Default: model-dependent

Description
The initial_samples keyword is used to define the number of initial samples (i.e., randomly chosen sets of variable values) at which to execute a model. The initial samples may later be augmented in an iterative process.

Default Behavior
By default, Dakota will use the minimum number of samples required by the chosen method.

Usage Tips
To obtain linear sensitivities or to construct a linear response surface, at least dim+1 samples should be used, where "dim" is the number of variables. For sensitivities to quadratic terms or quadratic response surfaces, at least (dim+1)(dim+2)/2 samples are needed. For uncertainty quantification, we recommend at least 10*dim samples. For variance_based_decomp, we recommend hundreds to thousands of samples. Note that for variance_based_decomp, the number of simulations performed will be N*(dim+2).
Examples

```
method
  sampling
    sample_type random
    initial_samples = 20
    refinement_samples = 5
```

**sample_type**

- **Keywords Area**
- **model**
- **active_subspace**
- **sample_type**

Selection of sampling strategy

**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** random

<table>
<thead>
<tr>
<th>Required/-Optional Required (Choose One)</th>
<th>Description of Group Sample Type (Group 1)</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td><strong>lhs</strong></td>
<td>Uses Latin Hypercube Sampling (LHS) to sample variables</td>
</tr>
<tr>
<td></td>
<td></td>
<td><strong>random</strong></td>
<td>Uses purely random Monte Carlo sampling to sample variables</td>
</tr>
</tbody>
</table>

**Description**

The `sample_type` keyword allows the user to select between two types of sampling: Monte Carlo (pure random) and Latin hypercube (stratified) sampling.

The incremental keywords are deprecated; instead use `samples` together with `refinement_samples`.

**Default Behavior**

If the `sample_type` keyword is present, it must be accompanied by `lhs` or `random`. In most contexts, `lhs` is the default (exception: multilevel_sampling uses Monte Carlo by default).

**Examples**

```
method
  sampling
    sample_type lhs
    samples = 20
    seed = 83921
```
6.3. MODEL

lhs

- Keywords Area
- model
- active_subspace
- sample_type
- lhs

Uses Latin Hypercube Sampling (LHS) to sample variables

Specification

Alias: none
Argument(s): none

Description

The `lhs` keyword invokes Latin Hypercube Sampling as the means of drawing samples of uncertain variables according to their probability distributions. This is a stratified, space-filling approach that selects variable values from a set of equi-probable bins.

Default Behavior

Latin Hypercube Sampling is the default sampling mode in most contexts (exception: multilevel_sampling). To explicitly specify LHS in the Dakota input file, the `lhs` keyword must appear in conjunction with the `sample_type` keyword.

Usage Tips

Latin Hypercube Sampling is very robust and can be applied to any problem. It is fairly effective at estimating the mean of model responses and linear correlations with a reasonably small number of samples relative to the number of variables.

Examples

```plaintext
method sampling
  sample_type lhs
  samples = 20
```

random

- Keywords Area
- model
- active_subspace
- sample_type
- random

Uses purely random Monte Carlo sampling to sample variables
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none
  Argument(s): none

Description

The `random` keyword invokes Monte Carlo sampling as the means of drawing samples of uncertain variables according to their probability distributions.

  Default Behavior
  In most contexts, Monte Carlo sampling is not the default sampling mode (exception: `multilevel_sampling`). To change this behavior, the `random` keyword must be specified in conjunction with the `sample_type` keyword.

  Usage Tips
  Monte Carlo sampling is more computationally expensive than Latin Hypercube Sampling as it requires a larger number of samples to accurately estimate statistics.

Examples

```plaintext
method
  sampling
    sample_type random
    samples = 200
```

truncation_method

- Keywords Area
- model
- active_subspace
- truncation_method

Metric that estimates active subspace size

Specification

Alias: none
  Argument(s): none
  Default: constantine

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>bing_li</td>
<td></td>
<td>Use the Bing Li &quot;ladle&quot; diagnostic to truncate subspace</td>
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</tbody>
</table>
6.3. MODEL

<table>
<thead>
<tr>
<th>Optional</th>
<th>constantine</th>
<th>Use the Constantine diagnostic to truncate subspace</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>energy</td>
<td>Truncate the subspace based on eigenvalue energy</td>
</tr>
<tr>
<td>Optional</td>
<td>cross_validation</td>
<td>Truncate the subspace to minimize surrogate cross-validation error</td>
</tr>
</tbody>
</table>

**Description**

Metric that controls how many basis vectors are retained in the active subspace.

**Default Behavior**

The default is to use the constantine diagnostic.

**Usage Tips**

If the automated subspace identification methods do not yield desirable results, consider using the explicit dimension truncation option.

**bing_li**

- **Keywords** Area
- model
- active_subspace
- truncation_method
- bing_li

Use the Bing Li "ladle" diagnostic to truncate subspace

**Specification**

**Alias**: none

**Argument(s)**: none

**Description**

Uses a trade-off criterion to determine where to truncate the active subspace. The criterion is a function of the eigenvalues and eigenvectors of the active subspace gradient matrix. This function compares the decrease in eigenvalue amplitude with the increase in eigenvector variability under bootstrap sampling of the gradient matrix. The active subspace size is taken to be the index of the first minimum of this quantity.

**Usage Tips**

If this automated diagnostic does not yield desirable results, consider using the explicit dimension truncation option or one of the other truncation methods.
CHAPTER 6. KEYWORDS AREA

**Theory**

Below is a brief outline of the Bing Li method of active subspace identification. The first two steps are common to all active subspace truncation methods.

1. Compute the gradient of the quantity of interest, $q = f(x)$, at several locations sampled from the input space,
   \[ \nabla_x f_i = \nabla f(x_i). \]

2. Compute the eigendecomposition of the matrix $\hat{C}$,
   \[ \hat{C} = \frac{1}{M} \sum_{i=1}^{M} \nabla_x f_i \nabla_x f_i^T = \hat{W} \hat{\Lambda} \hat{W}^T, \]
   where $\hat{W}$ has eigenvectors as columns, $\hat{\Lambda} = \text{diag}(\hat{\lambda}_1, \ldots, \hat{\lambda}_N)$ contains eigenvalues, and $N$ is the total number of parameters.

3. Normalize the eigenvalues,
   \[ \lambda_i = \frac{\hat{\lambda}_i}{\sum_j^N \hat{\lambda}_j}. \]

4. Use bootstrap sampling of the gradients found in step 1 to compute replicate eigendecompositions,
   \[ \hat{C}_j^* = \hat{W}_j^* \hat{\Lambda}_j^* \left( \hat{W}_j^* \right)^T. \]

5. Compute variability of eigenvectors,
   \[ f_i^0 = \frac{1}{M_{\text{boot}}} \sum_{j}^{M_{\text{boot}} \{ 1 - \left| \det \left( \hat{W}_i^T \hat{W}_{j,i}^* \right) \right| \}}, \]
   where $\hat{W}_i$ and $\hat{W}_{j,i}^*$ both contain only the first $i$ eigenvectors and $M_{\text{boot}}$ is the number of bootstrap samples. The value of the variability at the first index, $f_1^0$, is defined as zero.

6. Normalize the eigenvector variability,
   \[ f_i = \frac{f_i^0}{\sum_j^N f_j^0}. \]

7. The criterion, $g_i$, is defined as,
   \[ g_i = \lambda_i + f_i. \]

8. The index of first minimum of $g_i$ is then the estimated active subspace rank.

For additional information, see Luo, Wei, and Bing Li. "Combining eigenvalues and variation of eigenvectors for order determination." SIAM, 2015.

---

**constantine**

- Keywords Area
- model
- active_subspace
- truncation_method
- constantine

Use the Constantine diagnostic to truncate subspace
6.3. MODEL

Specification

Alias: none

Argument(s): none

Description

Uses a criterion based on the variability of the subspace estimate. Eigenvectors are computed for bootstrap samples of the gradient matrix. The subspace size associated with the minimum distance between bootstrap eigenvectors and the nominal eigenvectors is the estimated active subspace size.

Usage Tips

If this automated diagnostic does not yield desirable results, consider using the explicit dimension truncation option or one of the other truncation methods.

Theory

Below is a brief outline of the Constantine method of active subspace identification. The first two steps are common to all active subspace truncation methods.

1. Compute the gradient of the quantity of interest, \( q = f(x) \), at several locations sampled from the input space,
   \[
   \nabla_x f_i = \nabla f(x_i).
   \]

2. Compute the eigendecomposition of the matrix \( \dot{C} \),
   \[
   \dot{C} = \frac{1}{M} \sum_{i=1}^{M} \nabla_x f_i \nabla_x f_i^T = \dot{W} \dot{\Lambda} \dot{W}^T,
   \]
   where \( \dot{W} \) has eigenvectors as columns, \( \dot{\Lambda} = \text{diag}(\dot{\lambda}_1, \ldots, \dot{\lambda}_N) \) contains eigenvalues, and \( N \) is the total number of parameters.

3. Use bootstrap sampling of the gradients found in step 1 to compute replicate eigendecompositions,
   \[
   \dot{C}^*_j = \dot{W}^*_j \dot{\Lambda}^*_j \left( \dot{W}^*_j \right)^T.
   \]

4. Compute the average distance between nominal and bootstrap subspaces,
   \[
   e^*_n = \frac{1}{M_{\text{boot}}} \sum_j \text{dist}(\text{ran}(\dot{W}_n), \text{ran}(\dot{W}^*_j,n)) = \frac{1}{M_{\text{boot}}} \sum_j \| \dot{W}_n \dot{W}_n^T - \dot{W}^*_j,n \left( \dot{W}^*_j,n \right)^T \|,
   \]
   where \( M_{\text{boot}} \) is the number of bootstrap samples, \( \dot{W}_n \) and \( \dot{W}^*_j,n \) both contain only the first \( n \) eigenvectors, and \( n < N \).

5. The estimated subspace rank, \( r \), is then,
   \[
   r = \arg \min_n e^*_n.
   \]

For additional information, see Constantine, Paul G. "Active Subspaces: Emerging Ideas for Dimension Reduction in Parameter Studies". Vol. 2. SIAM, 2015.
energy

- Keywords Area
- model
- active_subspace
- truncation_method
- energy

Truncate the subspace based on eigenvalue energy

**Specification**

**Alias:** none

**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword</th>
</tr>
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<tbody>
<tr>
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<td>Group</td>
<td>truncation_</td>
<td>Description</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>tolerance</td>
<td>Specify the</td>
</tr>
</tbody>
</table>

maximum percentage (as a decimal) of the
eigenvalue energy not captured by the
active subspace representation.

**Description**

Uses a criterion based on the derivative matrix eigenvalue energy.

**Usage Tips**

This subspace truncation method may work best when working with non-normally distributed uncertain variables. If this automated diagnostic does not yield desirable results, consider using the explicit dimension truncation option or one of the other truncation methods.

**Theory**

Using the eigenvalue energy truncation metric, the subspace size is determined using the following equation:

\[
n = \inf \left\{ d \in \mathbb{Z} \mid 1 \leq d \leq N \land 1 - \frac{\sum_{i=1}^{d} \lambda_i}{\sum_{i=1}^{N} \lambda_i} < \epsilon \right\}
\]

where \(\epsilon\) is the truncation_tolerance, \(n\) is the estimated subspace size, \(N\) is the size of the full space, and \(\lambda_i\) are the eigenvalues of the derivative matrix.
truncation_tolerance

- Keywords Area
- model
- active_subspace
- truncation_method
- energy
- truncation_tolerance

Specify the maximum percentage (as a decimal) of the eigenvalue energy not captured by the active subspace representation.

**Specification**

Alias: none

Argument(s): REAL

**Description**

The truncation_tolerance is used in the energy truncation method to identify an active subspace. The truncation tolerance is used in the following equation to determine the subspace size:

\[
 n = \inf \left\{ d \in \mathbb{Z} \left| 1 \leq d \leq N \land 1 - \frac{\sum_{i=1}^{d} \lambda_i}{\sum_{i=1}^{N} \lambda_i} < \epsilon \right. \right\}
\]

where \( \epsilon \) is the truncation_tolerance, \( n \) is the estimated subspace size, \( N \) is the size of the full space, and \( \lambda_i \) are the eigenvalues of the derivative matrix.

The default value for truncation_tolerance is \( 1 \times 10^{-6} \).

cross_validation

- Keywords Area
- model
- active_subspace
- truncation_method
- cross_validation

Truncate the subspace to minimize surrogate cross-validation error

**Specification**

Alias: none

Argument(s): none

Default: relative
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<th>Required/Optional</th>
<th>Description of Group CV Selection Criterion (Group 1)</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<tbody>
<tr>
<td>Optional (Choose One)</td>
<td>minimum</td>
<td>relative</td>
<td>Select subspace to minimize cross-validation error</td>
</tr>
<tr>
<td>Optional</td>
<td>relative</td>
<td>decrease</td>
<td>Choose subspace with cross-validation error less than tolerance</td>
</tr>
<tr>
<td>Optional</td>
<td>decrease</td>
<td>decrease_tolerance</td>
<td>Choose subspace where cross-validation error stabilizes</td>
</tr>
<tr>
<td>Optional</td>
<td>max_rank</td>
<td>max_rank</td>
<td>Maximum subspace dimension to consider</td>
</tr>
<tr>
<td>Optional</td>
<td>exhaustive</td>
<td>exhaustive</td>
<td>Assess all admissible subspace dimensions</td>
</tr>
</tbody>
</table>

**Description**

Select the subspace dimension that minimizes the 10-fold cross-validation error when constructing a moving least squares surrogate model.

**minimum**
- Keywords Area
- model
- active_subspace
- truncation_method
• cross_validation

• minimum

Select subspace to minimize cross-validation error

**Specification**

**Alias:** none  
**Argument(s):** none

**Description**

Select the subspace dimension that minimizes the cross-validation error across sizes considered.

**relative**

• Keywords Area

• model

• active_subspace

• truncation_method

• cross_validation

• relative

Choose subspace with cross-validation error less than tolerance

**Specification**

**Alias:** none  
**Argument(s):** none

**Description**

Select smallest subspace with cross-validation error less than specified tolerance.

**decrease**

• Keywords Area

• model

• active_subspace

• truncation_method

• cross_validation

• decrease

Choose subspace where cross-validation error stabilizes
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none
Argument(s): none

Description

Select smallest subspace where change in cross-validation error to next larger subspace falls below specified tolerance.

relative_tolerance

- Keywords Area
- model
- active_subspace
- truncation_method
- cross_validation
- relative_tolerance

Tolerance for cross-validation error value

Specification

Alias: none
Argument(s): REAL
Default: 1.0e-6

Description

Select smallest subspace where change in cross-validation error falls below specified tolerance.

decrease_tolerance

- Keywords Area
- model
- active_subspace
- truncation_method
- cross_validation
- decrease_tolerance

Tolerance for cross-validation error stabilization
6.3. MODEL

**Specification**

**Alias:** none

**Argument(s):** REAL

**Default:** 1.0e-6

**Description**

Select smallest subspace where change in cross-validation error falls below specified tolerance.

- `max_rank`
  - **Keywords Area**
  - **model**
  - **active_subspace**
  - **truncation_method**
  - **cross_validation**
  - **max_rank**

Maximum subspace dimension to consider

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** number fullspace vars

**Description**

In cross-validation, only consider subspace dimensions from 1 to `max_rank`.

- `exhaustive`
  - **Keywords Area**
  - **model**
  - **active_subspace**
  - **truncation_method**
  - **cross_validation**
  - **exhaustive**

Assess all admissible subspace dimensions
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none
 Argument(s): none
 Default: on

Description

Assess cross-validation error for all admissible subspace dimensions, even if a particular dimension meets specified cross-validation tolerance(s).

dimension

- Keywords Area
- model
- active_subspace
- dimension

Explicitly specify the desired subspace size

Specification

Alias: none
 Argument(s): INTEGER

Description

This control explicitly indicates the number of basis vectors to retain. The subspace model will include exactly dimension variables.

Default Behavior
Not active; the number of basis vectors will be chosen by one of the truncation methods.

Usage Tips
This control can be helpful when a priori studies give insight to the appropriate subspace size.

bootstrap_samples

- Keywords Area
- model
- active_subspace
- bootstrap_samples

Number of bootstrap replicates used in truncation metrics

Specification

Alias: none
 Argument(s): INTEGER
6.3. **MODEL**

**Description**

The number of bootstrap replicates used to estimate the active subspace size.

**Default Behavior**

Use 100 replicates.

**build_surrogate**

- **Keywords Area**

- **model**

- **active_subspace**

- **build_surrogate**

Construct moving least squares surrogate over active subspace

**Specification**

**Alias:** none

**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td></td>
<td>refinement_-</td>
<td>Number of supplementary</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td></td>
<td>samples</td>
<td>surrogate build samples</td>
</tr>
</tbody>
</table>

**Description**

Once the active subspace variables have been identified, replace the fullspace truth model with a moving least squares surrogate model over the reduced variables. The surrogate is constructed using the fullspace function value samples collected during subspace identification, possibly supplemented with additional `refinement_samples` in the fullspace.

**Default Behavior**

No surrogate is constructed by default.

**Examples**

```plaintext
model
  active_subspace
    id_model = 'SUBSPACE'
    actual_model_pointer = 'FULLSPACE'
    initial_samples 100
  build_surrogate
    refinement_samples 10
```
refinement_samples

- Keywords Area
- model
- active_subspace
- build_surrogate
- refinement_samples

Number of supplementary surrogate build samples

**Specification**

**Alias:** none

**Argument(s):** INTEGERLIST

**Default:** 0

**Description**

Augment the function value data collected during subspace identification with the specified number of refinement_samples to build the surrogate model.

**normalization**

- Keywords Area
- model
- active_subspace
- normalization

Normalize gradient samples

**Specification**

**Alias:** none

**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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</thead>
<tbody>
<tr>
<td><strong>Required (Choose One)</strong></td>
<td>Normalize By... (Group 1)</td>
<td>mean_value</td>
<td>Normalize by sample mean of function values</td>
</tr>
</tbody>
</table>
6.3. MODEL

<table>
<thead>
<tr>
<th></th>
<th>mean_gradient</th>
<th>local_gradient</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Normalize by</td>
<td>Normalize each</td>
</tr>
<tr>
<td></td>
<td>sample mean of</td>
<td>gradient sample by</td>
</tr>
<tr>
<td></td>
<td>gradient norms</td>
<td>its norm</td>
</tr>
</tbody>
</table>

**Description**

Normalize the matrix of sampled gradients before identifying subspace.

**Default Behavior**

The default is `local_gradient`.

**mean_value**

- **Keywords Area**
- **model**
- **active_subspace**
- **normalization**
- **mean_value**

Normalize by sample mean of function values

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

For each response function $f_i$, normalize its gradient data by the mean $m_i$ of the function values taken across samples $j = 1, ..., J$:

$$m_i = \frac{1}{J} \sum_{j=1}^{J} f_i^j$$

**mean_gradient**

- **Keywords Area**
- **model**
- **active_subspace**
- **normalization**
- **mean_gradient**

Normalize by sample mean of gradient norms
CHAPTER 6. KEYWORDS AREA

Specification
Alias: none
Argument(s): none

Description
For each response function \( f_i \), normalize its gradient data by the mean \( m_i \) of the gradient two-norms taken across samples \( j = 1, \ldots, J \):

\[
m_i = \frac{1}{J} \sum_{j=1}^{J} \| \nabla^j f_i \|_2
\]

localGradient
- Keywords Area
- model
- active_subspace
- normalization
- localGradient

Normalize each gradient sample by its norm.

Specification
Alias: none
Argument(s): none

Description
For each response function \( f_i \), normalize each gradient sample \( \nabla^j f_i \) by its two-norm \( \| \nabla^j f_i \| \)

6.3.6 adapted_basis
- Keywords Area
- model
- adapted_basis

Unused (reserved for future Adapted Basis Model)

Specification
Alias: none
Argument(s): none
### Description

**Default Behavior**

- Expected Output
- Usage Tips
- Additional Discussion

### actual_model_pointer

- Keywords Area
- model
- adapted_basis
- actual_model_pointer

Pointer to specify a "truth" model, from which to construct a surrogate

### Topics

This keyword is related to the topics:

- block_pointer

### Specification

**Alias:** none  
**Argument(s):** STRING

**Description**

This must point to a model block, identified by id_model. That model will be run to generate training data, from which a surrogate model will be constructed.

See block_pointer for details about pointers.
sparse_grid_level
  • Keywords Area
  • model
  • adapted_basis
  • sparse_grid_level

Unused (reserved for future Adapted Basis Model)

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Description**

**Default Behavior**

**Expected Output**

**Usage Tips**

**Additional Discussion**

expansion_order
  • Keywords Area
  • model
  • adapted_basis
  • expansion_order

Unused (reserved for future Adapted Basis Model)

**Specification**

**Alias:** none

**Argument(s):** INTEGER

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<tr>
<th>Required/Optional Required</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<tr>
<td></td>
<td></td>
<td>collocation_ratio</td>
<td>Unused (reserved for future Adapted Basis Model)</td>
</tr>
</tbody>
</table>

**Description**

**Default Behavior**

**Expected Output**

**Usage Tips**

**Additional Discussion**
6.3. MODEL

colocation_ratio

- Keywords Area
- model
- adapted_basis
- expansion_order
- collocation_ratio

Unused (reserved for future Adapted Basis Model)

Specification

Alias: none

Argument(s): REAL

Description

Default Behavior

Expected Output

Usage Tips

Additional Discussion

6.3.7 random_field

- Keywords Area
- model
- random_field

Experimental capability to generate a random field representation from data, from simulation runs, or from a covariance matrix. The representation may then be sampled for use as a random field input to another simulation. THIS IS AN EXPERIMENTAL CAPABILITY.

Specification

Alias: none

Argument(s): none
<table>
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<th>Description of</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>Group</td>
<td>build_source</td>
<td>Specify how the random field will be built: from a data file, from simulation runs, or from a covariance matrix. THIS IS AN EXPERIMENTAL CAPABILITY.</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>expansion_form</td>
<td>Specify the form of the expansion to be used in the random field representation. THIS IS AN EXPERIMENTAL CAPABILITY.</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>expansion_bases</td>
<td>Specify the number of basis functions to be used in the random field representation. THIS IS AN EXPERIMENTAL CAPABILITY.</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>truncation_tolerance</td>
<td>Specify a percent of the response variance that should be captured with the random field representation. THIS IS AN EXPERIMENTAL CAPABILITY.</td>
</tr>
</tbody>
</table>
**Required**

- **propagation_model_pointer**: Pointer to the model that will accept realizations of the random field and use them for subsequent analysis. Typically, this model will take the random field as inputs, e.g. a random field defining a pressure boundary or temperature boundary condition over a structure. **THIS IS AN EXPERIMENTAL CAPABILITY.**

### Description

Capability to generate a random field representation from data, from simulation runs, or from a covariance matrix. The random field may then be sampled for use as a random field input to another simulation. **THIS IS AN EXPERIMENTAL CAPABILITY UNDER ACTIVE DEVELOPMENT.**

**Default Behavior** There are three main sections of the random field model. The first section tells Dakota what data to use to build the random field. This is specified with `build_source`. The source of data to build the random field may be a file with data (where the N rows of data correspond to N samples of the random field and the M columns correspond to field values), or it may be a simulation that generates field data, or it may be specified given a mesh and a covariance matrix governing how the field varies over the mesh. In the case of using a simulation to generate field data, the simulation is defined with `dace_method_pointer`. In the case of using a mesh and a covariance, the form of the covariance is defined with `analytic_covariance`.

The next section of the random field model specifies the form of the expansion, `expansion_form`. This can be either a Karhunen-Loeve expansion or a Principal components analysis. These are very similar: both involve the eigenvalues of the covariance matrix of the field data. The only difference is in the treatment of the estimation of the coefficients of the eigenvector basis functions. In the PCA case, we have developed an approach which makes the coefficients explicit functions of the uncertain variables used to generate the random field. The specification of the random field can also include the number of bases to retain or a truncation tolerance, which defines the percent variance that the expansion should capture.

The final section of the random field model allows the user to specify a pointer to a model over which the random field will be propagated, meaning the model which will be driven with the random field input. This part of the specification is optional: one can build a random field but not use it in a downstream model.

### Examples

As stated above, this is an emerging capability. The syntax currently looks like the following:

```plaintext
random_field
   build_source
      rf_data_file | dace_method_pointer | analytic_covariance
```
CHAPTER 6. KEYWORDS AREA

expansion_form
karhunen_loeve | principal_components
expansion_bases
truncation_tolerance
propagation_model_pointer

build_source

- Keywords Area
- model
- random_field
- build_source

Specify how the random field will be built: from a data file, from simulation runs, or from a covariance matrix. THIS IS AN EXPERIMENTAL CAPABILITY.

Specification

Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required (Choose One)</td>
<td>Build Data Source (Group 1)</td>
<td>rf_data_file</td>
<td>Specify that the random field will be built from a file of data. THIS IS AN EXPERIMENTAL CAPABILITY.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>dace_method_pointer</td>
<td>Pointer to a DACE method for purposes of generating an ensemble of field responses to be used in estimating a random field model. THIS IS AN EXPERIMENTAL CAPABILITY.</td>
</tr>
</tbody>
</table>
6.3. MODEL

| analytic_covariance | Use an analytic covariance function for the purposes of generating a random field model. THIS IS AN EXPERIMENTAL CAPABILITY. |

**Description**

As part of the capability to generate a random field representation, the user needs to specify the data used to generate the random field representation. This data may reside in a data file, it may be generated by running a set of simulations and generating field responses, or it may be generated by a covariance matrix defined over a mesh. THIS IS AN EXPERIMENTAL CAPABILITY UNDER ACTIVE DEVELOPMENT.

**Default Behavior**  
Currently, the build_source that is fully working is the dace_method_pointer. The others are not fully operational.

**rf_data_file**

- **Keywords Area**
- **model**
- **random_field**
- **build_source**
- **rf_data_file**

Specify that the random field will be built from a file of data. THIS IS AN EXPERIMENTAL CAPABILITY.

**Specification**

**Alias:** none  
**Argument(s):** STRING  
**Default:** none

**Description**

As part of the capability to generate a random field representation, the user needs to specify the data used to generate the random field representation. In the case of rf_data_file, the data should reside in that file. The rows of this file represent separate samples, and the columns represent the field data. For example, if you have 100 samples of a random field of length 500, the data file will be of dimension 100 x 500. Currently, this option is not operational. THIS IS AN EXPERIMENTAL CAPABILITY UNDER ACTIVE DEVELOPMENT.

**Default Behavior**  
Currently, the build_source that is fully working is the dace_method_pointer. The others are not fully operational.
dace_method_pointer

- Keywords Area
- model
- random_field
- build_source
- dace_method_pointer

Pointer to a DACE method for purposes of generating an ensemble of field responses to be used in estimating a random field model. **THIS IS AN EXPERIMENTAL CAPABILITY.**

**Specification**

**Alias:** none

**Argument(s):** STRING

**Default:** no design of experiments data

**Description**

As part of the capability to generate a random field representation, the user needs to specify the data used to generate the random field representation. One way to do this is to run a set of simulations and generating field responses. Dakota will then take the full set of field responses (e.g. multiple samples, where each sample has a field response) and construct a random field model representing the uncertainty in the ensemble. The dace_method_pointer is a pointer to a Design and Analysis of Computer Experiments (DACE) method, typically which is a sampling method. In this case, the sampling method should be on a simulation which can generate field responses (e.g. field_responses, field_objectives, or field_calibration terms.**

**Default Behavior** Currently, the build_source that is fully working is the dace_method_pointer. The others are not fully operational.

analytic_covariance

- Keywords Area
- model
- random_field
- build_source
- analytic_covariance

Use an analytic covariance function for the purposes of generating a random field model. **THIS IS AN EXPERIMENTAL CAPABILITY.**

**Specification**

**Alias:** none

**Argument(s):** none
## Description

As part of the capability to generate a random field representation, the user needs to specify the data used to generate the random field representation. If `analytic_covariance` is specified, an analytic covariance function will be used to generate instantiations of a random field over a mesh. The form of the covariance function must be specified (e.g. `exponential` or `squared_exponential`). THIS IS AN EXPERIMENTAL CAPABILITY UNDER ACTIVE DEVELOPMENT.

### Default Behavior

Currently, the `build_source` that is fully working is the `dace_method_pointer`.

The others are not fully operational.

### squared_exponential

- **Keywords Area**
  - model
  - random_field
  - build_source
  - analytic_covariance
  - squared_exponential

  Specify a squared exponential covariance in the case where the random field is built from an analytic covariance function. THIS IS AN EXPERIMENTAL CAPABILITY.
CHAPTER 6. KEYWORDS AREA

Specification
Alias: none
  Argument(s): none

Description
THIS IS AN EXPERIMENTAL CAPABILITY UNDER ACTIVE DEVELOPMENT.
  Default Behavior  Currently, the build_source that is fully working is the dace_method_pointer. The others are not fully operational.

  exponential
  • Keywords Area
  • model
  • random_field
  • build_source
  • analytic_covariance
  • exponential

Specify an exponential covariance in the case where the random field is built from an analytic covariance function. THIS IS AN EXPERIMENTAL CAPABILITY.

Specification
Alias: none
  Argument(s): none

Description
THIS IS AN EXPERIMENTAL CAPABILITY UNDER ACTIVE DEVELOPMENT.
  Default Behavior  Currently, the build_source that is fully working is the dace_method_pointer. The others are not fully operational.

  expansion_form
  • Keywords Area
  • model
  • random_field
  • expansion_form

Specify the form of the expansion to be used in the random field representation. THIS IS AN EXPERIMENTAL CAPABILITY.

Specification
Alias: none
  Argument(s): none
### 6.3. MODEL

<table>
<thead>
<tr>
<th>Required/-Optional Required/(Choose One)</th>
<th>Description of Group Reduced Basis Type (Group 1)</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>karhunen_loeve</td>
<td>Specify Karhunen-Loeve as the expansion form to be used in the random field representation. THIS IS AN EXPERIMENTAL CAPABILITY.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>principal-components</td>
<td>Specify Principal Components as the form of the expansion to be used in the random field representation. THIS IS AN EXPERIMENTAL CAPABILITY.</td>
</tr>
</tbody>
</table>

### Description

This control allows the user to specify the form of the random field representation (e.g. either a Karhunen-Loeve or Principal Components expansion). THIS IS AN EXPERIMENTAL CAPABILITY UNDER ACTIVE DEVELOPMENT.

**Default Behavior**  The default expansion form is Karhunen-Loeve.

**karhunen_loeve**

- **Keywords Area**
- **model**
- **random_field**
- **expansion_form**
- **karhunen_loeve**

Specify Karhunen-Loeve as the expansion form to be used in the random field representation. THIS IS AN EXPERIMENTAL CAPABILITY.

### Specification

**Alias:** none  
**Argument(s):** none
CHAPTER 6. KEYWORDS AREA

**Description**

THIS IS AN EXPERIMENTAL CAPABILITY UNDER ACTIVE DEVELOPMENT.

**Default Behavior** The default expansion form is Karhunen-Loeve.

**principal_components**

- Keywords Area
- model
- random_field
- expansion_form
- principal_components

Specify Principal Components as the form of the expansion to be used in the random field representation. THIS IS AN EXPERIMENTAL CAPABILITY.

**Specification**

Alias: none

**Argument(s):** none

**Description**

Principal Components and Karhunen-Loeve are very similar functional forms of the expansion. They both use basis functions which are eigenvectors of the covariance matrix of the random field data. However, in principal components, we parameterize the coefficients of the expansion to be Gaussian process models which are functions of the uncertain parameters used to generate the initial ensemble of data representing the random field. THIS IS AN EXPERIMENTAL CAPABILITY UNDER ACTIVE DEVELOPMENT.

**Default Behavior** The default expansion form is Karhunen-Loeve.

**expansion_bases**

- Keywords Area
- model
- random_field
- expansion_bases

Specify the number of basis functions to be used in the random field representation. THIS IS AN EXPERIMENTAL CAPABILITY.

**Specification**

Alias: none

**Argument(s):** INTEGER
6.3. **MODEL**

**Description**

This control allows the user to specify the number of basis functions to be used in the random field representation (e.g. either a Karhunen-Loeve or Principal Components expansion). Typically, a small number of basis functions (3-5) will be sufficient to represent a significant amount of the variance in the response field. However, this depends on the particulars of the problem. **THIS IS AN EXPERIMENTAL CAPABILITY UNDER ACTIVE DEVELOPMENT.**

**Default Behavior**  If the user specifies neither truncation_tolerance nor expansion_bases, then the number of expansion bases that captures 95% of the variance will be used.

**truncation_tolerance**

- Keywords Area
- model
- random_field
- truncation_tolerance

Specify a percent of the response variance that should be captured with the random field representation. **THIS IS AN EXPERIMENTAL CAPABILITY.**

**Specification**

**Alias:** none

**Argument(s):** REAL

**Description**

This control allows the user to specify the percent variance to be capture in the random field representation (e.g. either a Karhunen-Loeve or Principal Components expansion). Typically, the user would specify something like 0.9 or 0.95, where 0.9 means that 90% of the variance of the response field will be captured by the random field. **THIS IS AN EXPERIMENTAL CAPABILITY UNDER ACTIVE DEVELOPMENT.**

**Default Behavior**  If the user specifies neither truncation_tolerance nor expansion_bases, then the truncation tolerance is set to 0.95 and the number of expansion bases that captures 95% of the variance will be used.

**propagation_model_pointer**

- Keywords Area
- model
- random_field
- propagation_model_pointer

Pointer to the model that will accept realizations of the random field and use them for subsequent analysis. Typically, this model will take the random field as inputs, e.g. a random field defining a pressure boundary or temperature boundary condition over a structure. **THIS IS AN EXPERIMENTAL CAPABILITY.**
CHAPTER 6. KEYWORDS AREA

Specification
Alias: none
Argument(s): STRING

Description
After a random field representation has been generated, Dakota will generate samples of that random field based on the representation. These sample realizations can then be used to drive another set of simulation analyses. The propagation_model_pointer is the model on which the random field realizations will be propagated. THIS IS AN EXPERIMENTAL CAPABILITY UNDER ACTIVE DEVELOPMENT.

Default Behavior

6.3.8 variables_pointer
- Keywords Area
- model
- variables_pointer

Specify which variables block will be included with this model block

Topics
This keyword is related to the topics:
- block_pointer

Specification
Alias: none
Argument(s): STRING
Default: model use of last variables parsed

Description
The variables_pointer is used to specify which variables block will be used by the model, by cross-referencing with id_variables keyword in the variables block.
See block_pointer for details about pointers.
Default Behavior
When a variables pointer is not specified, the model will use the last variables block parsed from the input file.

6.3.9 responses_pointer
- Keywords Area
- model
- responses_pointer

Specify which responses block will be used by this model block
6.3. MODEL

Topics
This keyword is related to the topics:

- block_pointer

Specification
Alias: none
Argument(s): STRING
Default: model use of last responses parsed

Description
The responses_pointer is used to specify which responses block will be used by the model, by cross-referencing with id_responses keyword in the responses block.

See block_pointer for details about pointers.

Default Behavior
When a responses pointer is not specified, the model will use the last responses block parsed from the input file.

6.3.10 hierarchical_tagging

- Keywords Area
- model
- hierarchical_tagging

Enables hierarchical evaluation tagging

Specification
Alias: none
Argument(s): none
Default: no hierarchical tagging

Description
The hierarchical tagging option is useful for studies involving multiple models with a nested or hierarchical relationship. For example a nested model has a sub-method, which itself likely operates on a sub-model, or a hierarchical approximation involves coordination of low and high fidelity models. Specifying hierarchical_tagging will yield function evaluation identifiers ("tags") composed of the evaluation IDs of the models involved, e.g., outermodel.innermodel.interfaceid = 4.9.2. This communicates the outer contexts to the analysis driver when performing a function evaluation.

Examples
test/dakota_uq_timeseries_ivp_optinterf.in test/dakota_uq_timeseries_sop_optinterf.in
See Also

These keywords may also be of interest:

- file_tag model-nested

6.4 variables

- Keywords Area
- variables

Specifies the parameter set to be iterated by a particular method.

Topics

This keyword is related to the topics:

- block

Specification

Alias: none

<table>
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<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<td></td>
<td>id_variables</td>
<td>Name the variables block; helpful when there are multiple</td>
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<td>Optional</td>
<td></td>
<td>active</td>
<td>Set the active variables view a method will see</td>
</tr>
<tr>
<td>Optional(Choose One)</td>
<td>Group 1</td>
<td>mixed</td>
<td>Maintain continuous/discrete variable distinction</td>
</tr>
<tr>
<td></td>
<td></td>
<td>relaxed</td>
<td>Allow treatment of discrete variables as continuous</td>
</tr>
<tr>
<td>Optional</td>
<td>continuous_design</td>
<td>Design variable - continuous</td>
<td></td>
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<tr>
<td>--------------------------</td>
<td>--------------------------------</td>
<td>-----------------------------</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>discrete_design_range</td>
<td>Design variable - discrete</td>
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<td></td>
<td>range-valued</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>discrete_design_set</td>
<td>Design variable - discrete</td>
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</tr>
<tr>
<td></td>
<td></td>
<td>set-valued</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>normal_uncertain</td>
<td>Aleatory uncertain variable - normal (Gaussian)</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>lognormal_uncertain</td>
<td>Aleatory uncertain variable - lognormal</td>
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<td>Optional</td>
<td>uniform_uncertain</td>
<td>Aleatory uncertain variable - uniform</td>
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<td>Optional</td>
<td>loguniform_uncertain</td>
<td>Aleatory uncertain variable - loguniform</td>
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<td>Aleatory uncertain variable - triangular</td>
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<td>Aleatory uncertain variable - exponential</td>
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<td>Aleatory uncertain variable - beta</td>
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<td>Optional</td>
<td>gamma_uncertain</td>
<td>Aleatory uncertain variable - gamma</td>
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<td>Optional</td>
<td>gumbel_uncertain</td>
<td>Aleatory uncertain variable - gumbel</td>
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<tr>
<td>Optional</td>
<td>frechet_uncertain</td>
<td>Aleatory uncertain variable - Frechet</td>
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<tr>
<td>Optional</td>
<td>weibull_uncertain</td>
<td>Aleatory uncertain variable - Weibull</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>histogram_bin_uncertain</td>
<td>Aleatory uncertain variable - continuous histogram</td>
<td></td>
</tr>
</tbody>
</table>
### Optional keywords

<table>
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<th>Description</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>poisson_uncertain</td>
<td>Aleatory uncertain discrete variable - Poisson</td>
<td>discrete</td>
</tr>
<tr>
<td>binomial_uncertain</td>
<td>Aleatory uncertain discrete variable - binomial</td>
<td>discrete</td>
</tr>
<tr>
<td>negative_binomial_uncertain</td>
<td>Aleatory uncertain discrete variable - negative binomial</td>
<td>discrete</td>
</tr>
<tr>
<td>geometric_uncertain</td>
<td>Aleatory uncertain discrete variable - geometric</td>
<td>discrete</td>
</tr>
<tr>
<td>hypergeometric_uncertain</td>
<td>Aleatory uncertain discrete variable - hypergeometric</td>
<td>discrete</td>
</tr>
<tr>
<td>histogram_point_uncertain</td>
<td>Aleatory uncertain discrete variable - discrete histogram</td>
<td>discrete</td>
</tr>
<tr>
<td>uncertain_correlation_matrix</td>
<td>Correlation among aleatory uncertain variables</td>
<td>nominal</td>
</tr>
<tr>
<td>continuous_interval_uncertain</td>
<td>Epistemic uncertain variable - values from one or more continuous intervals</td>
<td>interval</td>
</tr>
<tr>
<td>discrete_interval_uncertain</td>
<td>Epistemic uncertain variable - values from one or more discrete intervals</td>
<td>interval</td>
</tr>
<tr>
<td>discrete_uncertain_set</td>
<td>Epistemic uncertain variable - discrete set-valued</td>
<td>set</td>
</tr>
<tr>
<td>continuous_state</td>
<td>State variable - continuous</td>
<td>state</td>
</tr>
</tbody>
</table>
### Description

The *variables* specification in a Dakota input file specifies the parameter set to be iterated by a particular method. In the case of

- An optimization study: These variables are adjusted in order to locate an optimal design.
- Parameter studies/sensitivity analysis/design of experiments: These parameters are perturbed to explore the parameter space.
• Uncertainty analysis: The variables are associated with distribution/interval characterizations which are used to compute corresponding distribution/interval characterizations for response functions.

To accommodate these different studies, Dakota supports different:

• Variable types
  – design
  – aleatory uncertain
  – epistemic uncertain
  – state

• Variable domains
  – continuous
  – discrete
    * discrete range
    * discrete integer set
    * discrete string set
    * discrete real set

Use the variables page to browse the available variables by type and domain.

**Variable Types**

• Design Variables
  – Design variables are those variables which are modified for the purposes of seeking an optimal design.
  – The most common type of design variables encountered in engineering applications are of the continuous type. These variables may assume any real value within their bounds.
  – All but a handful of the optimization algorithms in Dakota support continuous design variables exclusively.

• Aleatory Uncertain Variables
  – Aleatory uncertainty is also known as inherent variability, irreducible uncertainty, or randomness.
  – Aleatory uncertainty is predominantly characterized using probability theory. This is the only option implemented in Dakota.

• Epistemic Uncertain Variables
  – Epistemic uncertainty is uncertainty due to lack of knowledge.
  – In Dakota, epistemic uncertainty is assessed by interval analysis or the Dempster-Shafer theory of evidence
  – Continuous or discrete interval or set-valued variables are used to define set-valued probabilities or basic probability assignments (BPA) which define a belief structure.
  – Note that epistemic uncertainty can also be modeled with probability density functions (as done with aleatory uncertainty). Dakota does not support this capability.

• State Variables
6.4. VARIABLES

- State variables consist of "other" variables which are to be mapped through the simulation interface, in that they are not to be used for design and they are not modeled as being uncertain.
- State variables provide a convenient mechanism for managing additional model parameterizations such as mesh density, simulation convergence tolerances, and time step controls.
- Only parameter studies and design of experiments methods will iterate on state variables.
- The initial_value is used as the only value for the state variable for all other methods, unless active_state is invoked.
- See more details on the state_variables page.

Variable Domains
Continuous variables are typically defined by bounds. Discrete variables can be defined in one of three ways, which are discussed on the page discrete_variables.

Ordering of Variables
The ordering of variables is important, and a consistent ordering is employed throughout the Dakota software. The ordering is shown in dakota.input.summary (and in the hierarchical order of this reference manual) and can be summarized as:

1. design
   (a) continuous
   (b) discrete integer
   (c) discrete string
   (d) discrete real

2. aleatory uncertain
   (a) continuous
   (b) discrete integer
   (c) discrete string
   (d) discrete real

3. epistemic uncertain
   (a) continuous
   (b) discrete integer
   (c) discrete string
   (d) discrete real

4. state
   (a) continuous
   (b) discrete integer
   (c) discrete string
   (d) discrete real
Ordering of variable types below this granularity (e.g., from normal to histogram bin within aleatory uncertain - continuous) is defined somewhat arbitrarily, but is enforced consistently throughout the code.

**Active Variables**

The reason variable types exist is that methods have the capability to treat variable types differently. All methods have default behavior that determines which variable types are "active" and will be assigned values by the method. For example, optimization methods will only vary the design variables - by default.

The default behavior should be described on each method page, or on topics pages that relate to classes of methods. In addition, the default behavior can be modified using the active keyword.

At least one type of variables that are active for the method in use must have nonzero size (at least 1 active variable) or an input error message will result.

**Inferred Default Values and Bounds**

The concept of active variables allows any Dakota variable type to be used in any method context. Some methods, e.g., bound-constrained optimization or multi-dimensional or centered parameter studies, require bounds and/or an initial point on the variables, however uncertain variables may not be naturally defined in terms of these characteristics.

Distribution lower and upper bounds are explicit portions of the normal, lognormal, uniform, loguniform, triangular, and beta specifications, whereas they are implicitly defined for others. For example, bounds are naturally defined for histogram bin, histogram point, and interval variables (from the extreme values within the bin/point/interval specifications) as well as for binomial (0 to num_trials) and hypergeometric (0 to min(num_drawn, num_selected)) variables.

If not specified, distribution bounds are also inferred for normal and lognormal (if optional bounds are unspecified) as well as for exponential, gamma, gumbel, frechet, weibull, poisson, negative binomial, and geometric (which have no bounds specifications); these bounds are [0, $\mu + 3\sigma$] for exponential, gamma, frechet, weibull, poisson, negative binomial, geometric, and unspecified lognormal, and [$\mu - 3\sigma$, $\mu + 3\sigma$] for gumbel and unspecified normal.

When an initial point is needed, uncertain variables are initialized to their means, where mean values for bounded normal and bounded lognormal may be further adjusted to satisfy any user-specified distribution bounds, mean values for discrete integer range distributions are rounded down to the nearest integer, and mean values for discrete set distributions are rounded to the nearest set value.

**Examples**

Several examples follow. In the first example, two continuous design variables are specified:

```plaintext
variables,
  continuous_design = 2
  initial_point 0.9 1.1
  upper_bounds 5.8 2.9
  lower_bounds 0.5 -2.9
  descriptors 'radius' 'location'
```

In the next example, defaults are employed. In this case, initial_point will default to a vector of 0. values, upper bounds will default to vector values of DBL_MAX (the maximum number representable in double precision for a particular platform), lower bounds will default to a vector of -DBL_MAX values, and descriptors will default to a vector of 'cdv_i' strings, where i ranges from one to two:

```plaintext
variables,
  continuous_design = 2
```

In the following example, the syntax for a normal-lognormal distribution is shown. One normal and one lognormal uncertain variable are completely specified by their means and standard deviations. In addition, the dependence structure between the two variables is specified using the uncertain_correlation_matrix.
variables,
    normal_uncertain  = 1
    means             = 1.0
    std_deviations   = 1.0
    descriptors      = 'TF1n'
    lognormal_uncertain = 1
    means            = 2.0
    std_deviations   = 0.5
    descriptors      = 'TF2ln'
    uncertain_correlation_matrix = 1.0 0.2
                                    0.2 1.0

An example of the syntax for a state variables specification follows:

variables,
    continuous_state = 1
    initial_state   = 4.0
    lower_bounds    = 0.0
    upper_bounds    = 8.0
    descriptors     = 'CS1'
    discrete_state_range = 1
    initial_state   = 104
    lower_bounds    = 100
    upper_bounds    = 110
    descriptors     = 'DS1'

And in a more advanced example, a variables specification containing a set identifier, continuous and discrete
design variables, normal and uniform uncertain variables, and continuous and discrete state variables is shown:

variables,
    id_variables = 'V1'
    continuous_design = 2
    initial_point  = 0.9 1.1
    upper_bounds   = 5.8 2.9
    lower_bounds   = 0.5 -2.9
    descriptors    = 'radius' 'location'
    discrete_design_range = 1
    initial_point  = 2
    upper_bounds   = 1
    lower_bounds   = 3
    descriptors    = 'material'
    normal_uncertain = 2
    means           = 248.89, 593.33
    std_deviations  = 12.4, 29.7
    descriptors     = 'TF1n' 'TF2n'
    uniform_uncertain = 2
    lower_bounds    = 199.3, 474.63
    upper_bounds    = 298.5, 712.
    descriptors     = 'TF1u' 'TF2u'
    continuous_state = 2
    initial_state   = 1.e-4 1.e-6
    descriptors     = 'EPSIT1' 'EPSIT2'
    discrete_state_set
    integer = 1
    initial_state   = 100
    set_values      = 100 212 375
    descriptors     = 'load_case'

6.4.1 id_variables

• Keywords Area
Name the variables block; helpful when there are multiple

**Topics**

This keyword is related to the topics:

- `block_identifier`

**Specification**

**Alias:** none

**Argument(s):** STRING

**Default:** use of last variables parsed

**Description**

The optional `id_variables` keyword accepts a string that uniquely identifies this variables block. A model can then use these variables by specifying the same string in its `variables_pointer` specification.

**Default Behavior**

If the `id_variables` specification is omitted, a particular variables specification will be used by a model only if that model does not include an `variables_pointer` and the variables block was the last (or only) one parsed.

**Usage Tips**

- It is a best practice to always use explicit variables IDs and pointers to avoid confusion.
- If only one variables block exists, then `id_variables` can be safely omitted from the variables block (and `variables_pointer` omitted from the model specification(s)), since there is no ambiguity.

**Examples**

For example, a model specification including

```plaintext
model
  variables_pointer = 'V1'
```

will link to a response set with

```plaintext
id_variables = 'V1'
```

### 6.4.2 active

- **Keywords Area**
- **variables**
- **active**

Set the active variables view a method will see
6.4. VARIABLES

Specification

Alias: none

Argument(s): none

Default: Infer from response or method specification
CHAPTER 6. KEYWORDS AREA

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword</th>
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<tbody>
<tr>
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<td>Group</td>
<td></td>
<td>Description</td>
</tr>
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<td>Option for the active keyword</td>
</tr>
<tr>
<td></td>
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<td>uncertain</td>
<td>Option for the active keyword</td>
</tr>
<tr>
<td></td>
<td></td>
<td>aleatory</td>
<td>Option for the active keyword</td>
</tr>
<tr>
<td></td>
<td></td>
<td>epistemic</td>
<td>Option for the active keyword</td>
</tr>
<tr>
<td></td>
<td></td>
<td>state</td>
<td>Option for the active keyword</td>
</tr>
</tbody>
</table>

**Description**

There are certain situations where the user may want to explicitly control the subset of variables that is considered active for a certain Dakota method. This is done by specifying the keyword `active` in the variables specification block, followed by one of the following: `all`, `design`, `uncertain`, `aleatory`, `epistemic`, or `state`.

Specifying one of these subsets of variables will allow the Dakota method to operate on the specified variable types and override the default active subset.

If the user does not specify any explicit override of the active view of the variables, Dakota first considers the response function specification.

- If the user specifies objective functions or calibration terms in the response specification block, then we can infer that the active variables should be the design variables (since design variables are used within optimization and least squares methods).

- If the user instead specifies the generic response type of `response_functions`, then Dakota cannot infer the active variable subset from the response specification and will instead infer it from the method selection.

1. If the method is a parameter study, or any of the methods available under dace, psuade, or fsu methods, the active view is set to all variables.

2. For uncertainty quantification methods, if the method is sampling, then the view is set to aleatory if only aleatory variables are present, epistemic if only epistemic variables are present, or uncertain (covering both aleatory and epistemic) if both are present.

3. If the uncertainty method involves interval estimation or evidence calculations, the view is set to epistemic.

4. For other uncertainty quantification methods not mentioned in the previous sentences (e.g., reliability methods or stochastic expansion methods), the default view is set to aleatory.

5. Finally, for verification studies using the Richardson extrapolation method, the active view is set to state.

6. Note that in surrogate-based optimization, where the surrogate is built on points defined by the method defined by the `dace_method_pointer`, the sampling used to generate the points is performed only over the design variables as a default unless otherwise specified (e.g., state variables will not be sampled for surrogate construction).
As alluded to in the previous section, the iterative method selected for use in Dakota determines what subset, or view, of the variables data is active in the iteration. The general case of having a mixture of various different types of variables is supported within all of the Dakota methods even though certain methods will only modify certain types of variables (e.g., optimizers and least squares methods only modify design variables, and uncertainty quantification methods typically only utilize uncertain variables). This implies that variables which are not under the direct control of a particular iterator will be mapped through the interface in an unmodified state. This allows for a variety of parameterizations within the model in addition to those which are being used by a particular iterator, which can provide the convenience of consolidating the control over various modeling parameters in a single file (the Dakota input file). An important related point is that the variable set that is active with a particular iterator is the same variable set for which derivatives are typically computed.

Examples

For example, the default behavior for a nondeterministic sampling method is to sample the uncertain variables. However, if the user specified \texttt{active all} in the variables specification block, the sampling would be performed over all variables (e.g. design and state variables in addition to the uncertain variables). This may be desired in situations such as surrogate-based optimization under uncertainty, where a surrogate may be constructed to span both design and uncertain variables. This is an example where we expand the active subset beyond the default, but in other situations, we may wish to restrict from the default. An example of this would be performing design of experiments in the presence of multiple variable types (for which all types are active by default), but only wanting to sample over the design variables for purposes of constructing a surrogate model for optimization.

Theory

The optional status of the different variable type specifications allows the user to specify only those variables which are present (rather than explicitly specifying that the number of a particular type of variables is zero). However, at least one type of variables that are active for the iterator in use must have nonzero size or an input error message will result.

\texttt{all}

- \texttt{Keywords Area}
- \texttt{variables}
- \texttt{active}
- all

Option for the \texttt{active} keyword

Specification

\textbf{Alias}: none
- \textbf{Argument(s)}: none

Description

See the \texttt{active} keyword
design

- Keywords Area
- variables
- active
- design

Option for the active keyword

**Specification**

Alias: none
Argument(s): none

**Description**

See the active keyword

uncertain

- Keywords Area
- variables
- active
- uncertain

Option for the active keyword

**Specification**

Alias: none
Argument(s): none

**Description**

See the active keyword

aleatory

- Keywords Area
- variables
- active
- aleatory

Option for the active keyword
6.4. VARIABLES

**Specification**

Alias: none
  Argument(s): none

**Description**

See the active keyword

epistemic
  - Keywords Area
  - variables
  - active
  - epistemic

Option for the active keyword

**Specification**

Alias: none
  Argument(s): none

**Description**

See the active keyword

state
  - Keywords Area
  - variables
  - active
  - state

Option for the active keyword

**Specification**

Alias: none
  Argument(s): none

**Description**

See the active keyword
6.4.3 mixed

- Keywords Area
- variables
- mixed

Maintain continuous/discrete variable distinction

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** relaxed (branch and bound), mixed (all other methods)

**Description**

The variables domain specifies how the discrete variables are treated. If the user specifies *mixed* in the variable specification block, the continuous and discrete variables are treated separately. If the user specifies *relaxed* in the variable specification block, the discrete variables are relaxed and treated as continuous variables. This may be useful in optimization problems involving both continuous and discrete variables when a user would like to use an optimization method that is designed for continuous variable optimization. All Dakota methods have a default value of mixed for the domain type except for the branch-and-bound method which has a default domain type of relaxed. Note that the branch-and-bound method is under development at this time. Finally, note that the domain selection applies to all variable types: design, aleatory uncertain, epistemic uncertain, and state.

With respect to domain type, if the user does not specify an explicit override of *mixed* or *relaxed*, Dakota infers the domain type from the method. As mentioned above, all methods currently use a mixed domain as a default, except the branch-and-bound method which is under development.

**See Also**

These keywords may also be of interest:

- relaxed

6.4.4 relaxed

- Keywords Area
- variables
- relaxed

Allow treatment of discrete variables as continuous

**Specification**

**Alias:** none

**Argument(s):** none
6.4. VARIABLES

Description
The variables domain specifies how the discrete variables are treated. If the user specifies mixed in the variable specification block, the continuous and discrete variables are treated separately. If the user specifies relaxed in the variable specification block, the discrete variables are relaxed and treated as continuous variables. This may be useful in optimization problems involving both continuous and discrete variables when a user would like to use an optimization method that is designed for continuous variable optimization. All Dakota methods have a default value of mixed for the domain type except for the branch-and-bound method which has a default domain type of relaxed. Note that the branch-and-bound method is under development at this time. Finally, note that the domain selection applies to all variable types: design, aleatory uncertain, epistemic uncertain, and state.

With respect to domain type, if the user does not specify an explicit override of mixed or relaxed, Dakota infers the domain type from the method. As mentioned above, all methods currently use a mixed domain as a default, except the branch-and-bound method which is under development.

See Also
These keywords may also be of interest:

- mixed

6.4.5 continuous_design

- Keywords Area
- variables
- continuous_design

Design variable - continuous

Topics
This keyword is related to the topics:

- continuous_variables
- design_variables

Specification

Alias: none

Argument(s): INTEGER

Default: no continuous design variables
CHAPTER 6. KEYWORDS AREA

<table>
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<tr>
<th>Optional</th>
<th>lower_bounds</th>
<th>Specify minimum values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>upper_bounds</td>
<td>Specify maximum values</td>
</tr>
<tr>
<td>Optional</td>
<td>scale_types</td>
<td>Specify scaling for the variables</td>
</tr>
<tr>
<td>Optional</td>
<td>scales</td>
<td>Specify scaling for the variable.</td>
</tr>
<tr>
<td>Optional</td>
<td>descriptors</td>
<td>Labels for the variables</td>
</tr>
</tbody>
</table>

Description

Continuous variables are defined by a real interval and are changed during the search for the optimal design.

initial_point

- Keywords Area
- variables
- continuous_design
- initial_point

Initial values

Specification

Alias: cdv_initial_point

Argument(s): REALLIST
Default: 0.0

Description

The initial_point specifications provide the point in design space (variable values) from which an iterator is started. These default to the midpoint of bounds (continuous design variables) or the middle value (discrete design variables).

lower_bounds

- Keywords Area
- variables
- continuous_design
- lower_bounds

Specify minimum values
6.4. VARIABLES

Specification

Alias: cdv_lower_bounds
  Argument(s): REALLIST
  Default: -infinity

Description

Specify minimum values

upper_bounds
  • Keywords Area
  • variables
  • continuous_design
  • upper_bounds

Specify maximum values

Specification

Alias: cdv_upper_bounds
  Argument(s): REALLIST
  Default: infinity

Description

Specify maximum values

scale_types
  • Keywords Area
  • variables
  • continuous_design
  • scale_types

Specify scaling for the variables

Specification

Alias: cdv_scale_types
  Argument(s): STRINGLIST
  Default: vector values = ‘none’
Description

For continuous variables, the `scale_types` specification includes strings specifying the scaling type for each component of the continuous design variables vector in methods that support scaling, when scaling is enabled.

Each entry in `scale_types` may be selected from ‘none’, ‘value’, ‘auto’, or ‘log’, to select no, characteristic value, automatic, or logarithmic scaling, respectively. If a single string is specified it will apply to all components of the continuous design variables vector. Each entry in `scales` may be a user-specified nonzero real characteristic value to be used in scaling each variable component. These values are ignored for scaling type ‘none’, required for ‘value’, and optional for ‘auto’ and ‘log’. If a single real value is specified it will apply to all components of the continuous design variables vector.

Examples

Two continuous design variables, one scaled by a value, the other log scaled,

```plaintext
continuous_design = 2
initial_point -1.2 1.0
lower_bounds -2.0 0.001
upper_bounds 2.0 2.0
descriptors 'x1' 'x2'
scale_types = 'value' 'log'
scales = 4.0 0.1
```

scales

- Keywords Area
- variables
- continuous_design
- scales

Specify scaling for the variable.

Specification

Alias: cdv_scales

Argument(s): REALLIST

Default: vector values = 1. (no scaling)

Description

For continuous variables, the `scale_types` specification includes strings specifying the scaling type for each component of the continuous design variables vector in methods that support scaling, when scaling is enabled. Each entry in `scale_types` may be selected from ‘none’, ‘value’, ‘auto’, or ‘log’, to select no, characteristic value, automatic, or logarithmic scaling, respectively. If a single string is specified it will apply to all components of the continuous design variables vector. Each entry in `scales` may be a user-specified nonzero real characteristic value to be used in scaling each variable component. These values are ignored for scaling type ‘none’, required for ‘value’, and optional for ‘auto’ and ‘log’. If a single real value is specified it will apply to all components of the continuous design variables vector.
6.4. VARIABLES

Examples
Two continuous design variables, both scaled by the characteristic value 4.0

```plaintext
continuous_design = 2
    initial_point  -1.2  1.0
    lower_bounds   -200  0.001
    upper_bounds   200   2.0
    descriptors    'x1'  'x2'
    scale_types    'value' 'none'
    scales         10.0
```

descriptors

- Keywords Area
- variables
- continuous_design
- descriptors

Labels for the variables

Specification

Alias: cdv_descriptors

Argument(s): STRINGLIST

Default: cdv_{i}

Description

The optional variable labels specification descriptors is a list of strings which identify the variables. These are used in console and tabular output.

The default descriptor strings use a variable type-dependent root string plus a numeric identifier.

6.4.6 discrete_design_range

- Keywords Area
- variables
- discrete_design_range

Design variable - discrete range-valued

Topics

This keyword is related to the topics:

- discrete_variables
- design_variables
**Specification**

Alias: none

Argument(s): INTEGER

Default: no discrete design variables
## Description

These variables take on a range of integer values from the specified lower bound to the specified upper bound (integer interval). The details of how to specify this discrete variable are located on the `discrete_variables` page.

### initial_point

- **Keywords Area**
- **variables**
- **discrete_design_range**
- **initial_point**

Initial values

### Specification

**Alias:** ddv_initial_point  
**Argument(s):** INTEGERLIST  
**Default:** 0

### Description

The `initial_point` specifications provide the point in design space (variable values) from which an iterator is started. These default to the midpoint of bounds (continuous design variables) or the middle value (discrete design variables).

### lower_bounds

- **Keywords Area**
- **variables**
- **discrete_design_range**
- **lower_bounds**

Specify minimum values
Specification

Alias: ddv_lower_bounds
Argument(s): INTEGERLIST
Default: INT_MIN

Description

Specify minimum values

upper_bounds

- Keywords Area
- variables
- discrete_design_range
- upper_bounds

Specify maximum values

Specification

Alias: ddv_upper_bounds
Argument(s): INTEGERLIST
Default: INT_MAX

Description

Specify maximum values

descriptors

- Keywords Area
- variables
- discrete_design_range
- descriptors

Labels for the variables

Specification

Alias: ddv_descriptors
Argument(s): STRINGLIST
Default: ddriv_{\{i\}}
Description

The optional variable labels specification `descriptors` is a list of strings which identify the variables. These are used in console and tabular output.

The default descriptor strings use a variable type-dependent root string plus a numeric identifier.

6.4.7 discrete_design_set

- Keywords
  - Area
  - variables
  - discrete_design_set

Design variable - discrete set-valued

Topics

This keyword is related to the topics:

- discrete_variables
- design_variables

Specification

Alias: none

Argument(s): none

<table>
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<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
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<td>integer</td>
<td>integer</td>
<td>Integer-valued discrete design variables</td>
</tr>
<tr>
<td>Optional</td>
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<td>string</td>
<td>String-valued discrete design set variables</td>
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<tr>
<td>Optional</td>
<td>real</td>
<td>real</td>
<td>Real-valued discrete design variables</td>
</tr>
</tbody>
</table>

Description

Discrete design variables whose values come from a set of admissible elements. Each variable specified must be of type integer, string, or real.
Integer-valued discrete design variables

Topics
This keyword is related to the topics:
- discrete_variables
- design_variables

Specification
Alias: none
Argument(s): INTEGER
Default: no discrete design set integer variables

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<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
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<tbody>
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</tr>
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<td></td>
<td>.per_.variable</td>
<td>elements for each discrete</td>
</tr>
<tr>
<td></td>
<td></td>
<td>elements</td>
<td>variable</td>
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<td>Whether the set-valued</td>
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6.4. VARIABLES

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<th>Initial values</th>
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Optional initial point

Initial values

<table>
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<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Labels for the variables</td>
<td></td>
</tr>
</tbody>
</table>

**Description**

A design variable whose values come from a specified set of admissible integers. The details of how to specify this discrete variable are located on the discrete_variables page.

**Examples**

Four integer variables whose values will be selected from the following sets during the search for an optimal design. \( y_1 \in \{0, 1\}, y_2 \in \{0, 1\}, y_3 \in \{0, 5\} \) and \( y_4 \in \{10, 15, 20, 23\} \).

```plaintext
discrete_design_set
    integer 4
    descriptors 'y1' 'y2' 'y3' 'y4'
    elements_per_variable 2 2 2 4
    elements 0 1 0 1 0 5 10 15 20 23
```

**elements_per_variable**

- Keywords Area
- variables
- discrete_design_set
- integer
- elements_per_variable

Number of admissible elements for each set variable

**Specification**

Alias: num_set_values

Argument(s): INTEGERLIST

Default: equal distribution

**Description**

Discrete set variables (including design, uncertain, and state) take on only a fixed set of values. For each type (integer, string, or real), this keyword specifies how many admissible values are provided for each variable. If not specified, equal apportionment of elements among variables is assumed, and the number of elements must be evenly divisible by the number of variables.
elements
  • Keywords Area
  • variables
  • discrete_design_set
  • integer
  • elements

The permissible values for each discrete variable

**Specification**

Alias: set_values

**Argument(s):** INTEGERLIST

**Description**

Specify the permissible values for discrete set variables (of type integer, string, or real). See the description on the discrete_variables page.

categorical
  • Keywords Area
  • variables
  • discrete_design_set
  • integer
  • categorical

Whether the set-valued variables are categorical or relaxable

**Specification**

Alias: none

**Argument(s):** STRINGLIST

| Required/- | Description of | Dakota Keyword | Dakota Keyword |
| Optional | Group | | Description |
| Optional | adjacency_matrix | 1-0 matrix defining which categorical variable levels are related. |

**Description**

A list of strings of length equal to the number of set (integer, string, or real) variables indicating whether they are strictly categorical, meaning may only take on values from the provided set, or relaxable, meaning may take on any integer or real value between the lowest and highest specified element. Valid categorical strings include 'yes', 'no', 'true', and 'false', or any abbreviation in [yYnNtTfF][.]*
6.4. VARIABLES

Examples

Discrete design_set variable, 'rotor_blades', can take on only integer values, 2, 4, or 7 by default. Since categorical is specified to be false, the integrality can be relaxed and 'rotor_blades' can take on any value between 2 and 7, e.g., 3, 6, or 5.5.

```
discrete_design_set
  integer 1
  elements 2 4 7
descriptor 'rotor_blades'
categorical 'no'
```

```
adjacency_matrix
```

- Keywords Area
- variables
- discrete_design_set
- integer
- categorical
- adjacency_matrix

1-0 matrix defining which categorical variable levels are related.

Specification

Alias: none

Argument(s): INTEGERLIST

Description

The adjacency_matrix keyword is associated with discrete_design_set variables that are specified to be categorical. Each such variable is associated with one $k \times k$ symmetric matrix, where $k$ is the number of values (or levels) of the variable. Entry $i,j$ of a matrix should be 1 if level $i$ and level $j$ are related by some subjective criteria or if $i = j$; it should be 0 otherwise. The matrices for all variables of the same type (string, real, or integer) are entered sequentially as a list of integers as shown in the examples below.

Default Behavior

The adjacency_matrix keyword is only relevant for discrete_design_set real and discrete_design_set integer variables if one or more of them have been specified to be categorical. It is always relevant for discrete_design_set string variables. If the user does not define an adjacency matrix, the default is method dependent. Currently, the only method that makes use of the adjacency matrix is mesh_adaptive_search, which uses a tri-diagonal adjacency matrix by default.

Expected Output

The expected output is method dependent.

Usage Tips

If an adjacency matrix is defined for one type of (categorical) discrete_design_set variable, it must be defined for all variables of that type, even for those not defined to be categorical. Those for the non-categorical set variables will be ignored.
Examples

The following example shows a variables specification where some real and some integer discrete design-set variables are categorical.

```plaintext
variables
  continuous_design = 3
  initial_point -1.0 1.5 2.0
  lower_bounds -10.0 -10.0 -10.0
  upper_bounds 10.0 10.0 10.0
  descriptors 'x1' 'x2' 'x3'
  discrete_design_range = 2
  initial_point 2 2
  lower_bounds 1 1
  upper_bounds 4 9
  descriptors 'y1' 'y2'
  discrete_design_set
    real = 2
      elements_per_variable = 4 5
      elements = 1.2 2.3 3.4 4.5 1.2 3.3 4.4 5.5 7.7
      descriptors 'y3' 'y4'
      categorical 'no' 'yes'
      adjacency_matrix
        1 1 0 0 # Begin entry of 4x4 matrix for y3
        1 1 1 0
        0 1 1 1
        0 0 1 1
        1 0 1 0 1 # Begin entry of 5x5 matrix for y4
        0 1 0 1 0
        1 0 1 0 1
        0 1 0 1 0
        1 0 1 0 1
  integer = 2
    elements_per_variable = 2 3
    elements = 4 7 8 9 12
    descriptors 'z1' 'z2'
    categorical 'yes' 'yes'
```

Note that for the real case, the user wants to define an adjacency matrix for the categorical variable, so adjacency matrices for both variables must be specified. The matrix for the first one will be ignored. Note that no adjacency matrix is specified for either integer categorical variable. The default will be used in both cases. Currently the only method taking advantage of adjacency matrices is `mesh_adaptive_search`, which uses a tri-diagonal adjacency matrix by default. Thus, the matrices used would be

```plaintext
z1:
1 1
1 1
z2:
1 1 0
1 1 1
0 1 1
```

The following example shows a variables specification for string variables. Note that string variables are always considered to be categorical. If an adjacency matrix is not specified, a method-dependent default matrix will be used.

```plaintext
variables,
  continuous_design = 2
  initial_point 0.5 0.5
  lower_bounds 0. 0.
  upper_bounds 1. 1.
  descriptors = 'x' 'y'
  discrete_design_set string = 1
```
6.4. VARIABLES

```plaintext
elements = 'aniso1' 'aniso2' 'iso1' 'iso2' 'iso3'
descriptors = 'ancomp'
adjacency_matrix
1 1 0 0 0
1 1 0 0 0
0 0 1 1 1
0 0 1 1 1
0 0 1 1 1
```

See Also

These keywords may also be of interest:

- mesh_adaptive_search

initial_point

- Keywords Area
- variables
- discrete_design_set
- integer
- initial_point

Initial values

Specification

Alias: none

Argument(s): INTEGERLIST

Default: middle set value, or rounded down

Description

The initial_point specifications provide the point in design space (variable values) from which an iterator is started. These default to the midpoint of bounds (continuous design variables) or the middle value (discrete design variables).

descriptors

- Keywords Area
- variables
- discrete_design_set
- integer
- descriptors

Labels for the variables
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): STRINGLIST

Description

The optional variable labels specification descriptors is a list of strings which identify the variables. These are used in console and tabular output.

The default descriptor strings use a variable type-dependent root string plus a numeric identifier.

string

- Keywords Area
- variables
- discrete_design_set
- string

String-valued discrete design set variables

Topics

This keyword is related to the topics:

- discrete_variables
- design_variables

Specification

Alias: none

Argument(s): INTEGER

Default: no discrete design set string variables

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<td>Number of admissible elements for each set variable</td>
<td>The permissible values for each discrete variable</td>
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Optional

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<th>I-0 matrix defining which categorical variable levels are related.</th>
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<td>Initial values</td>
</tr>
<tr>
<td>descriptors</td>
<td>Labels for the variables</td>
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</tbody>
</table>

Description

Discrete design variables whose values come from a specified set of admissible strings. The details of how to specify this discrete variable are located on the `discrete_variables` page. Each string element value must be quoted and may contain alphanumeric, dash, underscore, and colon. White space, quote characters, and backslash/metacharacters are not permitted.

Examples

Two string variables whose values will be selected from the set of provided elements. The first variable, 'linear solver', takes on values from a set of three possible elements and the second variable, 'mesh_file', from a set of two possible elements.

discrete_design_set
string 2
  descriptors 'linear_solver' 'mesh_file'
  elements_per_variable 3 2
  elements 'cg' 'gmres' 'direct'
       'mesh64.exo' 'mesh128.exo'

**elements_per_variable**

- Keywords Area
- variables
- discrete_design_set
- string
- elements_per_variable

Number of admissible elements for each set variable

Specification

**Alias:** `num_set_values`
**Argument(s):** INTEGERLIST
**Default:** equal distribution
**Description**

Discrete set variables (including design, uncertain, and state) take on only a fixed set of values. For each type (integer, string, or real), this keyword specifies how many admissible values are provided for each variable. If not specified, equal apportionment of elements among variables is assumed, and the number of elements must be evenly divisible by the number of variables.

** Specification**

**Alias:** set_values  
**Argument(s):** STRINGLIST

**Description**

Specify the permissible values for discrete set variables (of type integer, string, or real). See the description on the discrete_variables page.

**adjacency_matrix**

**Alias:** none  
**Argument(s):** INTEGERLIST

1-0 matrix defining which categorical variable levels are related.
6.4. VARIABLES

Description

The `adjacency_matrix` keyword is associated with `discrete_design_set` variables that are specified to be categorical. Each such variable is associated with one $k \times k$ symmetric matrix, where $k$ is the number of values (or levels) of the variable. Entry $i,j$ of a matrix should be 1 if level $i$ and level $j$ are related by some subjective criteria or if $i = j$; it should be 0 otherwise. The matrices for all variables of the same type (`string`, `real`, or `integer`) are entered sequentially as a list of integers as shown in the examples below.

Default Behavior

The `adjacency_matrix` keyword is only relevant for `discrete_design_set` `real` and `discrete_design_set` `integer` variables if one or more of them have been specified to be categorical. It is always relevant for `discrete_design_set` `string` variables. If the user does not define an adjacency matrix, the default is method dependent. Currently, the only method that makes use of the adjacency matrix is `mesh_adaptive_search`, which uses a tri-diagonal adjacency matrix by default.

Expected Output

The expected output is method dependent.

Usage Tips

If an adjacency matrix is defined for one type of (categorical) `discrete_design_set` variable, it must be defined for all variables of that type, even for those not defined to be categorical. Those for the non-categorical set variables will be ignored.

Examples

The following example shows a variables specification where some real and some integer `discrete_design_set` variables are categorical.

```plaintext
variables
  continuous_design = 3
  initial_point -1.0 1.5 2.0
  lower_bounds -10.0 -10.0 -10.0
  upper_bounds 10.0 10.0 10.0
  descriptors 'x1' 'x2' 'x3'
  discrete_design_set_range = 2
  initial_point 2 2
  lower_bounds 1 1
  upper_bounds 4 9
  descriptors 'y1' 'y2'
  discrete_design_set
    real = 2
      elements_per_variable = 4 5
      elements  1.2 2.3 3.4 4.5 1.2 3.3 4.4 5.5 7.7
      descriptors 'y3' 'y4'
      categorical 'no' 'yes'
      adjacency_matrix 1 1 0 0  # Begin entry of 4x4 matrix for y3
        1 1 1 0
        0 1 1 1
        0 0 1 1
        1 0 1 0 1  # Begin entry of 5x5 matrix for y4
        0 1 0 1 0
        1 0 1 0 1
        0 1 0 1 0
        1 0 1 0 1
    integer = 2
      elements_per_variable = 2 3
      elements  4 7 8 9 12
      descriptors 'z1' 'z2'
      categorical 'yes' 'yes'
```
Note that for the real case, the user wants to define an adjacency matrix for the categorical variable, so adjacency matrices for both variables must be specified. The matrix for the first one will be ignored. Note that no adjacency matrix is specified for either integer categorical variable. The default will be used in both cases. Currently the only method taking advantage of adjacency matrices is mesh_adaptive_search, which uses a tri-diagonal adjacency matrix by default. Thus, the matrices used would be

\[
\begin{array}{c}
z1: & 1 & 1 \\
 & 1 & 1 \\
z2: & 1 & 1 & 0 \\
 & 1 & 1 & 1 \\
 & 0 & 1 & 1 \\
\end{array}
\]

The following example shows a variables specification for string variables. Note that string variables are always considered to be categorical. If an adjacency matrix is not specified, a method-dependent default matrix will be used.

```plaintext
variables,
  continuous_design = 2
  initial_point 0.5 0.5
  lower_bounds 0. 0.
  upper_bounds 1. 1.
  descriptors = 'x' 'y'
discrete_design_set string = 1
  elements = 'aniso1' 'aniso2' 'iso1' 'iso2' 'iso3'
  descriptors = 'ancomp'
  adjacency_matrix 1 1 0 0 0
  1 1 0 0 0
  0 0 1 1 1
  0 0 1 1 1
  0 0 1 1 1
```

See Also

These keywords may also be of interest:

- `mesh_adaptive_search`
- `variable`
- `discrete_design_set`
- `string`
- `initial_point`

Initial values

**Specification**

**Alias:** none

**Argument(s):** STRINGLIST

**Default:** middle set value, or rounded down
Description

The initial_point specifications provide the point in design space (variable values) from which an iterator is started. These default to the midpoint of bounds (continuous design variables) or the middle value (discrete design variables).

descriptors

- Keywords Area
- variables
- discrete_design_set
- string
- descriptors

Labels for the variables

Specification

Alias: none
Argument(s): STRINGLIST

Description

The optional variable labels specification descriptors is a list of strings which identify the variables. These are used in console and tabular output.

The default descriptor strings use a variable type-dependent root string plus a numeric identifier.

real

- Keywords Area
- variables
- discrete_design_set
- real

Real-valued discrete design variables

Topics

This keyword is related to the topics:

- discrete_variables
- design_variables

Specification

Alias: none
Argument(s): INTEGER
Default: no discrete design set real variables
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<th>Dakota Keyword</th>
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<td>Number of</td>
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<td>elements for</td>
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<td>each set</td>
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<td></td>
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</tr>
</tbody>
</table>

**Description**

A design variable whose values come from a specified set of admissible reals. The details of how to specify this discrete variable are located on the discrete_variables page.

**Examples**

Two continuous, restricted variables whose values will be selected from the following sets during the search for an optimal design. \( y_1 \in \{0.25, 1.25, 2.25, 3.25, 4.25\} \), \( y_2 \in \{0, 5\} \)

```plaintext
discrete_design_set
real 2
    descriptors 'y1' 'y2'
    elements_per_variable 5 2
    elements 0.25 1.25 2.25 3.25 4.25 0 5
```

**elements_per_variable**

- Keywords Area
- variables
- discrete_design_set
- real
- elements_per_variable

Number of admissible elements for each set variable
6.4. VARIABLES

**Specification**

Alias: num_set_values

- **Argument(s):** INTEGERLIST
- **Default:** equal distribution

**Description**

Discrete set variables (including design, uncertain, and state) take on only a fixed set of values. For each type (integer, string, or real), this keyword specifies how many admissible values are provided for each variable. If not specified, equal apportionment of elements among variables is assumed, and the number of elements must be evenly divisible by the number of variables.

**elements**

- Keywords Area
- variables
- discrete_design_set
- real
- elements

The permissible values for each discrete variable

**Specification**

Alias: set_values

- **Argument(s):** REALLIST

**Description**

Specify the permissible values for discrete set variables (of type integer, string, or real). See the description on the discrete_variables page.

**categorical**

- Keywords Area
- variables
- discrete_design_set
- real
- categorical

Whether the set-valued variables are categorical or relaxable

**Specification**

Alias: none

- **Argument(s):** STRINGLIST
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<th>Dakota Keyword</th>
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<td>Optional</td>
<td></td>
<td>adjacency_matrix</td>
<td>1-0 matrix defining which categorical variable levels are related.</td>
</tr>
</tbody>
</table>

**Description**

A list of strings of length equal to the number of set (integer, string, or real) variables indicating whether they are strictly categorical, meaning may only take on values from the provided set, or relaxable, meaning may take on any integer or real value between the lowest and highest specified element. Valid categorical strings include ‘yes’, ‘no’, ‘true’, and ‘false’, or any abbreviation in [yYnNtTfF][.].

**Examples**

Discrete_design_set variable, 'rotor_blades', can take on only integer values, 2, 4, or 7 by default. Since categorical is specified to be false, the integrality can be relaxed and 'rotor_blades' can take on any value between 2 and 7, e.g., 3, 6, or 5.5.

```plaintext
discrete_design_set
   integer 1
   elements 2 4 7
   descriptor 'rotor_blades'
   categorical 'no'
```

**adjacency_matrix**

- **Keywords Area**
- **variables**
- **discrete_design_set**
- **real**
- **categorical**
- **adjacency_matrix**

1-0 matrix defining which categorical variable levels are related.

**Specification**

Alias: none

Argument(s): INTEGERLIST
Description

The **adjacency_matrix** keyword is associated with **discrete_design_set** variables that are specified to be categorical. Each such variable is associated with one $k \times k$ symmetric matrix, where $k$ is the number of values (or levels) of the variable. Entry $i, j$ of a matrix should be 1 if level $i$ and level $j$ are related by some subjective criteria or if $i = j$; it should be 0 otherwise. The matrices for all variables of the same type (**string**, **real**, or **integer**) are entered sequentially as a list of integers as shown in the examples below.

**Default Behavior**

The **adjacency_matrix** keyword is only relevant for **discrete_design_set** **real** and **discrete_design_set** **integer** variables if one or more of them have been specified to be categorical. It is always relevant for **discrete_design_set** **string** variables. If the user does not define an adjacency matrix, the default is method dependent. Currently, the only method that makes use of the adjacency matrix is **mesh_adaptive_search**, which uses a tri-diagonal adjacency matrix by default.

**Expected Output**

The expected output is method dependent.

**Usage Tips**

If an adjacency matrix is defined for one type of (categorical) **discrete_design_set** variable, it must be defined for all variables of that type, even for those not defined to be categorical. Those for the non-categorical set variables will be ignored.

**Examples**

The following example shows a variables specification where some real and some integer **discrete_design_set** variables are categorical.

```
variables
  continuous_design = 3
    initial_point  -1.0  1.5  2.0
    upper_bounds   10.0  10.0  10.0
    descriptors    'x1' 'x2' 'x3'
  discrete_design_range = 2
    initial_point   2  2
    upper_bounds   4  9
    descriptors    'y1' 'y2'
  discrete_design_set
    real = 2
      elements_per_variable = 4 5
      elements           = 1.2 2.3 3.4 4.5 1.2 3.3 4.4 5.5 7.7
      descriptors      'y3' 'y4'
      categorical     'no' 'yes'
      adjacency_matrix 1 1 0 0  # Begin entry of 4x4 matrix for y3
      1 1 1 0
      0 1 1 1
      0 0 1 1
      1 0 1 0
      0 1 0 1  # Begin entry of 5x5 matrix for y4
      0 1 0 1
      1 0 1 0
      0 1 0 1
      1 0 1 0
    integer = 2
      elements_per_variable = 2 3
      elements           = 4 7 8 9 12
      descriptors      'z1' 'z2'
      categorical     'yes' 'yes'
```
Note that for the real case, the user wants to define an adjacency matrix for the categorical variable, so adjacency matrices for both variables must be specified. The matrix for the first one will be ignored. Note that no adjacency matrix is specified for either integer categorical variable. The default will be used in both cases. Currently the only method taking advantage of adjacency matrices is `mesh_adaptive_search`, which uses a tri-diagonal adjacency matrix by default. Thus, the matrices used would be

\[
\begin{align*}
z1: & \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \\
z2: & \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 1 \\ 0 & 1 & 1 \end{bmatrix}
\end{align*}
\]

The following example shows a variables specification for string variables. Note that string variables are always considered to be categorical. If an adjacency matrix is not specified, a method-dependent default matrix will be used.

variables,
  continuous_design = 2
  initial_point 0.5 0.5
  lower_bounds 0. 0.
  upper_bounds 1. 1.
  descriptors = 'x' 'y'
discrete_design_set string = 1
  elements = 'aniso1' 'aniso2' 'iso1' 'iso2' 'iso3'
  descriptors = 'ancomp'
  adjacency_matrix
  1 1 0 0 0
  1 1 0 0 0
  0 0 1 1 1
  0 0 1 1 1
  0 0 1 1 1

See Also
These keywords may also be of interest:

- mesh_adaptive_search

initial_point

- Keywords Area
- variables
- discrete_design_set
- real
- initial_point

Initial values

Specification
Alias: none
Argument(s): REALLIST
Default: middle set value, or rounded down
6.4. VARIABLES

Description
The initial_point specifications provide the point in design space (variable values) from which an iterator is started. These default to the midpoint of bounds (continuous design variables) or the middle value (discrete design variables).

descriptors
- Keywords
- Area
- variables
- discrete_design_set
- real
- descriptors

Labels for the variables

Specification
Alias: none
Argument(s): STRINGLIST

Description
The optional variable labels specification descriptors is a list of strings which identify the variables. These are used in console and tabular output.

Aleatory uncertain variable - normal (Gaussian)

Topics
This keyword is related to the topics:
- continuous_variables
- aleatory_uncertain_variables

Specification
Alias: none
Argument(s): INTEGER
Default: no normal uncertain variables
### Description

Within the normal uncertain optional group specification, the number of normal uncertain variables, the means, and standard deviations are required specifications, and the distribution lower and upper bounds and variable descriptors are optional specifications. The normal distribution is widely used to model uncertain variables such as population characteristics. It is also used to model the mean of a sample: as the sample size becomes very large, the Central Limit Theorem states that the distribution of the mean becomes approximately normal, regardless of the distribution of the original variables.

The density function for the normal distribution is:

\[
f(x) = \frac{1}{\sqrt{2\pi}\sigma_N} e^{-\frac{1}{2}\left(\frac{x-\mu_N}{\sigma_N}\right)^2}
\]

where \(\mu_N\) and \(\sigma_N\) are the mean and standard deviation of the normal distribution, respectively.

Note that if you specify bounds for a normal distribution, the sampling occurs from the underlying distribution with the given mean and standard deviation, but samples are not taken outside the bounds (see “bounded normal” distribution type in[90]). This can result in the mean and the standard deviation of the sample data being different from the mean and standard deviation of the underlying distribution. For example, if you are sampling from a normal distribution with a mean of 5 and a standard deviation of 3, but you specify bounds of 1 and 7, the resulting mean of the samples will be around 4.3 and the resulting standard deviation will be around 1.6. This is because you have bounded the original distribution significantly, and asymetrically, since 7 is closer to the original mean than 1.

### Theory

When used with design of experiments and multidimensional parameter studies, distribution bounds are inferred. These bounds are \([\mu - 3\sigma, \mu + 3\sigma]\).

For vector and centered parameter studies, an inferred initial starting point is needed for the uncertain variables. These variables are initialized to their means for these studies.

### means

- Keywords Area
- variables
6.4. VARIABLES

- normal_uncertain
- means

First parameter of the distribution

**Specification**

Alias: nuv_means

**Argument(s):** REALLIST

**Description**

Means

**std_deviations**

- Keywords Area
- variables
- normal_uncertain
- std_deviations

Second parameter of the distribution

**Specification**

Alias: nuv_std_deviations

**Argument(s):** REALLIST

**Description**

Standard deviation

**lower_bounds**

- Keywords Area
- variables
- normal_uncertain
- lower_bounds

Specify minimum values

**Specification**

Alias: nuv_lower_bounds

**Argument(s):** REALLIST

**Default:** -infinity
**Description**

Specify minimum values

**upper_bounds**

- Keywords Area
- variables
- normal_uncertain
- upper_bounds

Specify maximum values

**Specification**

Alias: nuv_upper_bounds

Argument(s): REALLIST
Default: infinity

**Description**

Specify maximum values

**initial_point**

- Keywords Area
- variables
- normal_uncertain
- initial_point

Initial values

**Specification**

Alias: none

Argument(s): REALLIST

**Description**

The initial_point specifications provide the point in design space (variable values) from which an iterator is started. These default to the midpoint of bounds (continuous design variables) or the middle value (discrete design variables).
6.4. VARIABLES

descriptors

- Keywords Area
- variables
- normal_uncertain
- descriptors

Labels for the variables

Specification

Alias: nuv_descriptors

Argument(s): STRINGLIST
Default: nuv_{i}

Description

The optional variable labels specification descriptors is a list of strings which identify the variables. These are used in console and tabular output.

The default descriptor strings use a variable type-dependent root string plus a numeric identifier.

6.4.9 lognormal_uncertain

- Keywords Area
- variables
- lognormal_uncertain

Aleatory uncertain variable - lognormal

Topics

This keyword is related to the topics:

- continuous_variables
- aleatory_uncertain_variables

Specification

Alias: none

Argument(s): INTEGER
Default: no lognormal uncertain variables

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CHAPTER 6. KEYWORDS AREA

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**Description**

If the logarithm of an uncertain variable $X$ has a normal distribution, that is $\log X \sim N(\mu, \sigma)$, then $X$ is distributed with a lognormal distribution. The lognormal is often used to model:

1. time to perform some task
2. variables which are the product of a large number of other quantities, by the Central Limit Theorem
3. quantities which cannot have negative values.

Within the lognormal uncertain optional group specification, the number of lognormal uncertain variables, the means, and either standard deviations or error factors must be specified, and the distribution lower and upper bounds and variable descriptors are optional specifications. These distribution bounds can be used to truncate the tails of lognormal distributions, which as for bounded normal, can result in the mean and the standard deviation of the sample data being different from the mean and standard deviation of the underlying distribution (see “bounded lognormal” and “bounded lognormal-n” distribution types in [90]).

For the lognormal variables, one may specify either the mean $\mu$ and standard deviation $\sigma$ of the actual lognormal distribution (option 1), the mean $\mu$ and error factor $\epsilon$ of the actual lognormal distribution (option 2), or the mean $\lambda$ (“lambda”) and standard deviation $\zeta$ (“zeta”) of the underlying normal distribution (option 3).

The conversion equations from lognormal mean $\mu$ and either lognormal error factor $\epsilon$ or lognormal standard deviation $\sigma$ to the mean $\lambda$ and standard deviation $\zeta$ of the underlying normal distribution are as follows:

$$\zeta = \frac{\ln(\epsilon)}{1.645}$$

$$\zeta^2 = \ln\left(\frac{\sigma^2}{\mu^2} + 1\right)$$

$$\lambda = \ln(\mu) - \frac{\zeta^2}{2}$$

Conversions from $\lambda$ and $\zeta$ back to $\mu$ and $\epsilon$ or $\sigma$ are as follows:

$$\mu = e^{\lambda + \frac{\zeta^2}{2}}$$
6.4. VARIABLES

\[ \sigma^2 = e^{2\lambda + \zeta^2} (e^{\zeta^2} - 1) \]
\[ \epsilon = e^{1.645\zeta} \]

The density function for the lognormal distribution is:

\[ f(x) = \frac{1}{\sqrt{2\pi\zeta x}} e^{-\frac{1}{2} \left( \frac{\ln x - \lambda}{\zeta} \right)^2} \]

Theory

When used with design of experiments and multidimensional parameter studies, distribution bounds are inferred. These bounds are \([0, \mu + 3\sigma]\).

For vector and centered parameter studies, an inferred initial starting point is needed for the uncertain variables. These variables are initialized to their means for these studies.

**lambdas**
- **Keywords Area**
- **variables**
- **lognormal_uncertain**
- **lambdas**

First parameter of the lognormal distribution (option 3)

**Specification**

**Alias:** lnuv_lambdas

**Argument(s):** REALLIST

<table>
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<th>Dakota Keyword</th>
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<td>Description</td>
</tr>
<tr>
<td>Required</td>
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<td></td>
<td>Second parameter of the lognormal distribution (option 3)</td>
</tr>
</tbody>
</table>

**Description**

For the lognormal variables, one may specify the mean \(\lambda\) ("lambda") and standard deviation \(\zeta\) ("zeta") of the underlying normal distribution.

**zetas**
- **Keywords Area**
- **variables**
- **lognormal_uncertain**
- **lambdas**
- **zetas**

Second parameter of the lognormal distribution (option 3)
CHAPTER 6. KEYWORDS AREA

Specification

Alias: lnuv_zetas

Argument(s): REALLIST

Description

For the lognormal variables, one may specify the mean $\lambda$ ("lambda") and standard deviation $\zeta$ ("zeta") of the underlying normal distribution.

means

- Keywords Area
- variables
- lognormal_uncertain
- means

First parameter of the lognormal distribution (options 1 & 2)

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<th>Dakota Keyword</th>
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<tr>
<td></td>
<td></td>
<td>error_factors</td>
<td>Second parameter of the lognormal distribution (option 2)</td>
</tr>
</tbody>
</table>

Description

For the lognormal variables, one may specify either the mean $\mu$ and standard deviation $\sigma$ of the actual lognormal distribution, the mean $\mu$ and error factor $\epsilon$ of the actual lognormal distribution.

This corresponds to the mean of the lognormal random variable

std_deviations

- Keywords Area
- variables
- lognormal_uncertain
- means
- std_deviations

Second parameter of the lognormal distribution (option 1)
6.4. VARIABLES

**Specification**

*Alias:* lnuv_std_deviations

**Argument(s):** REALLIST

**Description**

For the lognormal variables, one may specify either the mean $\mu$ and standard deviation $\sigma$ of the actual lognormal distribution.

This corresponds to the standard deviation of the lognormal random variable.

**error_factors**

- **Keywords Area**
- variables
- lognormal_uncertain
- means
- error_factors

Second parameter of the lognormal distribution (option 2)

**Specification**

*Alias:* lnuv_error_factors

**Argument(s):** REALLIST

**Description**

For the lognormal variables, one may specify the mean $\mu$ and error factor $\epsilon$ of the actual lognormal distribution.

This specifies the error function of the lognormal random variable.

**lower_bounds**

- **Keywords Area**
- variables
- lognormal_uncertain
- lower_bounds

Specify minimum values

**Specification**

*Alias:* lnuv_lower_bounds

**Argument(s):** REALLIST

**Default:** 0
CHAPTER 6. KEYWORDS AREA

Description
Specify minimum values

upper_bounds

• Keywords Area
• variables
• lognormal_uncertain
• upper_bounds

Specify maximum values

Specification
Alias: lnuv_upper_bounds
Argument(s): REALLIST
Default: infinity

Description
Specify maximum values

initial_point

• Keywords Area
• variables
• lognormal_uncertain
• initial_point

Initial values

Specification
Alias: none
Argument(s): REALLIST

Description
The initial_point specifications provide the point in design space (variable values) from which an iterator is started. These default to the midpoint of bounds (continuous design variables) or the middle value (discrete design variables).
6.4. VARIABLES


descriptors

- Keywords Area
- variables
- lognormal_uncertain
- descriptors

Labels for the variables

Specification

Alias: lnuv_descriptors

Argument(s): STRINGLIST
Default: lnuv_{i}

Description

The optional variable labels specification descriptors is a list of strings which identify the variables. These are used in console and tabular output.

The default descriptor strings use a variable type-dependent root string plus a numeric identifier.

6.4.10 uniform_uncertain

- Keywords Area
- variables
- uniform_uncertain

Aleatory uncertain variable - uniform

Topics

This keyword is related to the topics:

- continuous_variables
- aleatory_uncertain_variables

Specification

Alias: none

Argument(s): INTEGER
Default: no uniform uncertain variables

<table>
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<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
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<td></td>
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</tr>
</tbody>
</table>
**Description**

Within the uniform uncertain optional group specification, the number of uniform uncertain variables and the distribution lower and upper bounds are required specifications, and variable descriptors is an optional specification. The uniform distribution has the density function:

\[
f(x) = \frac{1}{U_U - L_U}
\]

where \(U_U\) and \(L_U\) are the upper and lower bounds of the uniform distribution, respectively. The mean of the uniform distribution is \(\frac{U_U + L_U}{2}\) and the variance is \(\frac{(U_U - L_U)^2}{12}\).

**Theory**

Note that this distribution is a special case of the more general beta distribution.

**lower_bounds**

- **Keywords Area**
- **variables**
- **uniform_uncertain**
- **lower_bounds**

Specify minimum values

**Specification**

Alias: uuv_lower_bounds

Argument(s): REALLIST

**Description**

Specify minimum values
6.4. VARIABLES

upper_bounds

- Keywords Area
- variables
- uniform_uncertain
- upper_bounds

Specify maximum values

Specification

Alias: uuv_upper_bounds
Argument(s): REALLIST

Description

Specify maximum values

initial_point

- Keywords Area
- variables
- uniform_uncertain
- initial_point

Initial values

Specification

Alias: none
Argument(s): REALLIST

Description

The initial_point specifications provide the point in design space (variable values) from which an iterator is started. These default to the midpoint of bounds (continuous design variables) or the middle value (discrete design variables).

descriptors

- Keywords Area
- variables
- uniform_uncertain
- descriptors

Labels for the variables
CHAPTER 6. KEYWORDS AREA

Specification

Alias: uuv_descriptors

Argument(s): STRINGLIST

Default: uuv_,{i}

Description

The optional variable labels specification descriptors is a list of strings which identify the variables. These are used in console and tabular output.

The default descriptor strings use a variable type-dependent root string plus a numeric identifier.

6.4.11 loguniform uncertain

- Keywords Area
- variables
- loguniform uncertain

Aleatory uncertain variable - loguniform

Topics

This keyword is related to the topics:

- continuous_variables
- aleatory_uncertain_variables

Specification

Alias: none

Argument(s): INTEGER

Default: no loguniform uncertain variables

<table>
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<tr>
<td>Optional</td>
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<tr>
<td>Optional</td>
<td>descriptors</td>
<td></td>
<td>Labels for the variables</td>
</tr>
</tbody>
</table>
6.4. VARIABLES

Description

If the logarithm of an uncertain variable $X$ has a uniform distribution, that is $\log X \sim U(L_{LU}, U_{LU})$, then $X$ is distributed with a loguniform distribution. The distribution lower bound is $L_{LU}$ and upper bound is $U_{LU}$. The loguniform distribution has the density function:

$$f(x) = \frac{1}{x(lnU_{LU} - lnL_{LU})}$$

Theory

For vector and centered parameter studies, an inferred initial starting point is needed for the uncertain variables. These variables are initialized to their means for these studies.

lower_bounds

- Keywords Area
- variables
- loguniform_uncertain
- lower_bounds

Specify minimum values

Specification

Alias: luu_lower_bounds

Argument(s): REALLIST

Description

Specify minimum values

upper_bounds

- Keywords Area
- variables
- loguniform_uncertain
- upper_bounds

Specify maximum values

Specification

Alias: luu_upper_bounds

Argument(s): REALLIST
Description

Specify maximum values

**initial_point**

- **Keywords Area**
- **variables**
- **loguniform_uncertain**
- **initial_point**

Initial values

**Specification**

Alias: none

**Argument(s):** REALLIST

Description

The initial_point specifications provide the point in design space (variable values) from which an iterator is started. These default to the midpoint of bounds (continuous design variables) or the middle value (discrete design variables).

descriptors

- **Keywords Area**

- **variables**

- **loguniform_uncertain**

- **descriptors**

Labels for the variables

**Specification**

Alias: luuv_descriptors

**Argument(s):** STRINGLIST

**Default:** luuv_{i}

Description

The optional variable labels specification descriptors is a list of strings which identify the variables. These are used in console and tabular output.

The default descriptor strings use a variable type-dependent root string plus a numeric identifier.
6.4. VARIABLES

6.4.12 triangular_uncertain

• Keywords Area
• variables
• triangular_uncertain

Aleatory uncertain variable - triangular

Topics

This keyword is related to the topics:

• continuous_variables
• aleatory_uncertain_variables

Specification

Alias: none
Argument(s): INTEGER
Default: no triangular uncertain variables

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<td>Specify maximum values</td>
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<td>Optional</td>
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<td>descriptors</td>
<td>Initial values</td>
</tr>
<tr>
<td>Required</td>
<td></td>
<td></td>
<td>Labels for the variables</td>
</tr>
</tbody>
</table>

Description

The triangular distribution is often used when one does not have much data or information, but does have an estimate of the most likely value and the lower and upper bounds. Within the triangular uncertain optional group specification, the number of triangular uncertain variables, the modes, and the distribution lower and upper bounds are required specifications, and variable descriptors is an optional specification.

The density function for the triangular distribution is:

\[
f(x) = \frac{2(x - L_T)}{(U_T - L_T)(M_T - L_T)}
\]

if \(L_T \leq x \leq M_T\), and

\[
f(x) = \frac{2(U_T - x)}{(U_T - L_T)(U_T - M_T)}
\]

if \(M_T \leq x \leq U_T\), and 0 elsewhere. In these equations, \(L_T\) is the lower bound, \(U_T\) is the upper bound, and \(M_T\) is the mode of the triangular distribution.
modes
  • Keywords Area
  • variables
  • triangular_uncertain
  • modes

Distribution parameter

Specification
Alias: tuv_modes
  Argument(s): REALLIST

Description
Specify the modes

lower_bounds
  • Keywords Area
  • variables
  • triangular_uncertain
  • lower_bounds

Specify minimum values

Specification
Alias: tuv_lower_bounds
  Argument(s): REALLIST

Description
Specify minimum values

upper_bounds
  • Keywords Area
  • variables
  • triangular_uncertain
  • upper_bounds

Specify maximum values
6.4. VARIABLES

**Specification**

**Alias:** tvu_upper_bounds

**Argument(s):** REALLIST

**Description**

Specify maximum values

**initial_point**

- Keywords Area
- variables
- triangular_uncertain
- initial_point

Initial values

**Specification**

**Alias:** none

**Argument(s):** REALLIST

**Description**

The `initial_point` specifications provide the point in design space (variable values) from which an iterator is started. These default to the midpoint of bounds (continuous design variables) or the middle value (discrete design variables).

**descriptors**

- Keywords Area
- variables
- triangular_uncertain
- descriptors

Labels for the variables

**Specification**

**Alias:** tvu_descriptors

**Argument(s):** STRINGLIST

**Default:** tvu_{i}
CHAPTER 6. KEYWORDS AREA

Description

The optional variable labels specification descriptors is a list of strings which identify the variables. These are used in console and tabular output.

The default descriptor strings use a variable type-dependent root string plus a numeric identifier.

6.4.13 exponential_uncertain

- Keywords Area
- variables
- exponential_uncertain

Aleatory uncertain variable - exponential

Topics

This keyword is related to the topics:

- continuous_variables
- aleatory_uncertain_variables

Specification

Alias: none

Argument(s): INTEGER

Default: no exponential uncertain variables

<table>
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<td>Initial values</td>
</tr>
<tr>
<td>Optional</td>
<td>descriptors</td>
<td></td>
<td>Labels for the variables</td>
</tr>
</tbody>
</table>

Description

The exponential distribution is often used for modeling failure rates.

The density function for the exponential distribution is given by:

\[ f(x) = \frac{1}{\beta} e^{-\frac{x}{\beta}} \]

where \( \mu_E = \beta \) and \( \sigma_E^2 = \beta^2 \).

Note that this distribution is a special case of the more general gamma distribution.
6.4. VARIABLES

Theory
When used with design of experiments and multidimensional parameter studies, distribution bounds are inferred. These bounds are $[0, \mu + 3\sigma]$.

For vector and centered parameter studies, an inferred initial starting point is needed for the uncertain variables. These variables are initialized to their means for these studies.

betas
- Keywords Area
- variables
- exponential_uncertain
- betas

Parameter of the exponential distribution

Specification
Alias: euv_betas
Argument(s): REALLIST

Description
Specifies the list of $\beta$ parameters to define the distributions of the exponential random variables. Length must match the other parameters and the number of exponential random variables.

initial_point
- Keywords Area
- variables
- exponential_uncertain
- initial_point

Initial values

Specification
Alias: none
Argument(s): REALLIST

Description
The initial_point specifications provide the point in design space (variable values) from which an iterator is started. These default to the midpoint of bounds (continuous design variables) or the middle value (discrete design variables).
descriptors

- Keywords Area
- variables
- exponential_uncertain
- descriptors

Labels for the variables

Specification

Alias: euv_descriptors
Argument(s): STRINGLIST
Default: euv_{i}

Description

The optional variable labels specification descriptors is a list of strings which identify the variables. These are used in console and tabular output.

The default descriptor strings use a variable type-dependent root string plus a numeric identifier.

6.4.14 beta_uncertain

- Keywords Area
- variables
- beta_uncertain

Aleatory uncertain variable - beta

Topics

This keyword is related to the topics:

- continuous_variables
- aleatory_uncertain_variables

Specification

Alias: none
Argument(s): INTEGER
Default: no beta uncertain variables

<table>
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<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
</table>
Within the beta uncertain optional group specification, the number of beta uncertain variables, the alpha and beta parameters, and the distribution upper and lower bounds are required specifications, and the variable descriptors is an optional specification. The beta distribution can be helpful when the actual distribution of an uncertain variable is unknown, but the user has a good idea of the bounds, the mean, and the standard deviation of the uncertain variable. The density function for the beta distribution is

\[ f(x) = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} \frac{(x - L_B)^{\alpha-1}(U_B - x)^{\beta-1}}{(U_B - L_B)^{\alpha+\beta-1}} \]

where \( \Gamma(\alpha) \) is the gamma function and \( B(\alpha, \beta) = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha + \beta)} \) is the beta function. To calculate the mean and standard deviation from the alpha, beta, upper bound, and lower bound parameters of the beta distribution, the following expressions may be used.

\[ \mu_B = L_B + \frac{\alpha}{\alpha + \beta} (U_B - L_B) \]
\[ \sigma^2_B = \frac{\alpha\beta}{(\alpha + \beta)^2(\alpha + \beta + 1)} (U_B - L_B)^2 \]

Solving these for \( \alpha \) and \( \beta \) gives:

\[ \alpha = \frac{(\mu_B - L_B)(U_B - L_B) - \sigma^2_B}{\sigma^2_B(U_B - L_B)} \]
\[ \beta = \frac{(U_B - \mu_B)(U_B - \mu_B) - \sigma^2_B}{\sigma^2_B(U_B - L_B)} \]

Note that the uniform distribution is a special case of this distribution for parameters \( \alpha = \beta = 1 \).

**Theory**

For vector and centered parameter studies, an inferred initial starting point is needed for the uncertain variables. These variables are initialized to their means for these studies.
**alphas**

- **Keywords Area**
- **variables**
- **beta_uncertain**
- **alphas**

First parameter of the beta distribution

**Specification**

**Alias:** `buv_alphas`

**Argument(s):** `REALLIST`

**Description**

Specifies the list of $\alpha$ parameters to define the distributions of the beta random variables. Length must match the other parameters and the number of beta random variables.

**betas**

- **Keywords Area**
- **variables**
- **beta_uncertain**
- **betas**

Second parameter of the beta distribution

**Specification**

**Alias:** `buv_betals`

**Argument(s):** `REALLIST`

**Description**

Specifies the list of $\beta$ parameters to define the distributions of the beta random variables. Length must match the other parameters and the number of beta random variables.

**lower_bounds**

- **Keywords Area**
- **variables**
- **beta_uncertain**
- **lower_bounds**

Specify minimum values
6.4. VARIABLES

**Specification**

**Alias:** buv_lower_bounds

**Argument(s):** REALLIST

**Description**

Specify minimum values

**upper_bounds**

- Keywords Area
- variables
- beta_uncertain
- upper_bounds

Specify maximum values

**Specification**

**Alias:** buv_upper_bounds

**Argument(s):** REALLIST

**Description**

Specify maximum values

**initial_point**

- Keywords Area
- variables
- beta_uncertain
- initial_point

Initial values

**Specification**

**Alias:** none

**Argument(s):** REALLIST

**Description**

The **initial_point** specifications provide the point in design space (variable values) from which an iterator is started. These default to the midpoint of bounds (continuous design variables) or the middle value (discrete design variables).
Keywords Area

variables

beta_uncertain

descriptors

Labels for the variables

Specification

Alias: buv_descriptors
   Argument(s): STRINGLIST
   Default: buv_{i}

Description

The optional variable labels specification descriptors is a list of strings which identify the variables. These are used in console and tabular output.
   The default descriptor strings use a variable type-dependent root string plus a numeric identifier.

6.4.15 gamma_uncertain

variables

gamma_uncertain

Aleatory uncertain variable - gamma

Topics

This keyword is related to the topics:

   continuous_variables

   aleatory_uncertain_variables

Specification

Alias: none
   Argument(s): INTEGER
   Default: no gamma uncertain variables

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</thead>
<tbody>
<tr>
<td>Optional</td>
<td>Group</td>
<td></td>
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</table>
The gamma distribution is sometimes used to model time to complete a task, such as a repair or service task. It is a very flexible distribution with its shape governed by alpha and beta.

The density function for the gamma distribution is given by:

\[ f(x) = \frac{x^{\alpha-1}e^{-\frac{x}{\beta}}}{\beta^\alpha \Gamma(\alpha)} \]

where \( \mu_{GA} = \alpha \beta \) and \( \sigma^2_{GA} = \alpha \beta^2 \). Note that the exponential distribution is a special case of this distribution for parameter \( \alpha = 1 \).

**Theory**

When used with design of experiments and multidimensional parameter studies, distribution bounds are inferred. These bounds are \([0, \mu + 3\sigma]\).

For vector and centered parameter studies, an inferred initial starting point is needed for the uncertain variables. These variables are initialized to their means for these studies.

**alphas**

- Keywords Area
- variables
- gamma_uncertain
- alphas

First parameter of the gamma distribution

**Specification**

**Alias:** gauv_alphas

**Argument(s):** REALLIST

**Description**

Specifies the list of \( \alpha \) parameters to define the distributions of the gamma random variables. Length must match the other parameters and the number of gamma random variables.
betas

- Keywords Area
- variables
- gamma_uncertain
- betas

Second parameter of the gamma distribution

**Specification**

*Alias:* gauv.betas  
*Argument(s):* REALLIST

**Description**

Specifies the list of $\beta$ parameters to define the distributions of the gamma random variables. Length must match the other parameters and the number of gamma random variables.

initial_point

- Keywords Area
- variables
- gamma_uncertain
- initial_point

Initial values

**Specification**

*Alias:* none  
*Argument(s):* REALLIST

**Description**

The *initial_point* specifications provide the point in design space (variable values) from which an iterator is started. These default to the midpoint of bounds (continuous design variables) or the middle value (discrete design variables).

descriptors

- Keywords Area
- variables
- gamma_uncertain
- descriptors

Labels for the variables
### Specification

**Alias:** gauv_descriptors  
**Argument(s):** STRINGLIST  
**Default:** gauv_{i}

**Description**

The optional variable labels specification descriptors is a list of strings which identify the variables. These are used in console and tabular output.

The default descriptor strings use a variable type-dependent root string plus a numeric identifier.

#### 6.4.16 gumbel_uncertain

- **Keywords Area**
- **variables**
- **gumbel_uncertain**

Aleatory uncertain variable - gumbel

**Topics**

This keyword is related to the topics:

- **continuous_variables**
- **aleatory_uncertain_variables**

**Specification**

**Alias:** none  
**Argument(s):** INTEGER  
**Default:** no gumbel uncertain variables

<table>
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<td>Labels for the variables</td>
</tr>
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</table>
CHAPTER 6. KEYWORDS AREA

Description

The Gumbel distribution is also referred to as the Type I Largest Extreme Value distribution. The distribution of maxima in sample sets from a population with a normal distribution will asymptotically converge to this distribution. It is commonly used to model demand variables such as wind loads and flood levels.

The density function for the Gumbel distribution is given by:

\[ f(x) = \alpha e^{-\alpha(x-\beta)} \exp(-e^{-\alpha(x-\beta)}) \]

where \( \mu_{GU} = \beta + \frac{0.5772}{\alpha} \) and \( \sigma_{GU} = \frac{\pi}{\sqrt{6\alpha}} \).

Theory

When used with design of experiments and multidimensional parameter studies, distribution bounds are inferred. These bounds are \([\mu - 3\sigma, \mu + 3\sigma]\)

For vector and centered parameter studies, an inferred initial starting point is needed for the uncertain variables. These variables are initialized to their means for these studies.

alphas

- Keywords Area
- variables
- gumbel_uncertain
- alphas

First parameter of the gumbel distribution

Specification

Alias: guuv_alphas

Argument(s): REALLIST

Description

Specifies the list of \( \beta \) parameters to define the distributions of the gumbel random variables. Length must match the other parameters and the number of gumbel random variables.

betas

- Keywords Area
- variables
- gumbel_uncertain
- betas

Second parameter of the gumbel distribution
6.4. VARIABLES

**Specification**

**Alias:** guuv_betas

**Argument(s):** REALLIST

**Description**

Specifies the list of $\beta$ parameters to define the distributions of the gumbel random variables. Length must match the other parameters and the number of gumbel random variables.

**initial_point**

- **Keywords Area**
- **variables**
- **gumbel_uncertain**
- **initial_point**

Initial values

**Specification**

**Alias:** none

**Argument(s):** REALLIST

**Description**

The *initial_point* specifications provide the point in design space (variable values) from which an iterator is started. These default to the midpoint of bounds (continuous design variables) or the middle value (discrete design variables).

**descriptors**

- **Keywords Area**
- **variables**
- **gumbel_uncertain**
- **descriptors**

Labels for the variables

**Specification**

**Alias:** guuv_descriptors

**Argument(s):** STRINGLIST

**Default:** guuv_{i}
CHAPTER 6. KEYWORDS AREA

Description
The optional variable labels specification descriptors is a list of strings which identify the variables. These are used in console and tabular output.

The default descriptor strings use a variable type-dependent root string plus a numeric identifier.

6.4.17 frechet_uncertain
- Keywords Area
- variables
- frechet_uncertain

Aleatory uncertain variable - Frechet

Topics
This keyword is related to the topics:
- continuous_variables
- aleatory_uncertain_variables

Specification
Alias: none
Argument(s): INTEGER
Default: no frechet uncertain variables

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</tr>
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<td>Optional</td>
<td>descriptors</td>
<td></td>
<td>Labels for the variables</td>
</tr>
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Description
The Frechet distribution is also referred to as the Type II Largest Extreme Value distribution. The distribution of maxima in sample sets from a population with a lognormal distribution will asymptotically converge to this distribution. It is commonly used to model non-negative demand variables.

The density function for the frechet distribution is:

\[ f(x) = \frac{\alpha}{\beta} \left( \frac{\beta}{x} \right)^{\alpha+1} e^{-\left( \frac{\beta}{x} \right)^{\alpha}} \]

where \( \mu_F = \beta \Gamma(1 - \frac{1}{\alpha}) \) and \( \sigma_F^2 = \beta^2 \left[ \Gamma(1 - \frac{2}{\alpha}) - \Gamma^2(1 - \frac{1}{\alpha}) \right] \)
6.4. VARIABLES

Theory

When used with design of experiments and multidimensional parameter studies, distribution bounds are inferred. These bounds are \([0, \mu + 3\sigma]\).

For vector and centered parameter studies, an inferred initial starting point is needed for the uncertain variables. These variables are initialized to their means for these studies.

alphas

- Keywords Area
- variables
- frechet_uncertain
- alphas

First parameter of the Frechet distribution

Specification

Alias: fuv_alphas

Argument(s): REALLIST

Description

Specifies the list of \(\alpha\) parameters to define the distributions of the Frechet random variables. Length must match the other parameters and the number of Frechet random variables.

betas

- Keywords Area
- variables
- frechet_uncertain
- betas

Second parameter of the Frechet distribution

Specification

Alias: fuv_betas

Argument(s): REALLIST

Description

Specifies the list of \(\beta\) parameters to define the distributions of the Frechet random variables. Length must match the other parameters and the number of Frechet random variables.
initial_point

- Keywords Area
- variables
- frechet_uncertain
- initial_point

Initial values

**Specification**

**Alias:** none

**Argument(s):** REALLIST

**Description**

The `initial_point` specifications provide the point in design space (variable values) from which an iterator is started. These default to the midpoint of bounds (continuous design variables) or the middle value (discrete design variables).

descriptors

- Keywords Area
- variables
- frechet_uncertain
- descriptors

Labels for the variables

**Specification**

**Alias:** fuv_descriptors

**Argument(s):** STRINGLIST

**Default:** fuv_{i}

**Description**

The optional variable labels specification `descriptors` is a list of strings which identify the variables. These are used in console and tabular output.

The default descriptor strings use a variable type-dependent root string plus a numeric identifier.

**6.4.18 weibull_uncertain**

- Keywords Area
- variables
- weibull_uncertain

Aleatory uncertain variable - Weibull
### Topics

This keyword is related to the topics:

- continuous_variables
- aleatory_uncertain_variables

### Specification

**Alias:** none

**Argument(s):** INTEGER

**Default:** no weibull uncertain variables

<table>
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</tr>
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### Description

The Weibull distribution is also referred to as the Type III Smallest Extreme Value distribution. The Weibull distribution is commonly used in reliability studies to predict the lifetime of a device. It is also used to model capacity variables such as material strength.

The density function for the Weibull distribution is given by:

\[
f(x) = \frac{\alpha}{\beta} \left(\frac{x}{\beta}\right)^{\alpha-1} e^{-\left(\frac{x}{\beta}\right)^\alpha}
\]

where \( \mu_W = \beta \Gamma(1 + \frac{1}{\alpha}) \) and \( \sigma_W = \sqrt{\frac{\Gamma(1 + \frac{2}{\alpha})}{\Gamma^2(1 + \frac{1}{\alpha})}} - \mu_W \)

**alphas**

- Keywords Area
- variables
- weibull_uncertain
- alphas

First parameter of the Weibull distribution
**Specification**

Alias: wuv_alphas

**Argument(s):** REALLIST

**Description**

Specifies the list of $\alpha$ parameters to define the distributions of the Weibull random variables. Length must match the other parameters and the number of Weibull random variables.

**betas**

- **Keywords Area**
- **variables**
- **weibull_uncertain**
- **betas**

Second parameter of the Weibull distribution

**Specification**

Alias: wuv_betas

**Argument(s):** REALLIST

**Description**

Specifies the list of $\beta$ parameters to define the distributions of the Weibull random variables. Length must match the other parameters and the number of Weibull random variables.

**initial_point**

- **Keywords Area**
- **variables**
- **weibull_uncertain**
- **initial_point**

Initial values

**Specification**

Alias: none

**Argument(s):** REALLIST

**Description**

The `initial_point` specifications provide the point in design space (variable values) from which an iterator is started. These default to the midpoint of bounds (continuous design variables) or the middle value (discrete design variables).
6.4. VARIABLES

- **Keywords Area**
- **variables**
- **weibull_uncertain**
- **descriptors**

Labels for the variables

**Specification**

**Alias:** wuv_descriptors

- **Argument(s):** STRINGLIST
- **Default:** wuv_{i}

**Description**

The optional variable labels specification descriptors is a list of strings which identify the variables. These are used in console and tabular output.

The default descriptor strings use a variable type-dependent root string plus a numeric identifier.

6.4.19 **histogram_bin_uncertain**

- **Keywords Area**
- **variables**
- **histogram_bin_uncertain**

Aleatory uncertain variable - continuous histogram

**Topics**

This keyword is related to the topics:

- **continuous_variables**
- **aleatory_uncertain_variables**

**Specification**

**Alias:** none

- **Argument(s):** INTEGER
- **Default:** no histogram bin uncertain variables

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</tbody>
</table>
CHAPTER 6. KEYWORDS AREA

Optional

pairs_per_variable
Number of pairs defining each histogram bin variable

Required

abscissas
Real abscissas for a bin histogram

Required (Choose One)

ordinates
Ordinates specifying a “skyline” probability density function

(counts
Frequency or relative probability of each bin

Optional

initial_point
Initial values

Optional
descriptors
Labels for the variables

Description

Histogram uncertain variables are typically used to model a set of empirical data. The bin histogram (contrast: histogram_point_uncertain) is a continuous aleatory distribution characterized by bins of non-zero width where the uncertain variable may lie, together with the relative frequencies of each bin. Hence it can be used to specify a marginal probability density function arising from data.

The histogram_bin_uncertain keyword specifies the number of variables to be characterized as continuous histograms. The required sub-keywords are: abscissas (ranges of values the variable can take on) and either ordinates or counts (characterizing each variable’s frequency information). When using histogram bin variables, each variable must be defined by at least one bin (with two bounding value pairs). When more than one histogram bin variable is active, pairs_per_variable can be used to specify unequal apportionment of provided bin pairs among the variables.

The abscissas specification defines abscissa values ("x" coordinates) for the probability density function of each histogram variable. When paired with counts, the specifications provide sets of (x,c) pairs for each histogram variable where c defines a count (i.e., a frequency or relative probability) associated with a bin. If using bins of unequal width and specification of probability densities is more natural, then the counts specification can be replaced with an ordinates specification ("y" coordinates) in order to support interpretation of the input as (x,y) pairs defining the profile of a "skyline" probability density function.

Conversion between the two specifications is straightforward: a count/frequency is a cumulative probability quantity defined from the product of the ordinate density value and the x bin width. Thus, in the cases of bins of equal width, ordinate and count specifications are equivalent. In addition, ordinates and counts may be relative values; it is not necessary to scale them as all user inputs will be normalized.

To fully specify a bin-based histogram with n bins (potentially of unequal width), n+1 (x,c) or (x,y) pairs must be specified with the following features:

• x is the parameter value for the left boundary of a histogram bin and c is the corresponding count for that
6.4. VARIABLES

bin. Alternatively, \( y \) defines the ordinate density value for this bin within a skyline probability density function. The right boundary of the bin is defined by the left boundary of the next pair.

- the final pair specifies the right end of the last bin and must have a \( c \) or \( y \) value of zero.
- the \( x \) values must be strictly increasing.
- all \( c \) or \( y \) values must be positive, except for the last which must be zero.
- a minimum of two pairs must be specified for each bin-based histogram variable.

Examples

The \texttt{pairs\_per\_variable} specification provides for the proper association of multiple sets of \((x,c)\) or \((x,y)\) pairs with individual histogram variables. For example, in this input snippet

```plaintext
histogram\_bin\_uncertain = 2
pairs\_per\_variable = 3 4
abscissas = 5 8 10 1.1 1.2 1.3 1.4
counts = 17 21 0 12 24 12 0
descriptors = 'hbu_1' 'hbu_2'
```

\texttt{pairs\_per\_variable} associates the first 3 \((x,c)\) pairs from \texttt{abscissas} and \texttt{counts} \{(5,17),(8,21),(10,0)\} with one bin-based histogram variable, where one bin is defined between 5 and 8 with a count of 17 and another bin is defined between 8 and 10 with a count of 21. The following set of 4 \((x,c)\) pairs \{(1.1,12),(2.24),(3.12),(4.0)\} defines a second bin-based histogram variable containing three equal-width bins with counts 12, 24, and 12 (middle bin is twice as probable as the other two).

See Also

These keywords may also be of interest:

- \texttt{histogram\_point\_uncertain}

FAQ

**Difference between bin and point histograms:** A (continuous) bin histogram specifies bins of non-zero width, whereas a (discrete) point histogram specifies individual point values, which can be thought of as bins with zero width. In the terminology of LHS[90], the bin pairs specification defines a ”continuous linear” distribution and the point pairs specification defines a ”discrete histogram” distribution (although the points are real-valued, the number of possible values is finite).

\texttt{pairs\_per\_variable}

- Keywords Area
- \texttt{variables}
- \texttt{histogram\_bin\_uncertain}
- \texttt{pairs\_per\_variable}

Number of pairs defining each histogram bin variable
CHAPTER 6. KEYWORDS AREA

Specification
Alias: num_pairs
Argument(s): INTEGERLIST
Default: equal distribution

Description
By default, the list of 
abscissas and counts or ordinates will be evenly divided among the histogram_bin_uncertain variables. pairs_per_variable is a list of integers that specify the number of pairs to apportion to each variable.

abscissas

• Keywords Area
• variables
• histogram_bin_uncertain
• abscissas

Real abscissas for a bin histogram

Specification
Alias: huv_bin_abscissas
Argument(s): REALLIST

Description
A list of real abscissa ("x" coordinate) values characterizing the probability density function for each of the histogram_bin_uncertain variables. These are paired with either counts or ordinates. See histogram_bin_uncertain for details and examples.

ordinates

• Keywords Area
• variables
• histogram_bin_uncertain
• ordinates

Ordinates specifying a "skyline" probability density function

Specification
Alias: huv_bin_ordinates
Argument(s): REALLIST
6.4. VARIABLES

Description

The ordinates list of real values defines the profile of a "skyline" probability density function by pairing with the specified abscissas. See histogram_bin_uncertain for details.

counts

- Keywords Area
- variables
- histogram_bin_uncertain
- counts

Frequency or relative probability of each bin

Specification

Alias: huv_bin_counts

Argument(s): REALLIST

Description

The counts list of real values gives the frequency or relative probability for each bin in a histogram_bin_uncertain specification. These are paired with the specified abscissas. See histogram_bin_uncertain for details.

initial_point

- Keywords Area
- variables
- histogram_bin_uncertain
- initial_point

Initial values

Specification

Alias: none

Argument(s): REALLIST

Description

The initial_point specifications provide the point in design space (variable values) from which an iterator is started. These default to the midpoint of bounds (continuous design variables) or the middle value (discrete design variables).
descriptors

- Keywords Area
- variables
- histogram_bin_uncertain
- descriptors

Labels for the variables

Specification

Alias: huh_bin_descriptors
Argument(s): STRINGLIST
Default: huh_{i}

Description

The optional variable labels specification descriptors is a list of strings which identify the variables. These are used in console and tabular output.

The default descriptor strings use a variable type-dependent root string plus a numeric identifier.

6.4.20 poisson_uncertain

- Keywords Area
- variables
- poisson_uncertain

Aleatory uncertain discrete variable - Poisson

Topics

This keyword is related to the topics:

- discrete_variables
- aleatory_uncertain_variables

Specification

Alias: none
Argument(s): INTEGER
Default: no poisson uncertain variables

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6.4. VARIABLES

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</tr>
<tr>
<td>Optional</td>
<td>descriptors</td>
<td>Labels for the variables</td>
</tr>
</tbody>
</table>

### Description

The Poisson distribution is used to predict the number of discrete events that happen in a single time interval. The random events occur uniformly and independently. The expected number of occurrences in a single time interval is \( \lambda \), which must be a positive real number. For example, if events occur on average 4 times per year and we are interested in the distribution of events over six months, \( \lambda \) would be 2. However, if we were interested in the distribution of events occurring over 5 years, \( \lambda \) would be 20.

The density function for the Poisson distribution is given by:

\[
f(x) = \frac{\lambda^x e^{-\lambda}}{x!}
\]

where

- \( \lambda \) is the expected number of events occurring in a single time interval
- \( x \) is the number of events that occur in this time period
- \( f(x) \) is the probability that \( x \) events occur in this time period

### Theory

When used with design of experiments and multidimensional parameter studies, distribution bounds are inferred. These bounds are \([0, \mu + 3\sigma]\).

For vector and centered parameter studies, an inferred initial starting point is needed for the uncertain variables. These variables are initialized to their means for these studies.

### lambdas

- **Keywords** Area
- **variables**
- **poisson_uncertain**
- **lambdas**

The parameter for the Poisson distribution, the expected number of events in the time interval of interest

### Specification

**Alias:** none

**Argument(s):** REALLIST
CHAPTER 6. KEYWORDS AREA

Description

The density function for the poisson distribution is given by:

\[ f(x) = \frac{\lambda e^{-\lambda}}{x!} \]

where \( \lambda \) is the frequency of events happening, and \( x \) is the number of events that occur.

initial_point

- Keywords Area
- variables
- poisson_uncertain
- initial_point

Initial values

Specification

Alias: none
Argument(s): INTEGERLIST

Description

The initial_point specifications provide the point in design space (variable values) from which an iterator is started. These default to the midpoint of bounds (continuous design variables) or the middle value (discrete design variables).

descriptors

- Keywords Area
- variables
- poisson_uncertain
- descriptors

Labels for the variables

Specification

Alias: none
Argument(s): STRINGLIST
Default: puv_{i}

Description

The optional variable labels specification descriptors is a list of strings which identify the variables. These are used in console and tabular output.

The default descriptor strings use a variable type-dependent root string plus a numeric identifier.
6.4. VARIABLES

6.4.21 binomial_uncertain

- Keywords Area
- variables
- binomial_uncertain

Aleatory uncertain discrete variable - binomial

Topics

This keyword is related to the topics:
- discrete_variables
- aleatory_uncertain_variables

Specification

Alias: none
Argument(s): INTEGER
Default: no binomial uncertain variables

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<tr>
<td></td>
<td></td>
<td></td>
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</tr>
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</table>

Description

The binomial distribution describes probabilities associated with a series of independent Bernoulli trials. A Bernoulli trial is an event with two mutually exclusive outcomes, such as 0 or 1, yes or no, success or fail. The probability of success remains the same (the trials are independent).

The density function for the binomial distribution is given by:

\[ f(x) = \binom{n}{x} p^x (1 - p)^{n-x} \]

where \( p \) is the probability of failure per trial, \( n \) is the number of trials and \( x \) is the number of successes.

Theory

The binomial distribution is typically used to predict the number of failures or defective items in a total of \( n \) independent tests or trials, where each trial has the probability \( p \) of failing or being defective.
probability_per_trial
  • Keywords Area
  • variables
  • binomial_uncertain
  • probability_per_trial

A distribution parameter for the binomial distribution

**Specification**

Alias: prob_per_trial
  Argument(s): REALLIST

**Description**

The binomial distribution is typically used to predict the number of failures (or defective items or some type of event) in a total of \( n \) independent tests or trials, where each trial has the probability \( p \) of failing or being defective. Each particular test can be considered as a Bernoulli trial.

**num_trials**

• Keywords Area
  • variables
  • binomial_uncertain
  • num_trials

A distribution parameter

**Specification**

Alias: none
  Argument(s): INTEGERLIST

**Description**

The binomial distribution is typically used to predict the number of failures (or defective items or some type of event) in a total of \( n \) independent tests or trials, where each trial has the probability \( p \) of failing or being defective. Each particular test can be considered as a Bernoulli trial.

**initial_point**

• Keywords Area
  • variables
  • binomial_uncertain
  • initial_point

Initial values
6.4. VARIABLES

**Specification**

*Alias:* none

*Argument(s):* INTEGERLIST

**Description**

The *initial_point* specifications provide the point in design space (variable values) from which an iterator is started. These default to the midpoint of bounds (continuous design variables) or the middle value (discrete design variables).

descriptors

- **Keywords Area**
- **variables**
- **binomial_uncertain**
- **descriptors**

Labels for the variables

**Specification**

*Alias:* none

*Argument(s):* STRINGLIST

*Default:* biuv_{i}

**Description**

The optional variable labels specification *descriptors* is a list of strings which identify the variables. These are used in console and tabular output.

The default descriptor strings use a variable type-dependent root string plus a numeric identifier.

**6.4.22 negative_binomial_uncertain**

- **Keywords Area**
- **variables**
- **negative_binomial_uncertain**

Aleatory uncertain discrete variable - negative binomial

**Topics**

This keyword is related to the topics:

- **discrete_variables**
- **aleatory_uncertain_variables**
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): INTEGER

Default: no negative binomial uncertain variables

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<tr>
<td>Optional</td>
<td>descriptors</td>
<td></td>
<td>Labels for the variables</td>
</tr>
</tbody>
</table>

Description

The density function for the negative binomial distribution is given by:

\[
f(x) = \binom{n + x - 1}{x} p^n (1 - p)^x
\]

where

- \( p \) is the probability of success per trial
- \( n \) is the number of successful trials
- \( X \) is the number of failures

Theory

The negative binomial distribution is typically used to predict the number of failures observed when repeating a test until a total of \( n \) successes have occurred, where each test has a probability \( p \) of success.

probability_per_trial

- Keywords Area
- variables
- negative_binomial_uncertain
- probability_per_trial

A negative binomial distribution parameter
6.4. VARIABLES

Specification

Alias: prob_per_trial

Argument(s): REALLIST

Description

The negative binomial distribution is typically used to predict the number of failures observed when repeating a test until a total of \( n \) successes have occurred, where each test has a probability \( p \) of success.

The density function for the negative binomial distribution is given by:

\[
f(x) = \binom{n + x - 1}{x} p^n (1 - p)^x
\]

where

- \( p \) is the probability of success per trial
- \( n \) is the number of successful trials
- \( X \) is the number of failures

num_trials

- Keywords Area
- variables
- negative_binomial_uncertain
- num_trials

A negative binomial distribution parameter

Specification

Alias: none

Argument(s): INTEGERLIST

Description

The negative binomial distribution is typically used to predict the number of failures observed when repeating a test until a total of \( n \) successes have occurred, where each test has a probability \( p \) of success.

The density function for the negative binomial distribution is given by:

\[
f(x) = \binom{n + x - 1}{x} p^n (1 - p)^x
\]

where

- \( p \) is the probability of success per trial
- \( n \) is the number of successful trials
- \( X \) is the number of failures
**Initial Point**

- **Keywords Area**
- **variables**
- **negative_binomial_uncertain**
- **initial_point**

Initial values

**Specification**

**Alias:** none  
**Argument(s):** INTEGERLIST

**Description**

The *initial_point* specifications provide the point in design space (variable values) from which an iterator is started. These default to the midpoint of bounds (continuous design variables) or the middle value (discrete design variables).

**Descriptors**

- **Keywords Area**
- **variables**
- **negative_binomial_uncertain**
- **descriptors**

Labels for the variables

**Specification**

**Alias:** none  
**Argument(s):** STRINGLIST  
**Default:** nbuv_{i}

**Description**

The optional variable labels specification *descriptors* is a list of strings which identify the variables. These are used in console and tabular output.

The default descriptor strings use a variable type-dependent root string plus a numeric identifier.

**6.4.23 geometric_uncertain**

- **Keywords Area**
- **variables**
- **geometric_uncertain**

Aleatory uncertain discrete variable - geometric
6.4. VARIABLES

Topics
This keyword is related to the topics:

- discrete_variables
- aleatory_uncertain_variables

Specification

Alias: none
Argument(s): INTEGER
Default: no geometric uncertain variables

| Required/- | Description of Group | Dakota Keyword | Dakota Keyword Description |
| Optional/Required | | probability_per_trial | Geometric distribution parameter |
| Optional | initial_point | | Initial values |
| Optional | descriptors | | Labels for the variables |

Description
The geometric distribution represents the number of successful trials that might occur before a failure is observed. The density function for the geometric distribution is given by:

\[ f(x) = p(1 - p)^x \]

where \( p \) is the probability of failure per trial.

probability_per_trial

- Keywords Area
- variables
- geometric_uncertain
- probability_per_trial

Geometric distribution parameter

Specification
Alias: prob_per_trial
Argument(s): REALLIST
Description
The geometric distribution represents the number of successful trials that occur before a failure is observed.

The density function for the geometric distribution is given by:

\[ f(x) = p(1 - p)^x \]

where \( p \) is the probability of failure per trial and \( x \) is the number of successful trials.

initial_point

- Keywords Area
- variables
- geometric_uncertain
- initial_point

Initial values

Specification

Alias: none

Argument(s): INTEGERLIST

Description

The initial_point specifications provide the point in design space (variable values) from which an iterator is started. These default to the midpoint of bounds (continuous design variables) or the middle value (discrete design variables).

descriptors

- Keywords Area
- variables
- geometric_uncertain
- descriptors

Labels for the variables

Specification

Alias: none

Argument(s): STRINGLIST

Default: geuv_{i}

Description

The optional variable labels specification descriptors is a list of strings which identify the variables. These are used in console and tabular output.

The default descriptor strings use a variable type-dependent root string plus a numeric identifier.
6.4. VARIABLES

6.4.24 hypergeometric_uncertain

- Keywords Area
- variables
- hypergeometric_uncertain

Aleatory uncertain discrete variable - hypergeometric

Topics

This keyword is related to the topics:

- discrete_variables
- aleatory_uncertain_variables

Specification

**Alias:** none
**Argument(s):** INTEGER
**Default:** no hypergeometric uncertain variables

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Description

The hypergeometric probability density is used when sampling without replacement from a total population of elements where

- The resulting element of each sample can be separated into one of two non-overlapping sets
- The probability of success changes with each sample.
The density function for the hypergeometric distribution is given by:

\[ f(x) = \binom{m}{x} \binom{N - m}{n - x} \binom{N}{n} \]

where:
- \( N \) is the total population
- \( m \) is the number of items in the selected population (e.g. the number of white balls in the full urn of \( N \) items)
- \( n \) is the size of the sample drawn (e.g. number of balls drawn)
- \( x \) is the number of sucess (e.g. drawing a white ball)
- \( \binom{n}{x} \) is a binomial coefficient

**Theory**

The hypergeometric is often described using an urn model. For example, say we have a total population containing \( N \) balls, and we know that \( m \) of the balls are white and the remaining balls are green. If we draw \( n \) balls from the urn without replacement, the hypergeometric distribution describes the probability of drawing \( x \) white balls.

**total_population**
- **Keywords Area**
- **variables**
- **hyergeometric_uncertain**
- **total_population**

Parameter for the hypergeometric probability distribution

**Specification**

**Alias:** none

**Argument(s):** INTEGERLIST

**Description**

The density function for the hypergeometric distribution is given by:

\[ f(x) = \binom{m}{x} \binom{N - m}{n - x} \binom{N}{n} \]

where
6.4. VARIABLES

- **N** is the total population (e.g. the total number of balls in the urn)
- **m** is the number of items in the selected population (e.g. the number of white balls in the full urn of N items)
- **n** is the size of the sample (e.g. number of balls drawn)
- **x** is the number of sucess (e.g. drawing a white ball)
- \( \binom{a}{b} \) is a binomial coefficient

**selected_population**

- **Keywords Area**
- **variables**
- **hypergeometric_uncertain**
- **selected_population**

Distribution parameter for the hypergeometric distribution

**Specification**

**Alias:** none

**Argument(s):** INTEGERLIST

**Description**

The density function for the hypergeometric distribution is given by:

\[
f(x) = \binom{m}{x} \binom{N-m}{n-x} \binom{N}{n}
\]

where

- **N** is the total population (e.g. the total number of balls in the urn)
- **m** is the number of items in the selected population (e.g. the number of white balls in the full urn of N items)
- **n** is the size of the sample (e.g. number of balls drawn)
- **x** is the number of sucess (e.g. drawing a white ball)
- \( \binom{a}{b} \) is a binomial coefficient
num_drawn
- Keywords Area
- variables
- hypergeometric_uncertain
- num_drawn

Distribution parameter for the hypergeometric distribution

**Specification**

Alias: none

**Argument(s):** INTEGERLIST

**Description**

The density function for the hypergeometric distribution is given by:

\[
f(x) = \binom{m}{x} \frac{\binom{N - m}{n - x}}{\binom{N}{n}}
\]

where

- \( N \) is the total population (e.g. the total number of balls in the urn)
- \( m \) is the number of items in the selected population (e.g. the number of white balls in the full urn of \( N \) items)
- \( n \) is the size of the sample (e.g. number of balls drawn)
- \( x \) is the number of sucess (e.g. drawing a white ball)
- \( \binom{a}{b} \) is a binomial coeffecient

**initial_point**

- Keywords Area
- variables
- hypergeometric_uncertain
- initial_point

Initial values

**Specification**

Alias: none

**Argument(s):** INTEGERLIST
6.4. VARIABLES

Description

The initial point specifications provide the point in design space (variable values) from which an iterator is started. These default to the midpoint of bounds (continuous design variables) or the middle value (discrete design variables).

descriptors

- Keywords Area
- variables
- hypergeometric_uncertain
- descriptors

Labels for the variables

Specification

Alias: none

Argument(s): STRINGLIST
Default: hguv_{i}

Description

The optional variable labels specification descriptors is a list of strings which identify the variables. These are used in console and tabular output.

The default descriptor strings use a variable type-dependent root string plus a numeric identifier.

6.4.25 histogram_point_uncertain

- Keywords Area
- variables
- histogram_point_uncertain

Aleatory uncertain variable - discrete histogram

Topics

This keyword is related to the topics:

- discrete_variables
- aleatory_uncertain_variables

Specification

Alias: none

Argument(s): none
Default: no histogram point uncertain variables
CHAPTER 6. KEYWORDS AREA

| Required/- | Description of | Dakota Keyword | Dakota Keyword |
| Optional Optional Group | **integer** | **Description** | **integer** |
| **Optional** | **string** | **Integer valued point histogram variable** | **string** |
| **Optional** | **real** | **String (categorical) valued point histogram variable** | **real** |

**Description**

Histogram uncertain variables are typically used to model a set of empirical data. When the variables take on only discrete values or categories, a discrete, or point histogram is used to describe their probability mass function (one could think of this as a histogram_bin_uncertain variable with "bins" of zero width). Dakota supports integer-, string-, and real-valued point histograms.

Point histograms are similar to discrete_design_set and discrete_state_set, but as they are uncertain variables, include the relative probabilities of observing the different values within the set.

The histogram_point_uncertain keyword is followed by one or more of integer, string, or real, each of which specify the number of variables to be characterized as discrete histograms of that sub-type.

Each discrete histogram variable is specified by one or more abscissa/count pairs. The abscissas, are the possible values the variable can take on ("x" coordinates of type integer, string, or real), and must be specified in increasing order. These are paired with counts which provide the frequency of the given value or string, relative to other possible values/strings.

Thus, to fully specify a point-based histogram with n points, n (x,c) pairs must be specified with the following features:

- x is the point value (integer, string, or real) and c is the corresponding count for that value.
- the x values must be strictly increasing (lexicographically for strings).
- all c values must be positive.
- a minimum of one pair must be specified for each point-based histogram.

**Examples**

The pairs_per_variable specification provides for the proper association of multiple sets of (x,c) or (x,y) pairs with individual histogram variables. For example, in the following specification,

```
histogram_point_uncertain
  integer = 2
  pairs_per_variable = 2 3
  abscissas = 3 4 100 200 300
  counts = 1 1 1 2 1
```

pairs_per_variable associates the (x,c) pairs {(3,1),(4,1)} with one point-based histogram variable (where the values 3 and 4 are equally probable) and associates the (x,c) pairs {{100,1},{200,2},{300,1}} with a second point-based histogram variable (where the value 200 is twice as probable as either 100 or 300).
6.4. VARIABLES

See Also
These keywords may also be of interest:

- histogram_bin_uncertain

FAQ
**Difference between bin and point histograms:** A (continuous) bin histogram specifies bins of non-zero width, whereas a (discrete) point histogram specifies individual point values, which can be thought of as bins with zero width. In the terminology of LHS[90], the bin pairs specification defines a "continuous linear" distribution and the point pairs specification defines a "discrete histogram" distribution (although the points are real-valued, the number of possible values is finite).

**integer**
- Keywords Area
- variables
- histogram_point_uncertain
- integer

Integer valued point histogram variable

Specification
**Alias:** none
**Argument(s):** INTEGER

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**Description**

This probability mass function is integer-valued; the abscissa values must all be integers. The \( n \) abscissa values are paired with \( n \) counts which indicate the relative frequency (mass) of each integer relative to the other specified integers.

**Examples**

```plaintext
histogram_point_uncertain
  integer = 2
  pairs_per_variable = 2 3
  abscissas = 3 4 100 200 300
  counts = 1 1 1 2 1
```

There are two variables, the first one has two possible integer values which are equally probable. The second one has three options, and 200 is twice as probable as either 100 or 300.

**pairs_per_variable**

- Keywords Area
- variables
- histogram_point_uncertain
- integer
- pairs_per_variable

Number of pairs defining each histogram point integer variable

**Specification**

Alias: \texttt{num_pairs}

Argument(s): INTEGERLIST

Default: equal distribution

**Description**

By default, the list of \texttt{abscissas} and \texttt{counts} will be evenly divided among the histogram point integer variables. The number of \texttt{pairs_per_variable} specifies the apportionment of abscissa/count pairs among the histogram point integer variables. It must specify one integer \( \geq 1 \) per variable that indicates how many of the \((\text{abscissa}, \text{count}) = (x,c)\) pairs to associate with that variable.
6.4. VARIABLES

abscissas
- Keywords Area
- variables
- histogram_point_uncertain
- integer
- abscissas

Integer abscissas for a point histogram

Specification
Alias: none
Argument(s): INTEGERLIST

Description
A list of integer abscissa ("x" coordinate) values characterizing the probability density function for each of the integer histogram_point_uncertain variables. These must be listed in increasing order for each variable, and are paired with counts. See histogram_point_uncertain for details and examples.

counts
- Keywords Area
- variables
- histogram_point_uncertain
- integer
- counts

Counts for integer-valued point histogram

Specification
Alias: none
Argument(s): REALLIST

Description
Count or frequency for each of abscissas. See histogram_point_uncertain for details and examples.
initial_point

- Keywords Area
- variables
- histogram_point_uncertain
- integer
- initial_point

Initial values

**Specification**

**Alias:** none  
**Argument(s):** INTEGERLIST

**Description**

The `initial_point` specifications provide the point in design space (variable values) from which an iterator is started. These default to the midpoint of bounds (continuous design variables) or the middle value (discrete design variables).

descriptors

- Keywords Area
- variables
- histogram_point_uncertain
- integer
- descriptors

Labels for the variables

**Specification**

**Alias:** none  
**Argument(s):** STRINGLIST  
**Default:** hpiv_{i}

**Description**

The optional variable labels specification `descriptors` is a list of strings which identify the variables. These are used in console and tabular output.

The default descriptor strings use a variable type-dependent root string plus a numeric identifier.
6.4. VARIABLES

string

- Keywords Area
- variables
- histogram_point_uncertain
- string

String (categorical) valued point histogram variable

Specification

Alias: none

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Description

This probability mass function is string-valued; the abscissa values must all be strings. The \( n \) abscissa values are paired with \( n \) counts which indicate the relative frequency (mass) of each string relative to the other specified strings.

Examples

```
histogram_point_uncertain
string = 2
pairs_per_variable = 2  3
abscissas = 'no' 'yes'  'function1' 'function2' 'function3'
counts = 1 1 1 2 1
descriptors = 'vote' 'which_function'
```

Here there are two variables, the first one ('vote') has two possible string values 'yes' and 'no' which are equally probable. The second one has three options for 'which_function', and 'function2' is twice as probable as 'function1' or 'function3'.
pairs_per_variable

- Keywords Area
- variables
- histogram_point_uncertain
- string
- pairs_per_variable

Number of pairs defining each histogram point string variable

**Specification**

**Alias:** num_pairs

**Argument(s):** INTEGERLIST

**Default:** equal distribution

**Description**

By default, the list of abscissas and counts will be evenly divided among the histogram point string variables. The number of `pairs_per_variable` specifies the apportionment of abscissa/count pairs among the histogram point string variables. It must specify one integer \( \geq 1 \) per variable that indicates how many of the \((\text{abscissa}, \text{count}) = (x, c)\) pairs to associate with that variable.

abscissas

- Keywords Area
- variables
- histogram_point_uncertain
- string
- abscissas

String abscissas for a point histogram

**Specification**

**Alias:** none

**Argument(s):** STRINGLIST

**Description**

A list of string abscissa ("x" coordinate) values characterizing the probability density function for each of the string `histogram_point_uncertain` variables. These must be listed in (lexicographically) increasing order for each variable, and are paired with `counts`. See `histogram_point_uncertain` for details and examples.
counts

- Keywords Area
- variables
- histogram_point_uncertain
- string
- counts

Counts for string-valued point histogram

**Specification**

**Alias:** none

**Argument(s):** REALLIST

**Description**

Count or frequency for each of abscissas. See histogram_point_uncertain for details and examples.

**initial_point**

- Keywords Area
- variables
- histogram_point_uncertain
- string
- initial_point

Initial values

**Specification**

**Alias:** none

**Argument(s):** STRINGLIST

**Description**

The initial_point specifications provide the point in design space (variable values) from which an iterator is started. These default to the midpoint of bounds (continuous design variables) or the middle value (discrete design variables).
descriptors

- Keywords Area
- variables
- histogram_point_uncertain
- string
- descriptors

Labels for the variables

**Specification**

**Alias:** none

**Argument(s):** STRINGLIST

**Default:** hpsv_{i}

**Description**

The optional variable labels specification `descriptors` is a list of strings which identify the variables. These are used in console and tabular output.

The default descriptor strings use a variable type-dependent root string plus a numeric identifier.

**real**

- Keywords Area
- variables
- histogram_point_uncertain
- real

Real valued point histogram variable

**Specification**

**Alias:** none

**Argument(s):** INTEGER

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<td>descriptors</td>
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</table>

**Description**

This probability mass function is real-valued; the abscissa values must all be integers. The \( n \) abscissa values are paired with \( n \) counts which indicate the relative frequency (mass) of each real relative to the other specified reals.

**Examples**

```plaintext
histogram_point_uncertain
real = 2
pairs_per_variable = 2 3
abscissas = 3.1415 4.5389 100 200.112345 300
counts = 1 1 1 2 1
```

There are two variables, the first one has two possible real values which are equally probable. The second one has three possible real value options, and 200.112345 is twice as probable as either 100 or 300.

**pairs_per_variable**

- Keywords: Area
- variables
- histogram_point_uncertain
- real
- pairs_per_variable

Number of pairs defining each histogram point real variable

**Specification**

Alias: num_pairs

Argument(s): INTEGERLIST

Default: equal distribution
Description

By default, the list of abscissas and counts will be evenly divided among the histogram point real variables. The number of pairs_per_variable specifies the apportionment of abscissa/count pairs among the histogram point real variables. It must specify one integer >=1 per variable that indicates how many of the (abscissa, count) = (x,c) pairs to associate with that variable.

abscissas

- Keywords Area
- variables
- histogram_point_uncertain
- real
- abscissas

Real abscissas for a point histogram

Specification

Alias: none

Argument(s): REALLIST

Description

A list of real abscissa ("x" coordinate) values characterizing the probability density function for each of the real histogram_point_uncertain variables. These must be listed in increasing order for each variable, and are paired with counts. See histogram_point_uncertain for details and examples.

counts

- Keywords Area
- variables
- histogram_point_uncertain
- real
- counts

Counts for real-valued point histogram

Specification

Alias: none

Argument(s): REALLIST

Description

Count or frequency for each of abscissas. See histogram_point_uncertain for details and examples.
6.4. VARIABLES

initial_point
- Keywords Area
- variables
- histogram_point_uncertain
- real
- initial_point

Initial values

Specification
Alias: none
Argument(s): REALLIST

Description
The initial_point specifications provide the point in design space (variable values) from which an iterator is started. These default to the midpoint of bounds (continuous design variables) or the middle value (discrete design variables).

descriptors
- Keywords Area
- variables
- histogram_point_uncertain
- real
- descriptors

Labels for the variables

Specification
Alias: none
Argument(s): STRINGLIST
Default: hpruv.{i}

Description
The optional variable labels specification descriptors is a list of strings which identify the variables. These are used in console and tabular output.

The default descriptor strings use a variable type-dependent root string plus a numeric identifier.
6.4.26 uncertain_correlation_matrix

- Keywords Area
- variables
- uncertain_correlation_matrix

Correlation among aleatory uncertain variables

**Specification**

**Alias:** none

**Argument(s):** REALLIST

**Default:** identity matrix (uncorrelated)

**Description**

Aleatory uncertain variables may have correlations specified through use of an uncertain_correlation_matrix specification. This specification is generalized in the sense that its specific meaning depends on the nondeterministic method in use.

When the method is a nondeterministic sampling method (i.e., sampling), then the correlation matrix specifies rank correlations [52].

When the method is a reliability (i.e., local_reliability or global_reliability) or stochastic expansion (i.e., polynomial_chaos or stoch_collocation) method, then the correlation matrix specifies correlation coefficients (normalized covariance)[42].

In either of these cases, specifying the identity matrix results in uncorrelated uncertain variables (the default). The matrix input should be symmetric and have all \( n^2 \) entries where \( n \) is the total number of aleatory uncertain variables.

Ordering of the aleatory uncertain variables is:

1. normal
2. lognormal
3. uniform
4. loguniform
5. triangular
6. exponential
7. beta
8. gamma
9. gumbel
10. frechet
11. weibull
12. histogram bin
13. poisson
6.4. VARIABLES

14. binomial
15. negative binomial
16. geometric
17. hypergeometric
18. histogram point

When additional variable types are activated, they assume uniform distributions, and the ordering is as listed on variables.

Examples

Consider the following random variables, distributions and correlations:

- $X_1$, normal, uncorrelated with others
- $X_2$, normal, correlated with $X_3$, $X_4$ and $X_5$
- $X_3$, weibull, correlated with $X_5$
- $X_4$, exponential, correlated with $X_3$, $X_4$ and $X_5$
- $X_5$, normal, correlated with $X_5$

These correlations are captured by the following commands (order of the variables is respected).

```
uncertain_correlation_matrix
# ordering normal, exponential, weibull
# $X_1$ $X_2$ $X_5$ $X_4$ $X_3$
1.00 0.00 0.00 0.00 0.00
0.00 1.00 0.50 0.24 0.78
0.00 0.50 1.00 0.00 0.20
0.00 0.24 0.00 1.00 0.49
0.00 0.78 0.20 0.49 1.0
```

6.4.27 continuous_interval_uncertain

- **Keywords** Area
- **variables**
- **continuous_interval_uncertain**

Epistemic uncertain variable - values from one or more continuous intervals

Topics

This keyword is related to the topics:

- **continuous_variables**
- **epistemic_uncertain_variables**

Specification

**Alias:** interval_uncertain

**Argument(s):** INTEGER

**Default:** no continuous interval uncertain variables
CHAPTER 6. KEYWORDS AREA

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<td>num_intervals</td>
<td></td>
<td>Specify the number of intervals for each variable</td>
</tr>
<tr>
<td>Optional</td>
<td>interval_probabilities</td>
<td></td>
<td>Assign probability mass to each interval</td>
</tr>
<tr>
<td>Required</td>
<td>lower_bounds</td>
<td></td>
<td>Specify minimum values</td>
</tr>
<tr>
<td>Required</td>
<td>upper_bounds</td>
<td></td>
<td>Specify maximum values</td>
</tr>
<tr>
<td>Optional</td>
<td>initial_point</td>
<td></td>
<td>Initial values</td>
</tr>
<tr>
<td>Optional</td>
<td>descriptors</td>
<td></td>
<td>Labels for the variables</td>
</tr>
</tbody>
</table>

**Description**

Continuous interval uncertain variables are epistemic types. They can specify a single interval per variable which may be used in interval analysis, where the goal is to determine the interval bounds on the output corresponding to the interval bounds on the input. All values between the bounds are permissible. More detailed continuous interval representations can specify a set of belief structures based on intervals that may be contiguous, overlapping, or disjoint. This is used in specifying the inputs necessary for an epistemic uncertainty analysis using Dempster-Shafer theory of evidence.

Other epistemic types include:

- discrete_interval_uncertain
- discrete_uncertain_set integer
- discrete_uncertain_set string
- discrete_uncertain_set real

**Examples**

The following specification is for an interval analysis:

```plaintext
continuous_interval_uncertain = 2
lower_bounds = 2.0 4.0
upper_bounds = 2.5 5.0
```

The following specification is for a Dempster-Shafer analysis:

```plaintext
continuous_interval_uncertain = 2
num_intervals = 3 2
interval_probs = 0.25 0.5 0.25 0.4 0.6
lower_bounds = 2.0 4.0 4.5 1.0 3.0
upper_bounds = 2.5 5.0 6.0 5.0 5.0
```

Here there are 2 interval uncertain variables. The first one is defined by three intervals, and the second by two intervals. The three intervals for the first variable have basic probability assignments of 0.2, 0.5, and 0.3, respectively, while the basic probability assignments for the two intervals for the second variable are 0.4 and 0.6.
6.4. VARIABLES

The basic probability assignments for each interval variable must sum to one. The interval bounds for the first variable are [2, 2.5], [4, 5], and [4.5, 6], and the interval bounds for the second variable are [1.0, 5.0] and [3.0, 5.0]. Note that the intervals can be overlapping or disjoint. The BPA for the first variable indicates that it is twice as likely that the value occurs on the interval [4,5] than either [2,2.5] or [4.5,6].

Theory

The continuous interval uncertain variable is NOT a probability distribution. Although it may seem similar to a histogram, the interpretation of this uncertain variable is different. It is used in epistemic uncertainty analysis, where one is trying to model uncertainty due to lack of knowledge. The continuous interval uncertain variable is used in both interval analysis and in Dempster-Shafer theory of evidence.

- **interval analysis** - only one interval is allowed for each `continuous_interval_uncertain` variable - the interval is defined by lower and upper bounds - the value of the random variable lies somewhere in this interval - output is the minimum and maximum function value conditional on the specified interval

- **Dempster-Shafer theory of evidence** - multiple intervals can be assigned to each `continuous_interval_uncertain` variable - a Basic Probability Assignment (BPA) is associated with each interval. The BPA represents a probability that the value of the uncertain variable is located within that interval. - each interval is defined by lower and upper bounds - outputs are called "belief" and "plausibility." Belief represents the smallest possible probability that is consistent with the evidence, while plausibility represents the largest possible probability that is consistent with the evidence. Evidence is the intervals together with their BPA.

`num_intervals`

- **Keywords** Area
- **variables**
- **continuous_interval_uncertain**
- **num_intervals**

Specify the number of intervals for each variable

Specification

**Alias:** `iuv_num_intervals`

**Argument(s):** INTEGERLIST

**Default:** Equal apportionment of intervals among variables

Description

In Dakota, epistemic uncertainty analysis is performed using either interval estimation or Dempster-Shafer theory of evidence. In these approaches, one does not assign a probability distribution to each uncertain input variable. Rather, one divides each uncertain input variable into one or more intervals. The input parameters are only known to occur within intervals; nothing more is assumed. `num_intervals` specifies the number of such intervals associated with each interval uncertain parameter.
interval_probabilities

- Keywords Area
- variables
- continuous_interval_uncertain
- interval_probabilities

Assign probability mass to each interval

**Specification**

Alias: interval.probs iuv_interval.probs

Argument(s): REALLIST

**Default:** Equal probability assignments for each interval (1/num_intervals[i])

**Description**

The basic probability assignments for each interval variable must sum to one. For example, if an interval variable is defined with three intervals, the probabilities for these intervals could be 0.2, 0.5, and 0.3 which sum to one, but could not be 0.5,0.5, and 0.5 which do not sum to one.

lower_bounds

- Keywords Area
- variables
- continuous_interval_uncertain
- lower_bounds

Specify minimum values

**Specification**

Alias: none

Argument(s): REALLIST

**Description**

Specify minimum values

upper_bounds

- Keywords Area
- variables
- continuous_interval_uncertain
- upper_bounds

Specify maximum values
6.4. VARIABLES

Specification

Alias: none
Argument(s): REALLIST

Description

Specify maximum values

initial_point

- Keywords Area
- variables
- continuous_interval_uncertain
- initial_point

Initial values

Specification

Alias: none
Argument(s): REALLIST

Description

The initial_point specifications provide the point in design space (variable values) from which an iterator is started. These default to the midpoint of bounds (continuous design variables) or the middle value (discrete design variables).

descriptors

- Keywords Area
- variables
- continuous_interval_uncertain
- descriptors

Labels for the variables

Specification

Alias: iuv_descriptors
Argument(s): STRINGLIST
Default: ciuv_{i}
Description

The optional variable labels specification descriptors is a list of strings which identify the variables. These are used in console and tabular output. The default descriptor strings use a variable type-dependent root string plus a numeric identifier.

6.4.28  discrete_interval_uncertain

- Keywords Area
- variables
- discrete_interval_uncertain

Epistemic uncertain variable - values from one or more discrete intervals

Topics

This keyword is related to the topics:

- discrete_variables
- epistemic_uncertain_variables

Specification

Alias: discrete_uncertain_range

Argument(s): INTEGER

Default: No discrete interval uncertain variables

<table>
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<tr>
<th>Required/-</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<td>Specify the number of intervals for each variable</td>
</tr>
<tr>
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<td>interval_probs</td>
<td>probabilities</td>
<td>Assign probability mass to each interval</td>
</tr>
<tr>
<td>Required</td>
<td>lower_bounds</td>
<td></td>
<td>Specify minimum values</td>
</tr>
<tr>
<td>Required</td>
<td>upper_bounds</td>
<td></td>
<td>Specify maximum values</td>
</tr>
<tr>
<td>Optional</td>
<td>initial_point</td>
<td></td>
<td>Initial values</td>
</tr>
<tr>
<td>Optional</td>
<td>descriptors</td>
<td></td>
<td>Labels for the variables</td>
</tr>
</tbody>
</table>

Description

Discrete interval uncertain variables are epistemic types. They can specify a single interval per variable which may be used in interval analysis, where the goal is to determine the interval bounds on the output corresponding to the interval bounds on the input. Permissible values are any integer within the bound. More detailed continuous
6.4. VARIABLES

interval representations can specify a set of belief structures based on intervals that may be contiguous, overlapping, or disjoint. This is used in specifying the inputs necessary for an epistemic uncertainty analysis using Dempster-Shafer theory of evidence.

Other epistemic types include:

- continuous_interval_uncertain
- discrete_uncertain_set integer
- discrete_uncertain_set string
- discrete_uncertain_set real

Examples

Let d1 be 2, 3 or 4 with probability 0.2, 4 or 5 with probability 0.5 and 6 with probability 0.3. Let d2 be 4, 5 or 6 with probability 0.4 and 6, 7 or 8 with probability 0.6. The following specification is for a Dempster-Shafer analysis:

discrete_interval_uncertain = 2  
num_intervals = 3 2  
interval_probs = 0.2 0.5 0.3 0.4 0.6  
lower_bounds = 2 4 6 4 6  
upper_bounds = 4 5 6 6 8

Theory

- Dempster-Shafer theory of evidence - multiple intervals can be assigned to each discrete_interval_uncertain variable - a Basic Probability Assignment (BPA) is associated with each interval. The BPA represents a probability that the value of the uncertain variable is located within that interval. Each interval is defined by lower and upper bounds - outputs are called "belief" and "plausibility." Belief represents the smallest possible probability that is consistent with the evidence, while plausibility represents the largest possible probability that is consistent with the evidence. Evidence is the intervals together with their BPA.

num_intervals

- Keywords Area
- variables
- discrete_interval_uncertain
- num_intervals

Specify the number of intervals for each variable

Specification

Alias: none

Argument(s): INTEGERLIST

Default: Equal apportionment of intervals among variables
Description

In Dakota, epistemic uncertainty analysis is performed using either interval estimation or Dempster-Shafer theory of evidence. In these approaches, one does not assign a probability distribution to each uncertain input variable. Rather, one divides each uncertain input variable into one or more intervals. The input parameters are only known to occur within intervals; nothing more is assumed. `num_intervals` specifies the number of such intervals associated with each interval uncertain parameter.

`interval_probabilities`

- `Keywords Area`
- `variables`
- `discrete_interval_uncertain`
- `interval_probabilities`

Assign probability mass to each interval

Specification

Alias: `interval_probs` `range_probabilities` `range_probs`  
Argument(s): `REALLIST`  
Default: Equal probability assignments for each interval (1/num_intervals[i])

Description

The basic probability assignments for each interval variable must sum to one. For example, if an interval variable is defined with three intervals, the probabilities for these intervals could be 0.2, 0.5, and 0.3 which sum to one, but could not be 0.5,0.5, and 0.5 which do not sum to one.

`lower_bounds`

- `Keywords Area`
- `variables`
- `discrete_interval_uncertain`
- `lower_bounds`

Specify minimum values

Specification

Alias: `none`  
Argument(s): `INTEGERLIST`  
Default: Equal probability assignments for each interval (1/num_intervals[i])

Description

Specify minimum values
6.4. VARIABLES

**upper_bounds**
- Keywords Area
- variables
- discrete_interval_uncertain
- upper_bounds

Specify maximum values

**Specification**

**Alias:** none
**Argument(s):** INTEGERLIST

**Description**
Specify maximum values

**initial_point**
- Keywords Area
- variables
- discrete_interval_uncertain
- initial_point

Initial values

**Specification**

**Alias:** none
**Argument(s):** INTEGERLIST

**Description**
The *initial_point* specifications provide the point in design space (variable values) from which an iterator is started. These default to the midpoint of bounds (continuous design variables) or the middle value (discrete design variables).

**descriptors**
- Keywords Area
- variables
- discrete_interval_uncertain
- descriptors

Labels for the variables
CHAPTER 6. KEYWORDS AREA

Specification
Alias: none
Argument(s): STRINGLIST
Default: diuv_{i}

Description
The optional variable labels specification descriptors is a list of strings which identify the variables. These are used in console and tabular output.

The default descriptor strings use a variable type-dependent root string plus a numeric identifier.

6.4.29 discrete_uncertain_set

- Keywords Area
- variables
- discrete_uncertain_set

Epistemic uncertain variable - discrete set-valued

Topics
This keyword is related to the topics:
- discrete_variables
- epistemic_uncertain_variables

Specification
Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<tr>
<td>Optional</td>
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<td>integer</td>
<td>Discrete, epistemic uncertain variable - integers within a set</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>string</td>
<td>Discrete, epistemic uncertain variable - strings within a set</td>
</tr>
</tbody>
</table>
6.4. VARIABLES

| Optional | real | Discrete, epistemic uncertain variable - real numbers within a set |

**Description**

Discrete uncertain variables whose values come from a set of admissible elements. Each variable specified must be of type integer, string, or real.

**integer**

- Keywords Area
- variables
- discrete_uncertain_set
- integer

Discrete, epistemic uncertain variable - integers within a set

**Topics**

This keyword is related to the topics:

- discrete_variables
- epistemic_uncertain_variables

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** no discrete uncertain set integer variables

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
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<td>elements_per_variable</td>
</tr>
<tr>
<td>Required</td>
<td>elements</td>
<td></td>
</tr>
</tbody>
</table>

The permissible values for each discrete variable
CHAPTER 6. KEYWORDS AREA

<table>
<thead>
<tr>
<th>Optional</th>
<th>set_probabilities</th>
<th>This keyword defines the probabilities for the various elements of discrete sets. Whether the set-valued variables are categorical or relaxable</th>
</tr>
</thead>
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<tr>
<td>Optional</td>
<td>categorical</td>
<td>Whether the set-valued variables are categorical or relaxable.</td>
</tr>
<tr>
<td>Optional</td>
<td>initial_point</td>
<td>Initial values</td>
</tr>
<tr>
<td>Optional</td>
<td>descriptors</td>
<td>Labels for the variables</td>
</tr>
</tbody>
</table>

Description

Discrete set variables may be used to specify categorical choices which are epistemic. For example, if we have three possible forms for a physics model (model 1, 2, or 3) and there is epistemic uncertainty about which one is correct, a discrete uncertain set may be used to represent this type of uncertainty.

This variable is defined by a set of integers, in which the discrete value may take any value within the integer set (for example, the set may be defined as 1, 2, and 4).

Other epistemic types include:

- continuous_interval_uncertain
- discrete_interval_uncertain
- discrete_uncertain_set string
- discrete_uncertain_set real

Examples

Let d1 be 2 or 13 and d2 be 4, 5 or 26. The following specification is for an interval analysis:

```plaintext
discrete_uncertain_set
   integer
   num_set_values 2 3
   set_values   2 13 4 5 26
   descriptors 'di1' 'di2'
```

Theory

The `discrete_uncertain_set` variable is NOT a discrete random variable. It can be contrasted to a the histogram-defined random variables: `histogram_bin_uncertain` and `histogram_point_uncertain`. It is used in epistemic uncertainty analysis, where one is trying to model uncertainty due to lack of knowledge.

The discrete uncertain set integer variable is used in both interval analysis and in Dempster-Shafer theory of evidence.
6.4. VARIABLES

- interval analysis -the values are integers, equally weighted -the true value of the random variable is one of the integers in this set -output is the minimum and maximum function value conditional on the specified inputs

- Dempster-Shafer theory of evidence -the values are integers, but they can be assigned different weights -outputs are called "belief" and "plausibility." Belief represents the smallest possible probability that is consistent with the evidence, while plausibility represents the largest possible probability that is consistent with the evidence. Evidence is the values together with their weights.

elements_per_variable

- Keywords Area
- variables
- discrete_uncertain_set
- integer
- elements_per_variable

Number of admissible elements for each set variable

Specification

Alias: num_set_values

Argument(s): INTEGERLIST

Default: equal distribution

Description

Discrete set variables (including design, uncertain, and state) take on only a fixed set of values. For each type (integer, string, or real), this keyword specifies how many admissible values are provided for each variable. If not specified, equal apportionment of elements among variables is assumed, and the number of elements must be evenly divisible by the number of variables.

elements

- Keywords Area
- variables
- discrete_uncertain_set
- integer
- elements

The permissible values for each discrete variable

Specification

Alias: set_values

Argument(s): INTEGERLIST
**Description**

Specify the permissible values for discrete set variables (of type integer, string, or real). See the description on the discrete_variables page.

**set_probabilities**

- Keywords Area
- variables
- discrete_uncertain_set
- integer
- set_probabilities

This keyword defines the probabilities for the various elements of discrete sets.

**Specification**

**Alias:** set_probs

**Argument(s):** REALLIST

**Default:** Equal probability assignments for each set member (1/num_set_values[i])

**Description**

There are three types of discrete_uncertain_set variables: integer, string, or real sets. With each of these types, one defines the number of elements of the set per that variable, the values of those elements, and the associated probabilities. For example, if one has an integer discrete uncertain set variable with 3 elements {3,4,8}, then one could define the probabilities associated with those set elements as (for example) 0.2, 0.5, and 0.3. The set_probabilities for a particular variable should sum to one over all the elements in that set.

**categorical**

- Keywords Area
- variables
- discrete_uncertain_set
- integer
- categorical

Whether the set-valued variables are categorical or relaxable

**Specification**

**Alias:** none

**Argument(s):** STRINGLIST
6.4. VARIABLES

Description
A list of strings of length equal to the number of set (integer, string, or real) variables indicating whether they are strictly categorical, meaning may only take on values from the provided set, or relaxable, meaning may take on any integer or real value between the lowest and highest specified element. Valid categorical strings include 'yes', 'no', 'true', and 'false', or any abbreviation in [yYnNtTfF].

Examples
Discrete design set variable, 'rotor_blades', can take on only integer values, 2, 4, or 7 by default. Since categorical is specified to be false, the integrality can be relaxed and 'rotor_blades' can take on any value between 2 and 7, e.g., 3, 6, or 5.5.

```
discrete_design_set
  integer 1
    elements 2 4 7
  descriptor 'rotor_blades'
  categorical 'no'
```

initial_point
- Keywords Area
- variables
- discrete_uncertain_set
- integer
- initial_point

Initial values

Specification
Alias: none
Argument(s): INTEGERLIST

Description
The initial_point specifications provide the point in design space (variable values) from which an iterator is started. These default to the midpoint of bounds (continuous design variables) or the middle value (discrete design variables).

descriptors
- Keywords Area
- variables
- discrete_uncertain_set
- integer
- descriptors

Labels for the variables
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): STRINGLIST
Default: dusiv_{i}

Description

The optional variable labels specification descriptors is a list of strings which identify the variables. These are used in console and tabular output.

The default descriptor strings use a variable type-dependent root string plus a numeric identifier.

string

- Keywords Area
- variables
- discrete_uncertain_set
- string

Discrete, epistemic uncertain variable - strings within a set

Topics

This keyword is related to the topics:

- discrete_variables
- epistemic_uncertain_variables

Specification

Alias: none

Argument(s): INTEGER
Default: no discrete uncertain set string variables

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword elements_per_variable</th>
<th>Dakota Keyword Description</th>
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<td>Optional</td>
<td></td>
<td>Number of admissible elements for each set variable</td>
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</tbody>
</table>
6.4. VARIABLES

<table>
<thead>
<tr>
<th>Required</th>
<th>elements</th>
<th>The permissible values for each discrete variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>set_probabilities</td>
<td>This keyword defines the probabilities for the various elements of discrete sets. Initial values</td>
</tr>
<tr>
<td>Optional</td>
<td>initial_point</td>
<td>Initial values</td>
</tr>
<tr>
<td>Optional</td>
<td>descriptors</td>
<td>Labels for the variables</td>
</tr>
</tbody>
</table>

**Description**

Discrete set variables may be used to specify categorical choices which are epistemic. For example, if we have three possible forms for a physics model (model 1, 2, or 3) and there is epistemic uncertainty about which one is correct, a discrete uncertain set may be used to represent this type of uncertainty.

This variable is defined by a set of strings, in which the discrete value may take any value within the string set (for example, the set may be defined as 'coarse', 'medium', and 'fine')

Other epistemic types include:

- continuous_interval_uncertain
- discrete_interval_uncertain
- discrete_uncertain_set integer
- discrete_uncertain_set real

**Examples**

discrete_uncertain_set

```
string
num_set_values 2 3
set_values 'red' 'blue' 'coarse' 'medium' 'fine'
descriptors 'ds1' 'ds2'
```

**elements_per_variable**

- Keywords Area
- variables
- discrete_uncertain_set
- string
- elements_per_variable

Number of admissible elements for each set variable
CHAPTER 6. KEYWORDS AREA

Specification

Alias: num_set_values
Argument(s): INTEGERLIST
Default: equal distribution

Description

Discrete set variables (including design, uncertain, and state) take on only a fixed set of values. For each type (integer, string, or real), this keyword specifies how many admissible values are provided for each variable. If not specified, equal apportionment of elements among variables is assumed, and the number of elements must be evenly divisible by the number of variables.

elements

- Keywords Area
- variables
- discrete_uncertain_set
- string
- elements

The permissible values for each discrete variable

Specification

Alias: set_values
Argument(s): STRINGLIST

Description

Specify the permissible values for discrete set variables (of type integer, string, or real). See the description on the discrete_variables page.

set_probabilities

- Keywords Area
- variables
- discrete_uncertain_set
- string
- set_probabilities

This keyword defines the probabilities for the various elements of discrete sets.
6.4. VARIABLES

Specification

Alias: set_probs
Argument(s): REALLIST
Default: Equal probability assignments for each set member (1/num_set_values[i])

Description

There are three types of discrete_uncertain_set variables: integer, string, or real sets. With each of these types, one defines the number of elements of the set per that variable, the values of those elements, and the associated probabilities. For example, if one has an integer discrete uncertain set variable with 3 elements \{3,4,8\}, then one could define the probabilities associated with those set elements as (for example) 0.2, 0.5, and 0.3. The set_probabilities for a particular variable should sum to one over all the elements in that set.

initial_point

- Keywords Area
- variables
- discrete_uncertain_set
- string
- initial_point

Initial values

Specification

Alias: none
Argument(s): STRINGLIST

Description

The initial_point specifications provide the point in design space (variable values) from which an iterator is started. These default to the midpoint of bounds (continuous design variables) or the middle value (discrete design variables).

descriptors

- Keywords Area
- variables
- discrete_uncertain_set
- string
- descriptors

Labels for the variables
**Specification**

*Alias:* none

*Argument(s):* STRINGLIST

*Default:* `dussv_{i}`

**Description**

The optional variable labels specification *descriptors* is a list of strings which identify the variables. These are used in console and tabular output.

The default descriptor strings use a variable type-dependent root string plus a numeric identifier.

- **real**
  - Keywords Area
  - variables
  - discrete_uncertain_set
  - real

Discrete, epistemic uncertain variable - real numbers within a set

**Topics**

This keyword is related to the topics:

- discrete_variables
- epistemic_uncertain_variables

**Specification**

*Alias:* none

*Argument(s):* INTEGER

*Default:* no discrete uncertain set real variables

<table>
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<tr>
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<th>Description of</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword</th>
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<td>Group</td>
<td>elements_per_-variable</td>
<td>Description</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td></td>
<td>Number of admissible elements for each set variable</td>
</tr>
</tbody>
</table>
Description
Discrete set variables may be used to specify categorical choices which are epistemic. For example, if we have three possible forms for a physics model (model 1, 2, or 3) and there is epistemic uncertainty about which one is correct, a discrete uncertain set may be used to represent this type of uncertainty.

This variable is defined by a set of reals, in which the discrete variable may take any value defined within the real set (for example, a parameter may have two allowable real values, 3.285 or 4.79).

Other epistemic types include:
- continuous_interval_uncertain
- discrete_interval_uncertain
- discrete_uncertain_set integer
- discrete_uncertain_set string

Examples
Let d1 be 2.1 or 1.3 and d2 be 0.4, 5 or 2.6. The following specification is for an interval analysis:

```plaintext
discrete_uncertain_set
  integer
  num_set_values 2 3
  set_values 2.1 1.3 0.4 5 2.6
  descriptors 'd1' 'd2'
```

Theory
The `discrete_uncertain_set-integer` variable is NOT a discrete random variable. It can be contrasted to a the histogram-defined random variables: `histogram_bin_uncertain` and `histogram_point_uncertain`. It is used in epistemic uncertainty analysis, where one is trying to model uncertainty due to lack of knowledge.
The discrete uncertain set integer variable is used in both interval analysis and in Dempster-Shafer theory of evidence.

- Interval analysis - the values are integers, equally weighted - the true value of the random variable is one of the integers in this set - output is the minimum and maximum function value conditional on the specified inputs.

- Dempster-Shafer theory of evidence - the values are integers, but they can be assigned different weights - outputs are called "belief" and "plausibility." Belief represents the smallest possible probability that is consistent with the evidence, while plausibility represents the largest possible probability that is consistent with the evidence. Evidence is the values together with their weights.

**elements_per_variable**

- Keywords Area
- variables
- discrete_uncertain_set
- real
- elements_per_variable

Number of admissible elements for each set variable

**Specification**

Alias: num_set_values

**Argument(s):** INTEGERLIST

**Default:** equal distribution

**Description**

Discrete set variables (including design, uncertain, and state) take on only a fixed set of values. For each type (integer, string, or real), this keyword specifies how many admissible values are provided for each variable. If not specified, equal apportionment of elements among variables is assumed, and the number of elements must be evenly divisible by the number of variables.

**elements**

- Keywords Area
- variables
- discrete_uncertain_set
- real
- elements

The permissible values for each discrete variable
6.4. VARIABLES

Specification

Alias: set_values
  Argument(s): REALLIST

Description

Specify the permissible values for discrete set variables (of type integer, string, or real). See the description on the discrete_variables page.

set_probabilities

- Keywords Area
- variables
- discrete_uncertain_set
- real
- set_probabilities

This keyword defines the probabilities for the various elements of discrete sets.

Specification

Alias: set_probs
  Argument(s): REALLIST
  Default: Equal probability assignments for each set member (1/num_set_values[i])

Description

There are three types of discrete_uncertain_set variables: integer, string, or real sets. With each of these types, one defines the number of elements of the set per that variable, the values of those elements, and the associated probabilities. For example, if one has an integer discrete uncertain set variable with 3 elements \{3,4,8\}, then one could define the probabilities associated with those set elements as (for example) 0.2, 0.5, and 0.3. The set_probabilities for a particular variable should sum to one over all the elements in that set.

categorical

- Keywords Area
- variables
- discrete_uncertain_set
- real
- categorical

Whether the set-valued variables are categorical or relaxable
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): STRINGLIST

Description

A list of strings of length equal to the number of set (integer, string, or real) variables indicating whether they are strictly categorical, meaning may only take on values from the provided set, or relaxable, meaning may take on any integer or real value between the lowest and highest specified element. Valid categorical strings include 'yes', 'no', 'true', and 'false', or any abbreviation in [yYnNtTfF][.]*

Examples

Discrete design set variable, 'rotor_blades', can take on only integer values, 2, 4, or 7 by default. Since categorical is specified to be false, the integrality can be relaxed and 'rotor_blades' can take on any value between 2 and 7, e.g., 3, 6, or 5.5.

discrete_design_set
  integer 1
  elements 2 4 7
  descriptor 'rotor_blades'
  categorical 'no'

initial_point

- Keywords Area
- variables
- discrete_uncertain_set
- real
- initial_point

Initial values

Specification

Alias: none

Argument(s): REALLIST

Description

The initial_point specifications provide the point in design space (variable values) from which an iterator is started. These default to the midpoint of bounds (continuous design variables) or the middle value (discrete design variables).
6.4. VARIABLES

descriptors

- Keywords Area
- variables
- discrete_uncertain_set
- real
- descriptors

Labels for the variables

Specification

Alias: none
Argument(s): STRINGLIST
Default: dusrv_{i}

Description

The optional variable labels specification descriptors is a list of strings which identify the variables. These are used in console and tabular output.

The default descriptor strings use a variable type-dependent root string plus a numeric identifier.

6.4.30 continuous_state

- Keywords Area
- variables
- continuous_state

State variable - continuous

Topics

This keyword is related to the topics:

- state_variables
- continuous_variables

Specification

Alias: none
Argument(s): INTEGER
Default: No continuous state variables
### Description

Continuous state variables are defined by bounds.

Default behavior for most methods is that only the initial_state values are used. See the state_variables page for details on the behavior of state variables.

**initial_state**

- Keywords Area
- variables
- continuous_state
- initial_state

Initial values for the state variables

### Specification

**Alias:** csv_initial_state

**Argument(s):** REALLIST

**Default:** 0.0

### Description

The initial_state specifications provide the initial values for the state variables.

This is an optional keyword. If it is not specified, the initial state will be inferred from the other keywords that define the state variable.

Defaults are:

- Continuous state variables - use the midpoint of the bounds

- Set variables - use the value with the index closest to the middle of the set

- Range variables - use the midpoint of the range
6.4. VARIABLES

lower_bounds
- Keywords Area
- variables
- continuous_state
- lower_bounds

Specify minimum values

Specification
Alias: csv_lower_bounds
Argument(s): REALLIST
Default: -infinity

Description
Specify minimum values

upper_bounds
- Keywords Area
- variables
- continuous_state
- upper_bounds

Specify maximum values

Specification
Alias: csv_upper_bounds
Argument(s): REALLIST
Default: infinity

Description
Specify maximum values

descriptors
- Keywords Area
- variables
- continuous_state
- descriptors

Labels for the variables
CHAPTER 6. KEYWORDS AREA

Specification

Alias: csv_descriptors
  Argument(s): STRINGLIST
  Default: csv_{1}

Description

The optional variable labels specification descriptors is a list of strings which identify the variables. These are used in console and tabular output.

The default descriptor strings use a variable type-dependent root string plus a numeric identifier.

6.4.31 discrete_state_range

- Keywords Area
- variables
- discrete_state_range

State variables - discrete range-valued

Topics

This keyword is related to the topics:

- discrete_variables
- state_variables

Specification

Alias: none
  Argument(s): INTEGER
  Default: No discrete state variables

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
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<tr>
<td>Optional</td>
<td>initial_state</td>
<td></td>
<td>Initial values for the state variables</td>
</tr>
<tr>
<td>Optional</td>
<td>lower_bounds</td>
<td></td>
<td>Specify minimum values</td>
</tr>
<tr>
<td>Optional</td>
<td>upper_bounds</td>
<td></td>
<td>Specify maximum values</td>
</tr>
<tr>
<td>Optional</td>
<td>descriptors</td>
<td></td>
<td>Labels for the variables</td>
</tr>
</tbody>
</table>

Description

Discrete state variables defined by bounds (an integer interval).

The details of how to specify this discrete variable are located on the discrete_variables page.

See the state_variables page for details on the behavior of state variables.
6.4. VARIABLES

initial_state

- Keywords Area
- variables
- discrete_state_range
- initial_state

Initial values for the state variables

**Specification**

**Alias:** dsv_initial_state

**Argument(s):** INTEGERLIST

**Default:** 0

**Description**

The `initial_state` specifications provide the initial values for the state variables. This is an optional keyword. If it is not specified, the initial state will be inferred from the other keywords that define the state variable.

Defaults are:

- Continuous state variables - use the midpoint of the bounds
- Set variables - use the value with the index closest to the middle of the set
- Range variables - use the midpoint of the range

lower_bounds

- Keywords Area
- variables
- discrete_state_range
- lower_bounds

Specify minimum values

**Specification**

**Alias:** dsv_lower_bounds

**Argument(s):** INTEGERLIST

**Default:** INT_MIN

**Description**

Specify minimum values
**upper_bounds**

- Keywords Area
- variables
- discrete_state_range
- upper_bounds

Specify maximum values

**Specification**

Alias: dsv_upper_bounds

**Argument(s):** INTEGERLIST

**Default:** INT_MAX

**Description**

Specify maximum values

**descriptors**

- Keywords Area
- variables
- discrete_state_range
- descriptors

Labels for the variables

**Specification**

Alias: dsv_descriptors

**Argument(s):** STRINGLIST

**Default:** dsvri_{i}

**Description**

The optional variable labels specification descriptors is a list of strings which identify the variables. These are used in console and tabular output.

The default descriptor strings use a variable type-dependent root string plus a numeric identifier.

6.4.32 discrete_state_set

- Keywords Area
- variables
- discrete_state_set

State variable - discrete set-valued
6.4. VARIABLES

Topics
This keyword is related to the topics:

- discrete_variables
- state_variables

Specification
Alias: none
Argument(s): none

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<th>Dakota Keyword Description</th>
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<tr>
<td>Optional</td>
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<td>Discrete state variables, each defined by a set of permissible integers</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>string</td>
<td>String-valued discrete state set variables</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>real</td>
<td>Discrete state variables, each defined by a set of permissible real numbers</td>
</tr>
</tbody>
</table>

Description
Discrete state variables whose values come from a set of admissible elements. Each variable specified must be of type integer, string, or real.

integer
- Keywords Area
- variables
- discrete_state_set
- integer

Discrete state variables, each defined by a set of permissible integers

Topics
This keyword is related to the topics:

- discrete_variables
- state_variables
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): INTEGER

Default: no discrete state set integer variables

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>elements_per_variable</td>
<td>Number of admissible elements for each set variable</td>
</tr>
<tr>
<td>Required</td>
<td></td>
<td>elements</td>
<td>The permissible values for each discrete variable</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>categorical</td>
<td>Whether the set-valued variables are categorical or relaxable</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>initial_state</td>
<td>Initial values for the state variables</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>descriptors</td>
<td>Labels for the variables</td>
</tr>
</tbody>
</table>

Description

Discrete state variables defined by a set of permissible integers.

The details of how to specify this discrete variable are located on the discrete_variables page.

See the state_variables page for details on the behavior of state variables.

elements_per_variable

- Keywords Area
- variables
- discrete_state_set
- integer
- elements_per_variable

Number of admissible elements for each set variable

Specification

Alias: num_set_values

Argument(s): INTEGERLIST

Default: equal distribution
6.4. VARIABLES

Description
Discrete set variables (including design, uncertain, and state) take on only a fixed set of values. For each type (integer, string, or real), this keyword specifies how many admissible values are provided for each variable. If not specified, equal apportionment of elements among variables is assumed, and the number of elements must be evenly divisible by the number of variables.

elements
- Keywords Area
- variables
- discrete_state_set
- integer
- elements

The permissible values for each discrete variable

Specification
Alias: set_values
Argument(s): INTEGERLIST

Description
Specify the permissible values for discrete set variables (of type integer, string, or real). See the description on the discrete_variables page.

categorical
- Keywords Area
- variables
- discrete_state_set
- integer
- categorical

Whether the set-valued variables are categorical or relaxable

Specification
Alias: none
Argument(s): STRINGLIST

Description
A list of strings of length equal to the number of set (integer, string, or real) variables indicating whether they are strictly categorical, meaning may only take on values from the provided set, or relaxable, meaning may take on any integer or real value between the lowest and highest specified element. Valid categorical strings include 'yes', 'no', 'true', and 'false', or any abbreviation in [yYnNtTfF][.]*
Examples

Discrete design set variable, 'rotor blades', can take on only integer values, 2, 4, or 7 by default. Since categorical is specified to be false, the integrality can be relaxed and 'rotor blades' can take on any value between 2 and 7, e.g., 3, 6, or 5.5.

```
discrete_design_set
  integer 1
  elements 2 4 7
  descriptor 'rotor_blades'
  categorical 'no'
```

**initial_state**

- Keywords Area
- variables
- discrete_state_set
- integer
- initial_state

Initial values for the state variables

**Specification**

**Alias:** none

**Argument(s):** INTEGERLIST

**Default:** middle set value, or rounded down

**Description**

The *initial_state* specifications provide the initial values for the state variables. This is an optional keyword. If it is not specified, the initial state will be inferred from the other keywords that define the state variable.

Defaults are:

- Continuous state variables - use the midpoint of the bounds
- Set variables - use the value with the index closest to the middle of the set
- Range variables - use the midpoint of the range

**descriptors**

- Keywords Area
- variables
- discrete_state_set
- integer
- descriptors

Labels for the variables
6.4. VARIABLES

Specification

Alias: none
Argument(s): STRINGLIST
Default: dssiv_{i}

Description

The optional variable labels specification descriptors is a list of strings which identify the variables. These are used in console and tabular output.

The default descriptor strings use a variable type-dependent root string plus a numeric identifier.

string

- Keywords Area
- variables
- discrete_state_set
- string

String-valued discrete state set variables

Topics

This keyword is related to the topics:

- discrete_variables
- state_variables

Specification

Alias: none
Argument(s): INTEGER
Default: no discrete state set string variables

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<thead>
<tr>
<th>Required/-</th>
<th>Description of</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword</th>
</tr>
</thead>
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<td>Group</td>
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<td>Description</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>Number of admissible elements for each set variable</td>
<td></td>
</tr>
</tbody>
</table>
CHAPTER 6. KEYWORDS AREA

<table>
<thead>
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<th>Required</th>
<th>elements</th>
<th>The permissible values for each discrete variable</th>
</tr>
</thead>
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<tr>
<td>Optional</td>
<td>initial_state</td>
<td>Initial values for the state variables</td>
</tr>
<tr>
<td>Optional</td>
<td>descriptors</td>
<td>Labels for the variables</td>
</tr>
</tbody>
</table>

**Description**

Discrete state variables whose values come from a specified set of admissible strings. The details of how to specify this discrete variable are located on the `discrete_variables` page. See the `state_variables` page for details on the behavior of state variables. Each string element value must be quoted and may contain alphanumeric, dash, underscore, and colon. White space, quote characters, and backslash/metacharacters are not permitted.

**elements_per_variable**

- Keywords Area
- variables
- discrete_state_set
- string
- elements_per_variable

Number of admissible elements for each set variable

**Specification**

**Alias:** num_set_values  
**Argument(s):** INTEGERLIST  
**Default:** equal distribution

**Description**

Discrete set variables (including design, uncertain, and state) take on only a fixed set of values. For each type (integer, string, or real), this keyword specifies how many admissible values are provided for each variable. If not specified, equal apportionment of elements among variables is assumed, and the number of elements must be evenly divisible by the number of variables.

**elements**

- Keywords Area
- variables
- discrete_state_set
- string
6.4. VARIABLES

- **elements**

  The permissible values for each discrete variable

**Specification**

* Alias: set_values

  * **Argument(s):** STRINGLIST

**Description**

Specify the permissible values for discrete set variables (of type integer, string, or real). See the description on the discrete_variables page.

**initial_state**

- **Keywords Area**

  - **variables**

  - **discrete_state_set**

  - **string**

  - **initial_state**

  Initial values for the state variables

**Specification**

* **Alias:** none

  * **Argument(s):** STRINGLIST

  * **Default:** middle set value, or rounded down

**Description**

The initial_state specifications provide the initial values for the state variables. This is an optional keyword. If it is not specified, the initial state will be inferred from the other keywords that define the state variable.

Defaults are:

- Continuous state variables - use the midpoint of the bounds
- Set variables - use the value with the index closest to the middle of the set
- Range variables - use the midpoint of the range
CHAPTER 6. KEYWORDS AREA

descriptors
- Keywords Area
- variables
- discrete_state_set
- string
- descriptors

Labels for the variables

Specification
Alias: none
Argument(s): STRINGLIST
Default: dssv_{i}

Description
The optional variable labels specification descriptors is a list of strings which identify the variables. These are used in console and tabular output.

The default descriptor strings use a variable type-dependent root string plus a numeric identifier.

real
- Keywords Area
- variables
- discrete_state_set
- real

Discrete state variables, each defined by a set of permissible real numbers

Topics
This keyword is related to the topics:
- discrete_variables
- state_variables

Specification
Alias: none
Argument(s): INTEGER
Default: no discrete state set real variables
<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword Description</th>
<th>Dakota Keyword</th>
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<tbody>
<tr>
<td>Required</td>
<td>elements</td>
<td>Number of admissible elements for each set variable</td>
<td>elements_per_variable</td>
</tr>
<tr>
<td>Optional</td>
<td>categorical</td>
<td>The permissible values for each discrete variable</td>
<td>categorical</td>
</tr>
<tr>
<td>Optional</td>
<td>initial_state</td>
<td>Whether the set-valued variables are categorical or relaxable</td>
<td>initial_state</td>
</tr>
<tr>
<td>Optional</td>
<td>descriptors</td>
<td>Initial values for the state variables</td>
<td>descriptors</td>
</tr>
</tbody>
</table>

### Description

Discrete state variables defined by a set of permissible real numbers.

The details of how to specify this discrete variable are located on the discrete_variables page. See the state_variables page for details on the behavior of state variables.

**elements_per_variable**

- Keywords Area
- variables
- discrete_state_set
- real
- elements_per_variable

Number of admissible elements for each set variable

### Specification

**Alias:** num_set_values

**Argument(s):** INTEGERLIST

**Default:** equal distribution
**Description**

Discrete set variables (including design, uncertain, and state) take on only a fixed set of values. For each type (integer, string, or real), this keyword specifies how many admissible values are provided for each variable. If not specified, equal apportionment of elements among variables is assumed, and the number of elements must be evenly divisible by the number of variables.

**elements**

- Keywords Area
- variables
- discrete_state_set
- real
- elements

The permissible values for each discrete variable

**Specification**

Alias: set_values

**Argument(s):** REALLIST

**Description**

Specify the permissible values for discrete set variables (of type integer, string, or real). See the description on the discrete_variables page.

**categorical**

- Keywords Area
- variables
- discrete_state_set
- real
- categorical

Whether the set-valued variables are categorical or relaxable

**Specification**

Alias: none

**Argument(s):** STRINGLIST

**Description**

A list of strings of length equal to the number of set (integer, string, or real) variables indicating whether they are strictly categorical, meaning may only take on values from the provided set, or relaxable, meaning may take on any integer or real value between the lowest and highest specified element. Valid categorical strings include 'yes', 'no', 'true', and 'false', or any abbreviation in [yYnNtTfF][.,]*
6.4. VARIABLES

Examples
Discrete design set variable, 'rotor_blades', can take on only integer values, 2, 4, or 7 by default. Since categorical is specified to be false, the integrality can be relaxed and 'rotor_blades' can take on any value between 2 and 7, e.g., 3, 6, or 5.5.

discrete_design_set
  integer 1
  elements 2 4 7
  descriptor 'rotor_blades'
categorical 'no'

initial_state
- Keywords Area
- variables
- discrete_state_set
- real
- initial_state

Initial values for the state variables

Specification
Alias: none
Argument(s): REALLIST
Default: middle set value, or rounded down

Description
The initial_state specifications provide the initial values for the state variables. This is an optional keyword. If it is not specified, the initial state will be inferred from the other keywords that define the state variable.

Defaults are:
- Continuous state variables - use the midpoint of the bounds
- Set variables - use the value with the index closest to the middle of the set
- Range variables - use the midpoint of the range

descriptors
- Keywords Area
- variables
- discrete_state_set
- real
- descriptors

Labels for the variables
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): STRINGLIST

Default: dssrv_{i}

Description

The optional variable labels specification descriptors is a list of strings which identify the variables. These are used in console and tabular output.

The default descriptor strings use a variable type-dependent root string plus a numeric identifier.

6.4.33 linear_inequality_constraint_matrix

- Keywords Area
- variables
- linear_inequality_constraint_matrix

Define coefficients of the linear inequality constraints

Topics

This keyword is related to the topics:

- linear_constraints

Specification

Alias: none

Argument(s): REALLIST

Default: no linear inequality constraints

Description

In the inequality case, the constraint matrix $A$ provides coefficients for the variables in the two-sided formulation:

$$a_l \leq Ax \leq a_u$$

Where the bounds are optionally specified by linear_inequality_lower_bounds, and linear_inequality_upper_bounds. The bounds, if not specified, will default to -infinity, and 0, respectively, resulting in one-sided inequalities of the form

$$Ax \leq 0.0$$

The linear_constraints topics page (linked above) outlines a few additional things to consider when using linear constraints.
Examples
In the first example, an optimization involving two variables, \(x_1\) and \(x_2\), is to be performed. These variables must satisfy two constraints:

\[
1.5 \cdot x_1 + 1.0 \cdot x_2 \leq 5.0 \\
x_1 \leq x_2 \implies x_1 - x_2 \leq 0.0
\]

The pair of constraints can be written in matrix form as:

\[
\begin{bmatrix}
1.5 & 1.0 \\
1.0 & -1.0
\end{bmatrix}
\begin{bmatrix}
x_1 \\
x_2
\end{bmatrix}
\leq
\begin{bmatrix}
5.0 \\
0.0
\end{bmatrix}
\]

The coefficient matrix and right hand side of this matrix inequality are expressed to Dakota in the variables section of the input file:

variables
continuous_design 2
descriptors 'x1' 'x2'
linear_inequality_constraint_matrix = 1.5 1.0
1.0 -1.0
linear_inequality_upper_bounds = 5.0
0.0

The second example is more complex in two respects. First, some, but not all, of the constraints are "two sided", with both lower and upper bounds. Second, not all variables participate in all constraints.

There are four variables, \(x_1\), \(x_2\), \(x_3\), and \(x_4\), and four constraints.

\[
-2.0 \leq 5.0 \cdot x_1 + 2.0 \cdot x_2 \leq 9.0 \\
0.0 \leq x_1 + x_3 \\
-8.0 \leq x_2 + 6.0 \cdot x_4 \leq 8.0 \\
x_1 + x_2 + x_3 \leq 9.0
\]

Or, in matrix form,

\[
\begin{bmatrix}
-2.0 \\
0.0 \\
-8.0 \\
-\infty
\end{bmatrix}
\leq
\begin{bmatrix}
5.0 & 2.0 & 0.0 & 0.0 \\
1.0 & 0.0 & 1.0 & 0.0 \\
0.0 & 1.0 & 0.0 & 6.0 \\
1.0 & 1.0 & 1.0 & 0.0
\end{bmatrix}
\begin{bmatrix}
x_1 \\
x_2 \\
x_3 \\
x_4
\end{bmatrix}
\leq
\begin{bmatrix}
9.0 \\
\infty \\
8.0 \\
9.0
\end{bmatrix}
\]

The Dakota specification for this matrix inequality is:

variables
continuous_design 4

descriptors 'x1' 'x2' 'x3' 'x4'
linear_inequality_constraint_matrix = 5.0 2.0 0.0 0.0
1.0 0.0 1.0 0.0
0.0 1.0 0.0 6.0
1.0 1.0 1.0 0.0
linear_inequality_lower_bounds = -2.0
0.0
-8.0
6.4.34 `linear_inequality_lower_bounds`

- **Keywords Area**
- **variables**
- **linear_inequality_lower_bounds**

Define lower bounds for the linear inequality constraint

**Topics**

This keyword is related to the topics:

- **linear_constraints**

**Specification**

Alias: none  
**Argument(s):** REALLIST  
**Default:** vector values = -infinity  

**Description**

In the inequality case, the lower \( a_l \) and upper \( a_u \) bounds provide constraint limits for the two-sided formulation:

\[
-a_l \leq Ax \leq a_u
\]

Where \( A \) is the constrain matrix of variable coefficients.

As with nonlinear inequality constraints (see `objective_functions`), the default linear inequality constraint bounds are selected so that one-sided inequalities of the form

\[
Ax \leq 0.0
\]

result when there are no user bounds specifications (this provides backwards compatibility with previous Dakota versions).

In a user bounds specification, any upper bound values greater than +bigRealBoundSize (1.0e+30, as defined in Minimizer) are treated as +infinity and any lower bound values less than -bigRealBoundSize are treated as -infinity.

This feature is commonly used to drop one of the bounds in order to specify a 1-sided constraint (just as the default lower bounds drop out since -DBL_MAX < -bigRealBoundSize).

**Examples**

Examples of specifying linear inequality constraints to Dakota are provided on the `linear_inequality_constraint_matrix` page.
6.4.35  **linear_inequality_upper_bounds**

- **Keywords Area**
- **variables**
- **linear_inequality_upper_bounds**

Define upper bounds for the linear inequality constraint

**Topics**

This keyword is related to the topics:

- **linear_constraints**

**Specification**

**Alias:** none  
**Argument(s):** REALLIST  
**Default:** vector values = 0.

**Description**

In the inequality case, the lower $a_l$ and upper $a_u$ bounds provide constraint limits for the two-sided formulation:

$$ a_l \leq Ax \leq a_u $$

Where $A$ is the constrain matrix of variable coefficients.

As with nonlinear inequality constraints (see **objective_functions**), the default linear inequality constraint bounds are selected so that one-sided inequalities of the form

$$ Ax \leq 0.0 $$

result when there are no user bounds specifications (this provides backwards compatibility with previous Dakota versions).

In a user bounds specification, any upper bound values greater than $+\text{bigRealBoundSize}$ (1.e+30, as defined in Minimizer) are treated as $+\infty$ and any lower bound values less than $-\text{bigRealBoundSize}$ are treated as $-\infty$.

This feature is commonly used to drop one of the bounds in order to specify a 1-sided constraint (just as the default lower bounds drop out since $-\text{DBL_MAX} < -\text{bigRealBoundSize}$).

**Examples**

Examples of specifying linear inequality constraints to Dakota are provided on the **linear_inequality_constraint_matrix** page.

6.4.36  **linear_inequality_scale_types**

- **Keywords Area**
- **variables**
- **linear_inequality_scale_types**

Specify how each linear inequality constraint is scaled
CHAPTER 6. KEYWORDS AREA

Topics
This keyword is related to the topics:

- linear_constraints

Specification
Alias: none
Argument(s): STRINGLIST
Default: vector values = "none"

Description
linear_inequality_scale_types provide strings specifying the scaling type for each linear inequality constraint, in methods that support scaling.

An entry may be selected for each constraint. The options are:

- 'none' - no scaling
- 'value' - characteristic value if this is chosen, then linear_inequality_scales must be specified
- 'auto' - automatic scaling If a single string is specified it will apply to all constraints.

Scaling for linear constraints is applied after any continuous variable scaling. For example, for variable scaling on continuous design variables \( x \):

\[
\tilde{x}^j = \frac{x^j - x_O^j}{x_M^j}
\]

we have the following system for linear inequality constraints

\[
a_L \leq A_i x \leq a_U
\]

\[
a_L \leq A_i (\text{diag}(x_M) \tilde{x} + x_O) \leq a_U
\]

\[
a_L - A_i x_O \leq A_i \text{diag}(x_M) \tilde{x} \leq a_U - A_i x_O
\]

\[
\tilde{a}_L \leq \tilde{A}_i \tilde{x} \leq \tilde{a}_U
\]

and user-specified or automatically computed scaling multipliers are applied to this final transformed system, which accounts for continuous design variable scaling. When automatic scaling is in use for linear constraints they are linearly scaled by a computed characteristic value, but not affinely to \([0,1]\).

6.4.37 linear_inequality_scales

- Keywords Area
- variables
- linear_inequality_scales

Define the characteristic values to scale linear inequalities
6.4. VARIABLES

Topics
This keyword is related to the topics:

- linear_constraints

Specification
Alias: none
Argument(s): REALLIST
Default: vector values = 1. (no scaling)

Description
Each entry in linear_inequality_scales may be a user-specified, nonzero characteristic value to be used in scaling each constraint.

Behavior depends on the choice of linear_inequality_scale_type:

- scale_type - behavior of linear_inequality_scales
- 'none' - ignored
- 'value' - required
- 'auto' - optional

If a single real value is specified it will apply to all components of the constraint.
Scaling for linear constraints is applied after any continuous variable scaling. For example, for variable scaling on continuous design variables \( x \):\[
\tilde{x}^j = \frac{x^j - x^j_O}{x^j_M}
\]
we have the following system for linear inequality constraints
\[
a_L \leq A_i x \leq a_U
\]
\[
a_L \leq A_i (\text{diag}(x_M)\tilde{x} + x_O) \leq a_U
\]
\[
a_L - A_i x_O \leq A_i \text{diag}(x_M)\tilde{x} \leq a_U - A_i x_O
\]
\[
\tilde{a}_L \leq \tilde{A}_i \tilde{x} \leq \tilde{a}_U
\]
and user-specified or automatically computed scaling multipliers are applied to this final transformed system, which accounts for continuous design variable scaling. When automatic scaling is in use for linear constraints they are linearly scaled by a computed characteristic value, but not affinely to \([0,1]\).

6.4.38 linear_equality_constraint_matrix

- Keywords Area
- variables
- linear_equality_constraint_matrix

Define coefficients of the linear equalities
Topics
This keyword is related to the topics:

- linear_constraints

Specification
Alias: none
Argument(s): REALLIST
Default: no linear equality constraints

Description
In the equality case, the constraint matrix $A$ provides coefficients for the variables on the left hand side of:

$$Ax = a_t$$

The linear_constraints topics page (linked above) outlines a few additional things to consider when using linear constraints.

Examples
An optimization involving three variables, $x_1$, $x_2$, and $x_3$, is to be performed. These variables must satisfy a pair of linear equality constraints:

1. $1.5 \cdot x_1 + 1.0 \cdot x_2 = 5.0$
2. $3.0 \cdot x_1 - 4.0 \cdot x_3 = 0.0$

The pair of constraints can be written in matrix form as:

$$\begin{bmatrix} 1.5 & 1.0 & 0.0 \\ 3.0 & 0.0 & -4.0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 5.0 \\ 0.0 \end{bmatrix}$$

The coefficient matrix and right hand side are expressed to Dakota in the variables section of the input file:

```plaintext
variables
continuous_design 2
descriptors 'x1' 'x2'
linear_equality_constraint_matrix = 1.5 1.0 0.0
                                3.0 0.0 -4.0
linear_equality_targets = 5.0
                         0.0
```

For related examples, see the linear_inequality_constraint_matrix keyword page.

6.4.39 linear_equality_targets

- Keywords Area
- variables
- linear_equality_targets

Define target values for the linear equality constraints
6.4. VARIABLES

Topics
This keyword is related to the topics:

- linear_constraints

Specification
Alias: none
Argument(s): REALLIST
Default: vector values = 0 .

Description
In the equality case, the targets $a_t$ provide the equality constraint right hand sides:

$$Ax = a_t$$

If this is not specified, the defaults for the equality constraint targets enforce a value of 0. for each constraint: $Ax = 0.0$

Examples
Examples of specifying linear equality constraints to Dakota are provided on the linear_equality_constraint_matrix page.

6.4.40 linear_equality_scale_types

- Keywords Area
- variables
- linear_equality_scale_types

Specify how each linear equality constraint is scaled

Topics
This keyword is related to the topics:

- linear_constraints

Specification
Alias: none
Argument(s): STRINGLIST
Default: vector values = "none"
Description

`linear_equalitiescale_types` provide strings specifying the scaling type for each linear equality constraint, in methods that support scaling.

An entry may be selected for each constraint. The options are:

- `'none'` - no scaling
- `'value'` - characteristic value if this is chosen, then `linear_equalitiescales` must be specified
- `'auto'` - automatic scaling If a single string is specified it will apply to all constraints.

Scaling for linear constraints is applied after any continuous variable scaling.

For example, for variable scaling on continuous design variables $x$:

$$\bar{x}^j = \frac{x^j - x_O^j}{x_M^j}$$

we have the following system for linear equality constraints

$$a_L \leq A_i x \leq a_U$$

$$a_L \leq A_i (\text{diag}(x_M)\bar{x} + x_O) \leq a_U$$

$$a_L - A_i x_O \leq A_i \text{diag}(x_M)\bar{x} \leq a_U - A_i x_O$$

$$\tilde{a}_L \leq \tilde{A}_i \bar{x} \leq \tilde{a}_U$$

and user-specified or automatically computed scaling multipliers are applied to this final transformed system, which accounts for continuous design variable scaling. When automatic scaling is in use for linear constraints they are linearly scaled by a computed characteristic value, but not affinely to [0,1].

6.4.41 `linear_equalitiescales`

- **Keywords Area**
- **variables**
- **linear_equalitiescales**

Define the characteristic values to scale linear equalities

Topics

This keyword is related to the topics:

- **linear_constraints**

Specification

Alias: none

Argument(s): REALLIST

Default: vector values = 1 . (no scaling)
6.5. INTERFACE

Description

Each entry in `linear_equality_scales` may be a user-specified, nonzero characteristic value to be used in scaling each constraint.

See the scaling keyword in the method section for details on how to use this keyword.

Scaling for linear constraints is applied *after* any continuous variable scaling.

For example, for variable scaling on continuous design variables $x$:

$$\tilde{x}_j = \frac{x_j - x_{O}}{x_{M}}$$

we have the following system for linear inequality constraints

$$a_L \leq A_i x \leq a_U$$

$$a_L \leq A_i (\text{diag}(x_M)\tilde{x} + x_O) \leq a_U$$

$$a_L - A_i x_O \leq A_i (\text{diag}(x_M)\tilde{x}) \leq a_U - A_i x_O$$

$$\tilde{a}_L \leq \tilde{A}_i \tilde{x} \leq \tilde{a}_U$$

and user-specified or automatically computed scaling multipliers are applied to this final transformed system, which accounts for continuous design variable scaling. When automatic scaling is in use for linear constraints they are linearly scaled by a computed characteristic value, but not affinely to [0,1].

6.5 interface

- **Keywords Area**
- **interface**

Specifies how function evaluations will be performed in order to map the variables into the responses.

Topics

This keyword is related to the topics:

- **block**

Specification

**Alias:** none

**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>id_interface</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Name the interface block; helpful when there are multiple
<table>
<thead>
<tr>
<th>Optional</th>
<th>analysis_drivers</th>
<th>Define how Dakota should run a function evaluation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>algebraic mappings</td>
<td>Use AMPL to define algebraic input-output mappings</td>
</tr>
<tr>
<td>Optional</td>
<td>failure_capture</td>
<td>Determine how Dakota responds to analysis driver failure</td>
</tr>
<tr>
<td>Optional</td>
<td>deactivate</td>
<td>Deactivate Dakota interface features for simplicity or efficiency</td>
</tr>
<tr>
<td>Optional</td>
<td>asynchronous</td>
<td>Specify local evaluation or analysis concurrency</td>
</tr>
<tr>
<td>Optional</td>
<td>evaluation_servers</td>
<td>Specify the number of evaluation servers when Dakota is run in parallel</td>
</tr>
<tr>
<td>Optional</td>
<td>evaluation_scheduling</td>
<td>Specify the scheduling of concurrent evaluations when Dakota is run in parallel</td>
</tr>
</tbody>
</table>
6.5. INTERFACE

### Description

The interface section in a Dakota input file specifies how function evaluations will be performed in order to map the variables into the responses. The term "interface" refers to the bridge between Dakota and the underlying simulation code.

In this context, a "function evaluation" is the series of operations that takes the variables and computes the responses. This can be comprised of one or many codes, scripts, and glue, which are generically referred to as "analysis drivers" (and optional input/output filters). The mapping actions of analysis drivers may be combined with explicit algebraic mappings.

#### Parallelism Options

- The asynchronous keyword enables concurrent local function evaluations or analyses via operating system process management. Its child keywords allow tailoring the evaluation and analysis concurrency.

- The evaluation servers, scheduling mode (master, peer static or dynamic), and processor keywords allow a user to override Dakota’s default evaluation configuration when running in parallel (MPI) mode.

- The analysis servers and scheduling mode (master, peer static or dynamic) keywords allow a user to override Dakota’s default analysis configuration when running in parallel (MPI) mode.

Note: see direct for the specific processors_per_analysis specification supported for direct interfaces.


#### Theory

Function evaluations are performed using either interfaces to simulation codes, algebraic mappings, or a combination of the two.

When employing mappings with simulation codes, the interface invokes the simulation using either forks, direct function invocations, or computational grid invocations.

- In the fork case, Dakota will treat the simulation as a black-box and communication between Dakota and the simulation occurs through parameter and result files. This is the most common case.
• In the direct function case, the simulation is internal to Dakota and communication occurs through the function parameter list. The direct case can involve linked simulation codes or test functions which are compiled into the Dakota executable. The test functions allow for rapid testing of algorithms without process creation overhead or engineering simulation expense.

• The grid case is deprecated, but was an experiment in interfacing Dakota to distributed computing engines.

When employing algebraic mappings, the AMPL solver library[29] is used to evaluate a directed acyclic graph (DAG) specification from a separate stub.nl file. Separate stub.col and stub.row files are also required to declare the string identifiers of the subset of inputs and outputs, respectively, that will be used in the algebraic mappings.

6.5.1 id_interface

Keywords Area

interface

id_interface

Name the interface block; helpful when there are multiple

Topics

This keyword is related to the topics:

• block_identifier

Specification

Alias: none

Argument(s): STRING

Default: use of last interface parsed

Description

The optional id_interface keyword accepts a string that uniquely identifies this interface block. A model can then use this interface by specifying the same string in its interface_pointer specification.

Default Behavior

If the id_interface specification is omitted, a particular interface specification will be used by a model only if that model does not include an interface_pointer and the interface block was the last (or only) one parsed.

Usage Tips

• It is a best practice to always use explicit interface IDs and pointers to avoid confusion.

• If only one interface block exists, then id_interface can be safely omitted from the interface block (and interface_pointer omitted from the model specification(s)), since there is no ambiguity.

Examples

For example, a model specification including

```
model
    interface_pointer = 'I1'
```

will link to an interface with

```
id_interface = 'I1'
```
### 6.5.2 analysis_drivers

- **Keywords Area**
- **interface**
- **analysis_drivers**

Define how Dakota should run a function evaluation

#### Specification

**Alias:** none  
**Argument(s):** STRINGLIST

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>input_filter</td>
<td>Run a pre-processing script before the analysis drivers</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>output_filter</td>
<td>Run a post-processing script after the analysis drivers (Not recommended) Launch analysis drivers with a system call</td>
</tr>
<tr>
<td>Required (Choose One)</td>
<td>Interface Type (Group 1)</td>
<td>system</td>
<td>Launch analysis drivers using fork command</td>
</tr>
<tr>
<td></td>
<td></td>
<td>fork</td>
<td>Run analysis drivers that are linked-to or compiled-with Dakota</td>
</tr>
<tr>
<td></td>
<td></td>
<td>direct</td>
<td>Run analysis drivers that are linked-to or compiled-with Dakota</td>
</tr>
</tbody>
</table>
**Description**

The `analysis_drivers` keyword provides the names of one or more executable analysis programs or scripts, a.k.a. “drivers” which comprise a function evaluation. The optional and required sub-keywords specify how Dakota will manage directories and files, and run the driver(s).

**Types of Interfaces**

Dakota has two recommended ways of running analysis drivers:

- as an external processes (fork), or
- using internal code to couple to the analysis driver (direct)

Other options are available for advanced users, and are not as well documented, supported, or tested:

- external processes (system)
- internal coupling (python, matlab, scilab, grid)

**Use Cases**

The internally coupled codes have few options because many of the details are already handled with the coupling. Their behavior is described in the direct keyword.

For external processes using the fork keyword,

A function evaluation may comprise:

1. A *single analysis driver*: Function evaluation, including all pre- and post-processing is contained entirely within a single script/executable.
2. A single analysis driver with filters: Function evaluation is explicitly split into pre-processing (performed by the input filter), analysis, and post-processing (by the output filter).

3. A single analysis driver with environment variables: Function evaluation is contained within one analysis driver, but it requires environment variables to be set before running.

4. Multiple analysis drivers: Drivers are run sequentially or concurrently (See the asynchronous keyword) and can have any of the above options as well.

For fork and system interfaces, the analysis_driver list contains the names of one or more executable programs or scripts taking parameters files as input and producing results files as output. The first field in each analysis driver string must be an executable program or script for Dakota to spawn to perform the function evaluation. Drivers support:

- One set of nested quotes, for arguments with spaces
- Dakota will define special environment variables DAKOTA_PARAMETERS_FILE and DAKOTA_RESULTS_FILE which can be used in the driver script.
- Variable definitions preceding the executable program or script, such as 'MY_VAR=2 run_analysis.sh' are no longer supported.

For details and examples see the Simulation Interface Components section of the Interfaces chapter of the User’s Manual; for details on the filters and environment variables, see the subsection on Syntax for Filter and Driver Strings.

Examples

Examples:

1. analysis_drivers = ‘run_simulation_part1.sh’ ‘run_simulation_part2.sh’

2. analysis_driver = ‘run_simulation.sh -option "option 1”’

3. analysis_driver = ‘simulation.exe -option value -dakota_params $DAKOTA_PARAMETERS_FILE -input sim.in -dakota_results_file $DAKOTA_RESULTS_FILE’

FAQ

Where will Dakota look for the analysis_driver? Dakota will locate analysis_driver programs first in (or relative to) the present working directory (".", the interface-analysis_drivers-fork-work_directory if used, otherwise the directory in which Dakota is started), then the directory from which Dakota is started, then using the system $PATH environment variable (Path% on Windows).

Where should the driver be located? When the driver is a script it is most commonly placed in the same directory as the Dakota input file. When using a work_directory, Dakota will also look for drivers in the specified working directory, so link_files or copy_files may specify the driver to get copied or linked into the work directory. When executable programs are used as drivers, they are often elsewhere on the filesystem. These can be specified using absolute paths, or by prepending the PATH environment variable so Dakota finds them.

What if Dakota fails to run my analysis_driver? Prepend the absolute location of the driver to the PATH environment variable before running Dakota, or specify an absolute path to the driver in the Dakota input file.
input_filter

- Keywords Area
- interface
- analysis_drivers
- input_filter

Run a pre-processing script before the analysis drivers

Specification

Alias: none
Argument(s): STRING
Default: no input filter

Description

The optional input_filter and output_filter specifications provide the names of separate pre- and post-processing programs or scripts which assist in mapping Dakota parameters files into analysis input files and mapping analysis output files into Dakota results files, respectively.

If there is only a single analysis driver, then it is usually most convenient to combine pre- and post-processing requirements into a single analysis driver script and omit the separate input and output filters. However, in the case of multiple analysis drivers, the input and output filters provide a convenient location for non-repeated pre- and post-processing requirements. That is, input and output filters are only executed once per function evaluation, regardless of the number of analysis drivers, which makes them convenient locations for data processing operations that are shared among the analysis drivers.

output_filter

- Keywords Area
- interface
- analysis_drivers
- output_filter

Run a post-processing script after the analysis drivers

Specification

Alias: none
Argument(s): STRING
Default: no output filter
Description

The optional input_filter and output_filter specifications provide the names of separate pre- and post-processing programs or scripts which assist in mapping Dakota parameters files into analysis input files and mapping analysis output files into Dakota results files, respectively.

If there is only a single analysis driver, then it is usually most convenient to combine pre- and post-processing requirements into a single analysis driver script and omit the separate input and output filters. However, in the case of multiple analysis drivers, the input and output filters provide a convenient location for non-repeated pre- and post-processing requirements. That is, input and output filters are only executed once per function evaluation, regardless of the number of analysis drivers, which makes them convenient locations for data processing operations that are shared among the analysis drivers.

system

- Keywords Area
- interface
- analysis_drivers
- system

(Not recommended) Launch analysis drivers with a system call

Specification

Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>parameters_file</td>
<td>parameters_file</td>
<td>Specify the name of the parameters file</td>
</tr>
<tr>
<td>Optional</td>
<td>results_file</td>
<td>results_file</td>
<td>Specify the name of the results file</td>
</tr>
<tr>
<td>Optional</td>
<td>file_tag</td>
<td>file_tag</td>
<td>Tag each parameters &amp; results file name with the function evaluation number</td>
</tr>
<tr>
<td>Optional</td>
<td>file_save</td>
<td>file_save</td>
<td>Keep the parameters &amp; results files after the analysis driver completes</td>
</tr>
</tbody>
</table>
### Description

The system call interface is included in Dakota for portability and backward compatibility. Users are strongly encouraged to use the `fork` interface if possible, reverting to system only when necessary. To enable the system call interface, replace the `fork` keyword with `system`. All other keywords have identical meanings to those for the `fork` interface.

### See Also

These keywords may also be of interest:

- `fork`

### parameters_file

- `Keywords Area`
- `interface`
- `analysis_drivers`
- `system`
- `parameters_file`

Specify the name of the parameters file.
6.5. INTERFACE

Specification

Alias: none
  Argument(s): STRING
  Default: Unix temp files

Description

The parameters file is used by Dakota to pass the parameter values to the analysis driver. The name of the file can be optionally specified using the `parameters_file` keyword.

If this is not specified, the default data transfer files are temporary files with system-generated names (e.g., `/tmp/dakota_params_aaaa0886`).

results_file

- Keywords Area
- interface
- analysis_drivers
- system
- results_file

Specify the name of the results file

Specification

Alias: none
  Argument(s): STRING
  Default: Unix temp files

Description

The results file must be written by the analysis driver. It is read by Dakota to determine the response values for each function evaluation.

The name of the file can be optionally specified using the `results_file` keyword.

If this is not specified, the default data transfer files are temporary files with system-generated names (e.g., `/tmp/dakota_results_aaaa0886`).

file_tag

- Keywords Area
- interface
- analysis_drivers
- system
- file_tag

Tag each parameters & results file name with the function evaluation number
**Specification**

Alias: none  
Argument(s): none  
Default: no tagging

**Description**

If this keyword is used, Dakota will append a period and the function evaluation number to the names of the parameter and results files.

**Default Behavior** If this keyword is omitted, the default is no file tagging.

**Usage Tips**

- File tagging is most useful when multiple function evaluations are running simultaneously using files in a shared disk space. The analysis driver will be able to infer the function evaluation number from the file names.

- Note that when the `file_save` keyword is used, Dakota automatically renames parameters and results files, giving them tags after execution of the analysis driver if they otherwise would be overwritten by the next evaluation.

**Examples**

If the following is included in the `interface` section of the Dakota input:

```
parameters_file = params.in  
results_file = results.out  
file_tag
```

Then for the 3rd evaluation, Dakota will write `params.in.3`, and will expect `results.out.3` to be written by the analysis driver.

**file_save**

- Keywords Area  
- interface  
- analysis_drivers  
- system  
- file_save

Keep the parameters & results files after the analysis driver completes

**Specification**

Alias: none  
Argument(s): none  
Default: file cleanup
Description
If file_save is used, Dakota will not delete the parameters and results files after the function evaluation is completed.
- The default behavior is NOT to save these files.
- If file_tag is not specified and the saved files would be overwritten by a future evaluation, Dakota renames them after the analysis driver has run by tagging them with the evaluation number.
- File saving is most useful when debugging the data communication between Dakota and the simulation.

labeled
- Keywords Area
  - interface
  - analysis_drivers
  - system
  - labeled

  Requires correct function value labels in results file

Topics
This keyword is related to the topics:
- file_formats

Specification
Alias: none
  - Argument(s): none
  - Default: Function value labels optional

Description
The labeled keyword directs Dakota to enforce a stricter results file format and enables more detailed error reporting.
- When the labeled keyword is used, function values in results files must be accompanied by their corresponding descriptors. If the user did not supply response descriptors in her Dakota input file, then Dakota auto-generated descriptors are expected.
- Distinct error messages are emitted for function values that are out-of-order, repeated, or missing. Labels that appear without a function value and unexpected data are also reported as errors. Dakota attempts to report all errors in a results file, not just the first it encounters. After reporting results file errors, Dakota aborts.
- Labels for analytic gradients and Hessians currently are not supported.
  - Although the labeled keyword is optional, its use is recommended to help catch and identify problems with results files. The User’s Manual contains further information about the results file format.

Default Behavior
By default, Dakota does not require labels for function values, and ignores them if they are present.
aprepro

- Keywords Area
- interface
- analysis_drivers
- system
- aprepro

Write parameters files in APREPRO syntax

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: dprepro

Argument(s): none

Default: standard parameters file format

Description

The format of data in the parameters files can be modified for direct usage with the APREPRO pre-processing tool [75] using the aprepro specification.

Without this keyword, the parameters file are written in DPrePro format. DPrePro is a utility included with Dakota, described in the Users Manual[4].

work_directory

- Keywords Area
- interface
- analysis_drivers
- system
- work_directory

Perform each function evaluation in a separate working directory

Specification

Alias: none

Argument(s): none

Default: no work directory
6.5. INTERFACE

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>named</td>
<td>The base name of the work directory created by Dakota</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>directory_tag</td>
<td>Tag each work directory with the function evaluation number</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>directory_save</td>
<td>Preserve the work directory after function evaluation completion</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>link_files</td>
<td>Paths to be linked into each working directory</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>copy_files</td>
<td>Files and directories to be copied into each working directory</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>replace</td>
<td>Overwrite existing files within a work directory</td>
</tr>
</tbody>
</table>

**Description**

When performing concurrent evaluations, it is typically necessary to cloister simulation input and output files in separate directories to avoid conflicts. When the `work_directory` feature is enabled, Dakota will create a directory for each evaluation, with optional tagging (`directory_tag`) and saving (`directory_save`), as with files, and execute the analysis driver from that working directory.

The directory may be named with a string, or left anonymous to use an automatically-generated directory in the system’s temporary file space, e.g., `/tmp/dakota_work_c93vb71z`. The optional `link_files` and `copy_files` keywords specify files or directories which should appear in each working directory.

When using `work_directory`, the `analysis_drivers` may be given by an absolute path, located in (or relative to) the startup directory alongside the Dakota input file, in the list of template files linked or copied, or on the $PATH (Path% on Windows).

- **named**
  - Keywords Area
  - interface
  - analysis_drivers
  - system
• work_directory

• named

The base name of the work directory created by Dakota

**Specification**

Alias: none

---

**Argument(s):** STRING

**Default:** dakota_workxxxxxxxx

**Description**

The named keyword is followed by a string, indicating the name of the work directory created by Dakota. If relative, the work directory will be created relative to the directory from which Dakota is invoked.

If named is not used, the default work directory is a temporary directory with a system-generated name (e.g., /tmp/dakota_work_c93vb71z/).

**See Also**

These keywords may also be of interest:

• directory_tag

• directory_save

**directory_tag**

• Keywords Area

• interface

• analysis_drivers

• system

• work_directory

• directory_tag

Tag each work directory with the function evaluation number

**Specification**

Alias: dir_tag

---

**Argument(s):** none

**Default:** no work directory tagging

**Description**

If this keyword is used, Dakota will append a period and the function evaluation number to the work directory names.

If this keyword is omitted, the default is no tagging, and the same work directory will be used for ALL function evaluations. Tagging is most useful when multiple function evaluations are running simultaneously.
**directory_save**

- Keywords Area
- interface
- analysis_drivers
- system
- work_directory
- directory_save

Preserve the work directory after function evaluation completion

**Specification**

**Alias:** dir_save

**Argument(s):** none

**Default:** remove work directory

**Description**

By default, when a working directory is created by Dakota using the `work_directory` keyword, it is deleted after the evaluation is completed. The `directory_save` keyword will cause Dakota to leave (not delete) the directory.

**link_files**

- Keywords Area
- interface
- analysis_drivers
- system
- work_directory
- link_files

Paths to be linked into each working directory

**Specification**

**Alias:** none

**Argument(s):** STRINGLIST

**Default:** no linked files

**Description**

Specifies the paths (files or directories) that will be symbolically linked from each working directory. Wildcards using * and ? are permitted. Linking is space-saving and useful for files not modified during the function evaluation. However, not all filesystems support linking, for example, support on Windows varies.
Examples

Specifying

\[ \text{link\_files} = '\text{siminput*.in} ' '/\text{path/to/simdir1} ' '\text{simdir2/*}' \]

will create copies

\[
\begin{align*}
\text{workdir/siminput*.in} & \quad \# \text{links to each of rundir / siminput*.in} \\
\text{workdir/simdir1/} & \quad \# \text{whole directory simdir1 linked} \\
\text{workdir/*} & \quad \# \text{each entry in directory simdir2 linked}
\end{align*}
\]

\text{copy\_files}

- Keywords Area
- interface
- analysis.drivers
- system
- work.directory
- copy.files

Files and directories to be copied into each working directory

Specification

Alias: none

Argument(s): STRINGLIST

Default: no copied files

Description

Specifies the files or directories that will be recursively copied into each working directory. Wildcards using * and ? are permitted.

Examples

Specifying

\[ \text{copy\_files} = '\text{siminput*.in} ' '/\text{path/to/simdir1} ' '\text{simdir2/*}' \]

will create copies

\[
\begin{align*}
\text{workdir/siminput*.in} & \quad \# \text{files rundir/siminput*.in copied} \\
\text{workdir/simdir1/} & \quad \# \text{whole directory simdir1 recursively copied} \\
\text{workdir/*} & \quad \# \text{contents of directory simdir2 recursively copied}
\end{align*}
\]

where rundir is the directory in which Dakota was started.
replace

- Keywords Area
- interface
- analysis_drivers
- system
- work_directory
- replace

Overwrite existing files within a work directory

**Specification**

Alias: none
Argument(s): none
Default: do not overwrite files

**Description**

By default, Dakota will not overwrite any existing files in a work directory. The `replace` keyword changes this behavior to force overwriting.

allow_existing_results

- Keywords Area
- interface
- analysis_drivers
- system
- allow_existing_results

Change how Dakota deals with existing results files

**Specification**

Alias: none
Argument(s): none
Default: results files removed before each evaluation

**Description**

By default Dakota will remove existing results files before invoking the `analysis_driver` to avoid problems created by stale files in the current directory. To override this behavior and not delete existing files, specify `allow_existing_results`.
CHAPTER 6. KEYWORDS AREA

verbatim

- Keywords Area
- interface
- analysis_drivers
- system
- verbatim

Specify the command Dakota uses to launch analysis driver(s) and filters

Specification

Alias: none  
Argument(s): none

Default: driver/filter invocation syntax augmented with file names

Description

The typical commands that Dakota uses to launch analysis drivers are:

```> analysis_driver parameters_file_name results_file_name```

Dakota will automatically arrange the executables and file names.
If the analysis driver requires a different syntax, the entire command can be specified as the analysis driver and the `verbatim` keyword will tell Dakota to use this as the command.

Note, this will not allow the use of `file_tag`, because the exact command must be specified.
For additional information on invocation syntax, see the Interfaces chapter of the Users Manual[4].

Examples

In the following example, the analysis_driver command is run without any edits from Dakota.

```interface
  analysis_driver = "matlab -nodesktop -nojvm -r 'MatlabDriver_hardcoded_filenames; exit' 
  fork
    parameters_file 'params.in'
    results_file 'results.out'
  verbatim # this tells Dakota to fork the command exactly as written, instead of appending I/O filenames```

The `-r` flag identifies the commands that will be run by matlab. The Matlab script has the parameters_file and results_file names hardcoded, so no additional arguments are required.

fork

- Keywords Area
- interface
- analysis_drivers
- fork

Launch analysis drivers using fork command
6.5. INTERFACE

Specification

Alias: none

Argument(s): none

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>parameters_file</td>
<td>file</td>
<td>Specify the name of the parameters file</td>
</tr>
<tr>
<td>Optional</td>
<td>results_file</td>
<td></td>
<td>Specify the name of the results file</td>
</tr>
<tr>
<td>Optional</td>
<td>file_tag</td>
<td></td>
<td>Tag each parameters &amp; results file name with the function evaluation number</td>
</tr>
<tr>
<td>Optional</td>
<td>file_save</td>
<td>file_save</td>
<td>Keep the parameters &amp; results files after the analysis driver completes</td>
</tr>
<tr>
<td>Optional</td>
<td>labeled</td>
<td>labeled</td>
<td>Requires correct function value labels in results file</td>
</tr>
<tr>
<td>Optional</td>
<td>aprepro</td>
<td>aprepro</td>
<td>Write parameters files in APREPRO syntax</td>
</tr>
<tr>
<td>Optional</td>
<td>work_directory</td>
<td>work_directory</td>
<td>Perform each function evaluation in a separate working directory</td>
</tr>
<tr>
<td>Optional</td>
<td>allow_existing_results</td>
<td>allow_existing_results</td>
<td>Change how Dakota deals with existing results files</td>
</tr>
<tr>
<td>Optional</td>
<td>verbatim</td>
<td>verbatim</td>
<td>Specify the command Dakota uses to launch analysis driver(s) and filters</td>
</tr>
</tbody>
</table>

Description

The fork interface is the most common means by which Dakota launches a separate application analysis process.

The fork interface is recommended over system for most analysis drivers that are external to Dakota, i.e., any driver not linked in via the direct interface.
As explained in the Users Manual, the parameters and results file names are passed on the command line to the analysis driver(s). If input/output filters are specified, they will be run before/after the analysis drivers. The `verbatim` keyword is used to modify the default driver/filter commands.

For additional information on invocation syntax, see the Interfaces chapter of the Users Manual[4].

**Examples**

Spawn (fork) an external executable/script called 'rosenbrock' which reads variables from params.in and writes responses to results.out. Preserve the analysis files for each function evaluation with tag and save.

```plaintext
interface
   analysis_drivers = 'rosenbrock'
   fork
      parameters_file = 'params.in'
      results_file  = 'results.out'
      file_tag
      file_save
```

**parameters_file**

- **Keywords Area**
- **interface**
- **analysis_drivers**
- **fork**
- **parameters_file**

Specify the name of the parameters file

**Specification**

**Alias:** none

**Argument(s):** STRING

**Default:** Unix temp files

**Description**

The parameters file is used by Dakota to pass the parameter values to the analysis driver. The name of the file can be optionally specified using the `parameters_file` keyword.

If this is not specified, the default data transfer files are temporary files with system-generated names (e.g., `/tmp/dakota_params_aaaa0886`).

**results_file**

- **Keywords Area**
- **interface**
- **analysis_drivers**
- **fork**
- **results_file**

Specify the name of the results file
6.5. INTERFACE

Specification

Alias: none
  Argument(s): STRING
  Default: Unix temp files

Description

The results file must be written by the analysis driver. It is read by Dakota to determine the response values for each function evaluation.

The name of the file can be optionally specified using the results_file keyword.

If this is not specified, the default data transfer files are temporary files with system-generated names (e.g., /tmp/dakota_results_aaaa0886).

file_tag

  - Keywords Area
  - interface
  - analysis_drivers
  - fork
  - file_tag

Tag each parameters & results file name with the function evaluation number

Specification

Alias: none
  Argument(s): none
  Default: no tagging

Description

If this keyword is used, Dakota will append a period and the function evaluation number to the names of the parameter and results files.

Default Behavior If this keyword is omitted, the default is no file tagging.

Usage Tips

  - File tagging is most useful when multiple function evaluations are running simultaneously using files in a shared disk space. The analysis driver will be able to infer the function evaluation number from the file names.

  - Note that when the file_save keyword is used, Dakota automatically renames parameters and results files, giving them tags after execution of the analysis driver if they otherwise would be overwritten by the next evaluation.
Examples
If the following is included in the interface section of the Dakota input:

```
parameters_file = params.in
results_file = results.out
file_tag
```

Then for the 3rd evaluation, Dakota will write `params.in.3`, and will expect `results.out.3` to be written by the analysis driver.

**file_save**
- Keywords Area
- interface
- analysis_drivers
- fork
- file_save

Keep the parameters & results files after the analysis driver completes

**Specification**
Alias: none
Argument(s): none
Default: file cleanup

**Description**
If **file_save** is used, Dakota will not delete the parameters and results files after the function evaluation is completed.

The default behavior is NOT to save these files.

If **file_tag** is not specified and the saved files would be overwritten by a future evaluation, Dakota renames them after the analysis driver has run by tagging them with the evaluation number.

File saving is most useful when debugging the data communication between Dakota and the simulation.

**labeled**
- Keywords Area
- interface
- analysis_drivers
- fork
- labeled

Requires correct function value labels in results file
Topics
This keyword is related to the topics:

- fileformats

Specification
Alias: none
  Argument(s): none
  Default: Function value labels optional

Description
The labeled keyword directs Dakota to enforce a stricter results file format and enables more detailed error reporting.

When the labeled keyword is used, function values in results files must be accompanied by their corresponding descriptors. If the user did not supply response descriptors in her Dakota input file, then Dakota auto-generated descriptors are expected.

Distinct error messages are emitted for function values that are out-of-order, repeated, or missing. Labels that appear without a function value and unexpected data are also reported as errors. Dakota attempts to report all errors in a results file, not just the first it encounters. After reporting results file errors, Dakota aborts.

Labels for analytic gradients and Hessians currently are not supported.

Although the labeled keyword is optional, its use is recommended to help catch and identify problems with results files. The User’s Manual contains further information about the results file format.

Default Behavior
By default, Dakota does not require labels for function values, and ignores them if they are present.

aprepro
  - Keywords Area
  - interface
  - analysis_drivers
  - fork
  - aprepro

Write parameters files in APREPRO syntax

Topics
This keyword is related to the topics:

- fileformats

Specification
Alias: dprepro
  Argument(s): none
  Default: standard parameters file format
CHAPTER 6. KEYWORDS AREA

Description
The format of data in the parameters files can be modified for direct usage with the APREPRO pre-processing tool \cite{aprepro} using the \texttt{aprepro} specification

Without this keyword, the parameters file are written in DPrePro format. DPrePro is a utility included with Dakota, described in the Users Manual\cite{dakota_users_manual}. 

\texttt{work\_directory}

- Keywords Area
- interface
- analysis\_drivers
- fork
- work\_directory

Perform each function evaluation in a separate working directory

Specification

Alias: none
Argument(s): none
Default: no work directory

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>named</td>
<td></td>
<td>The base name of the work directory created by Dakota</td>
</tr>
<tr>
<td>Optional</td>
<td>directory_tag</td>
<td></td>
<td>Tag each work directory with the function evaluation number</td>
</tr>
<tr>
<td>Optional</td>
<td>directory_save</td>
<td></td>
<td>Preserve the work directory after function evaluation completion</td>
</tr>
<tr>
<td>Optional</td>
<td>link_files</td>
<td></td>
<td>Paths to be linked into each working directory</td>
</tr>
</tbody>
</table>
Optional

| copy_files | Files and directories to be copied into each working directory

Optional

| replace | Overwrite existing files within a work directory

**Description**

When performing concurrent evaluations, it is typically necessary to cloister simulation input and output files in separate directories to avoid conflicts. When the `work_directory` feature is enabled, Dakota will create a directory for each evaluation, with optional tagging (`directory_tag`) and saving (`directory_save`), as with files, and execute the analysis driver from that working directory.

The directory may be named with a string, or left anonymous to use an automatically-generated directory in the system’s temporary file space, e.g., `/tmp/dakota_work_c93vb71z`. The optional `link_files` and `copy_files` keywords specify files or directories which should appear in each working directory.

When using `work_directory`, the `analysis_drivers` may be given by an absolute path, located in (or relative to) the startup directory alongside the Dakota input file, in the list of template files linked or copied, or on the `$PATH` (Path% on Windows).

- **named**
- Keywords Area
- `interface`
- `analysis_drivers`
- `fork`
- `work_directory`
- `named`

The base name of the work directory created by Dakota

**Specification**

**Alias:** none

**Argument(s):** STRING

**Default:** dakota_work_xxxxxxx

**Description**

The `named` keyword is followed by a string, indicating the name of the work directory created by Dakota. If relative, the work directory will be created relative to the directory from which Dakota is invoked.

If `named` is not used, the default work directory is a temporary directory with a system-generated name (e.g., `/tmp/dakota_work_c93vb71z`).
See Also
These keywords may also be of interest:

- directory.tag
- directory.save

**directory.tag**
- Keywords Area
- interface
- analysis_drivers
- fork
- work.directory
- directory.tag

Tag each work directory with the function evaluation number

**Specification**

**Alias:** dir.tag

**Argument(s):** none

**Default:** no work directory tagging

**Description**
If this keyword is used, Dakota will append a period and the function evaluation number to the work directory names.

If this keyword is omitted, the default is no tagging, and the same work directory will be used for ALL function evaluations. Tagging is most useful when multiple function evaluations are running simultaneously.

**directory.save**
- Keywords Area
- interface
- analysis_drivers
- fork
- work.directory
- directory.save

Preserve the work directory after function evaluation completion
6.5. INTERFACE

Specification
Alias: dir_save
Argument(s): none
Default: remove work directory

Description
By default, when a working directory is created by Dakota using the work_directory keyword, it is deleted after the evaluation is completed. The directory_save keyword will cause Dakota to leave (not delete) the directory.

link_files
- Keywords Area
- interface
- analysis_drivers
- fork
- work_directory
- link_files

Paths to be linked into each working directory

Specification
Alias: none
Argument(s): STRINGLIST
Default: no linked files

Description
Specifies the paths (files or directories) that will be symbolically linked from each working directory. Wildcards using * and ? are permitted. Linking is space-saving and useful for files not modified during the function evaluation. However, not all filesystems support linking, for example, support on Windows varies.

Examples
Specifying

    link_files = 'siminput*.in' '/path/to/simdir1' 'simdir2/*'

will create copies

    workdir/siminput*.in  # links to each of rundir / siminput*.in
    workdir/simdir1/      # whole directory simdir1 linked
    workdir/*             # each entry in directory simdir2 linked
copy_files

- Keywords Area
- interface
- analysis_drivers
- fork
- work_directory
- copy_files

Files and directories to be copied into each working directory

**Specification**

**Alias:** none

**Argument(s):** STRINGLIST

**Default:** no copied files

**Description**

Specifies the files or directories that will be recursively copied into each working directory. Wildcards using * and ? are permitted.

**Examples**

Specifying

```bash
copy_files = 'siminput*.in' '/path/to/simdir1' 'simdir2/*'
```

will create copies

```bash
workdir/siminput*.in # files rundir/siminput*.in copied
gw
workdir/simdir1/ # whole directory simdir1 recursively copied
workdir/* # contents of directory simdir2 recursively copied
```

where rundir is the directory in which Dakota was started.

**replace**

- Keywords Area
- interface
- analysis_drivers
- fork
- work_directory
- replace

Overwrite existing files within a work directory
6.5. INTERFACE

Specification

Alias: none
  Argument(s): none
  Default: do not overwrite files

Description

By default, Dakota will not overwrite any existing files in a work directory. The replace keyword changes this behavior to force overwriting.

allow_existing_results

- Keywords Area
- interface
- analysis_drivers
- fork
- allow_existing_results

Change how Dakota deals with existing results files

Specification

Alias: none
  Argument(s): none
  Default: results files removed before each evaluation

Description

By default Dakota will remove existing results files before invoking the analysis_driver to avoid problems created by stale files in the current directory. To override this behavior and not delete existing files, specify allow_existing_results.

verbatim

- Keywords Area
- interface
- analysis_drivers
- fork
- verbatim

Specify the command Dakota uses to launch analysis driver(s) and filters
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none
Argument(s): none
Default: driver/filter invocation syntax augmented with file names

Description

The typical commands that Dakota uses to launch analysis drivers are:

> analysis_driver parameters_file_name results_file_name

Dakota will automatically arrange the executables and file names.
If the analysis driver requires a different syntax, the entire command can be specified as the analysis driver
and the `verbatim` keyword will tell Dakota to use this as the command.
Note, this will not allow the use of `file_tag`, because the exact command must be specified.
For additional information on invocation syntax, see the Interfaces chapter of the Users Manual[4].

Examples

In the following example, the analysis_driver command is run without any edits from Dakota.

```
interface
  analysis_driver = "matlab -nodesktop -nojvm -r 'MatlabDriver_hardcoded_filenames; exit' "
  fork
    parameters_file 'params.in'
    results_file 'results.out'
    verbatim # this tells Dakota to fork the command exactly as written, instead of appending I/O filenames
```

The `-r` flag identifies the commands that will be run by matlab. The Matlab script has the parameters_file and
results_file names hardcoded, so no additional arguments are required.

```
direct
  keywords Area
  interface
  analysis_drivers
  direct
```

Run analysis drivers that are linked-to or compiled-with Dakota

Specification

Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Optional processors_per_analysis
Specify the number of processors per analysis when Dakota is run in parallel

Description

Direct interfaces are used to compile/link simulation programs into Dakota and to invoke Dakota’s built-in algebraic test problems.

Direct simulation interfaces communicate variable and response data in-core instead of through the filesystem. This typically requires modification to simulator programs so that they can be linked into Dakota; however it can be more efficient due to elimination of external processes and auxiliary simulator output, more accurate due to higher numerics, and more flexible in terms of MPI parallelism.

Direct interfaces are also used to invoke internal test functions that perform parameter to response mappings for simple functions as inexpensively as possible. These problems are compiled directly into the Dakota executable as part of the direct function interface class and are used for algorithm testing.

Dakota supports direct interfaces to a few select simulation codes such as Matlab, Python, and Scilab. Another example is ModelCenter, a commercial simulation management framework from Phoenix Integration. To utilize this interface, a user must first define the simulation specifics within a ModelCenter session and then save these definitions to a ModelCenter configuration file. The analysis_components specification provides the means to communicate this configuration file to Dakota’s ModelCenter interface.

Examples

The rosenbrock function is available as an executable, which can be launched with fork, and is also compiled with Dakota. The internal version can be used with:

```
interface
  analysis_drivers = 'rosenbrock'
  direct
```

processors_per_analysis

- Keywords Area
- interface
- analysis_drivers
- direct
- processors_per_analysis

Specify the number of processors per analysis when Dakota is run in parallel

Topics

This keyword is related to the topics:

- concurrency_and_parallelism
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none

Argument(s): INTEGER

Default: automatic (see discussion)

Description

For direct function interfaces, *processors_per_analysis* can be used to specify multiprocessor analysis partitions. As with the *evaluation_servers*, *analysis_servers*, *analysis_self_scheduling*, *evaluation_static_scheduling*, *analysis_self_scheduling*, and *analysis_static_scheduling* specifications, *processors_per_analysis* provides a means for the user to override the automatic parallel configuration (refer to ParallelLibrary and the Parallel Computing chapter of the Users Manual [4]) for the number of processors used for each analysis partition.

Usage Tips

- If both *analysis_servers* and *processors_per_analysis* are specified and they are not in agreement, then *analysis_servers* takes precedence.

matlab

- Keywords Area
- interface
- *analysis_drivers*
- *matlab*

Run Matlab through a direct interface - requires special Dakota build

Specification

Alias: none

Argument(s): none

Description

Dakota supports a library-linked interface to Matlab, but it must be explicitly enabled when compiling Dakota from source. Consult the Users Manual[4] for discussion and examples. Contact the Dakota users mailing list for assistance building and using Dakota with these interfaces.

The *analysis_drivers* specifies a Matlab file which implements the parameter to response mapping.

Examples

See dakota/examples/linked_interfaces/Matlab
Run Python through a direct interface - requires special Dakota build

### Specification

**Alias:** none

<table>
<thead>
<tr>
<th>Argument(s): none</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Required/Optional</strong></td>
</tr>
<tr>
<td>---------------------</td>
</tr>
<tr>
<td>numpy</td>
</tr>
</tbody>
</table>

**Description**

Dakota supports a library-linked interface to Python, but it must be explicitly enabled when compiling Dakota from source. Consult the Users Manual[4] for discussion and examples. Contact the Dakota users mailing list for assistance building and using Dakota with these interfaces.

The `analysis_drivers` specifies a Python module:function which implements the parameter to response mapping. List data structures are the default, but NumPy is also supported, if enabled in the build.

**Examples**

See dakota/examples/linked_interfaces/Python

**numpy**

- **Keywords Area**
- **interface**
- **analysis_drivers**
- **python**
- **numpy**

Enable the use of numpy in Dakota’s Python interface

### Specification

**Alias:** none

**Argument(s):** none

**Default:** Python list dataflow
CHAPTER 6. KEYWORDS AREA

Description

When the numpy keyword is used, Dakota expects responses in the form of a Python dictionary of numpy arrays. See the example in examples/linked_interfaces/Python.

scilab

- Keywords Area
- interface
- analysis_drivers
- scilab

Run Scilab through a direct interface - requires special Dakota build

Specification

Alias: none

Argument(s): none

Description

Dakota supports a library-linked interface to Scilab, but it must be explicitly enabled when compiling Dakota from source. Consult the Users Manual[4] for discussion and examples. Contact the Dakota users mailing list for assistance building and using Dakota with these interfaces.

The analysis_drivers specifies a Scilab file which implements the parameter to response mapping.

Examples

See dakota/examples/linked_interfaces/Scilab

grid

- Keywords Area
- interface
- analysis_drivers
- grid

Deprecated grid computing interface

Specification

Alias: none

Argument(s): none
6.5. INTERFACE

Description

Interface Dakota directly to a grid (distributed) computing engine. This deprecated capability was historically used for interfaces with IDEA and JAVASpaces in the past and was intended as a placeholder for future work with Condor and/or Globus services. It is not currently operational.

**analysis_components**

- **Keywords Area**
- **interface**
- **analysis_drivers**
- **analysis_components**

Provide additional identifiers to analysis drivers.

Specification

**Alias:** none

**Argument(s):** STRINGLIST

**Default:** no additional identifiers

Description

The optional `analysis_components` specification allows the user to provide additional identifiers (e.g., mesh file names) for use by the analysis drivers. This is particularly useful when the same analysis driver is to be reused multiple times for slightly different analyses. The specific content within the strings is open-ended and can involve whatever syntax is convenient for a particular analysis driver. The number of analysis components $n_c$ should be an integer multiple of the number of drivers $n_d$, and the first $n_c/n_d$ component strings will be passed to the first driver, etc.

6.5.3 **algebraic_mappings**

- **Keywords Area**
- **interface**
- **algebraic_mappings**

Use AMPL to define algebraic input-output mappings

Specification

**Alias:** none

**Argument(s):** STRING

**Default:** no algebraic mappings
CHAPTER 6. KEYWORDS AREA

Description

Dakota can evaluate algebraic input-output mappings using AMPL [26]. The mappings are expressed in 3 files: stub.nl, stub.col, and stub.row, where stub is a particular root name describing a particular problem. The file names are communicated to Dakota using the algebraic_mappings keyword. It may either specify the full stub.nl filename, or alternatively, just the stub basename.

Dakota then extracts the input and output identifier strings from stub.col and stub.row and employs the AMPL solver library [29] to process the directed acyclic graph (DAG) specification in stub.nl. The variable and objective function names declared within AMPL should be a subset of the variable and response descriptors specified in the variables and responses blocks. Ordering is not important, as Dakota will reorder data as needed.

Examples

An interface employing both algebraic and simulation-based mappings. The results from the individual algebraic and simulation mappings are overlaid based on the variable and response descriptors used by the individual mappings.

interface,
  algebraic_mappings = 'ampl/fma.nl'
  fork
    analysis_driver = 'text_book'
    parameters_file = 'tb.in'
    results_file = 'tb.out'

6.5.4 failure_capture

- Keywords Area
- interface
- failure_capture

Determine how Dakota responds to analysis driver failure

Specification

Alias: none
Argument(s): none
Default: abort

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required (Choose One)</td>
<td>Failure Mitigation (Group 1)</td>
<td>abort</td>
<td>(Default) Abort the Dakota job</td>
</tr>
<tr>
<td></td>
<td></td>
<td>retry</td>
<td>Rerun failed analyses</td>
</tr>
</tbody>
</table>
Description

Dakota can deal with analysis failure in a few ways.

The first step is that Dakota must detect analysis failure. Importantly, Dakota always expects a results file to be written by the analysis driver, even when a failure has occurred. If the file does not exist when the analysis driver exits, a Dakota error results, causing Dakota itself to terminate. The analysis driver communicates an analysis failure to Dakota by writing a results file beginning with the (case-insensitive) word “fail”. Any file contents after “fail” are ignored.

Once Dakota detects analysis failure, the failure can be mitigated in four ways:

- interface-analysis_drivers-failure_capture-abort (the default)
- interface-analysis_drivers-failure_capture-retry
- interface-analysis_drivers-failure_capture-recover
- interface-analysis_drivers-failure_capture-continuation


abort

- Keywords Area
- interface
- failure_capture
- abort

(Default) Abort the Dakota job

Specification

Alias: none

Argument(s): none

Description

Stop the Dakota job, as well as any other running analysis drivers when a failure is communicated.
retry

- Keywords Area
- interface
- failure_capture
- retry

Rerun failed analyses

Specification

Alias: none
Argument(s): INTEGER

Description

Number of times to retry a failing analysis

recover

- Keywords Area
- interface
- failure_capture
- recover

Substitute dummy values for the responses

Specification

Alias: none
Argument(s): REALLIST

Description

When a simulation failure is detected, substitute the provided dummy function values in the response. Gradient and Hessian are not supported.

continuation

- Keywords Area
- interface
- failure_capture
- continuation

Cause Dakota to step toward the failed "target" simulation from a nearby successful "source"
6.5. INTERFACE

Specification

Alias: none
  Argument(s): none

Description

When failure_capture continuation is enabled and an evaluation fails, then Dakota will attempt to
march incrementally from a previous good evaluation (the "source") toward the failing one (the "target"). Further
details about the algorithm employed by Dakota are supplied in the User's Manual [4].

6.5.5 deactivate

- Keywords Area
- interface
- deactivate

Deactivate Dakota interface features for simplicity or efficiency

Specification

Alias: none
  Argument(s): none

Default: Active set vector control, function evaluation cache, and restart file features are active

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>active_set_vector</td>
<td>Deactivate the Active Set Vector</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>evaluation_cache</td>
<td>Do not retain function evaluation history in memory</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>strict_cache_-_equality</td>
<td>Do not require strict cache equality when finding duplicates</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>restart_file</td>
<td>Deactivate writing to the restart file</td>
</tr>
</tbody>
</table>

Description

The optional deactivate specification block allows a user to deactivate interface features in order to simplify
interface development, increase execution speed, and/or reduce memory and disk requirements. Any or all of
these features may be specified concurrently.
Active set vector (ASV) control: deactivate so that Dakota expects the same response data (all functions, gradients, Hessian) back from the simulation on every evaluation, instead of only those components required by the method for this particular function evaluation.

Function evaluation cache: save memory by not caching the function evaluation history. May result in additional (duplicate) function evaluations.

Strict cache equality: allow a relaxed tolerance when detecting duplicate function evaluations. Can be useful when importing data or restarting across machines.

Restart file: improve efficiency and eliminate restart file storage at the risk of not being able to recover a failed or partial Dakota study.

Deactivate the Active Set Vector

Alias: none
Argument(s): none

Description

Allows the user to turn off any variability in ASV values so that active set logic can be omitted in the user’s simulation interface. This option trades some efficiency for simplicity in interface development.

The default behavior is to request the minimum amount of data required by an algorithm at any given time, which implies that the ASV values may vary from one function evaluation to the next. Since the user’s interface must return the data set requested by the ASV values, this interface must contain additional logic to account for any variations in ASV content.

Deactivating this ASV control causes Dakota to always request a “full” data set (the full function, gradient, and Hessian data that is available from the interface as specified in the responses specification) on each function evaluation.

For example, if ASV control has been deactivated and the responses section specifies four response functions, analytic gradients, and no Hessians, then the ASV on every function evaluation will be \{3 3 3 3\}, regardless of what subset of this data is currently needed. While wasteful of computations in many instances, this simplifies the interface and allows the user to return the same data set on every evaluation. Conversely, if ASV control is active (the default behavior), then the ASV requests in this example might vary from \{1 1 1 1\} to \{2 0 0 2\}, etc., according to the specific data needed on a particular function evaluation. This will require the user’s interface to read the ASV requests and perform the appropriate logic in conditionally returning only the data requested.

Usage Tips

- In general, the default ASV behavior is recommended for the sake of computational efficiency, unless interface development time is a critical concern.
6.5. INTERFACE

- Whether active or inactive, the data returned to Dakota from the user's interface must match the ASV passed in, or else a response recovery error will result. However, when the ASV control is deactivated, the ASV values are invariant and need not be checked on every evaluation.

- Deactivating the ASV control can have a positive effect on load balancing for parallel Dakota executions. Thus, there is significant overlap in this ASV control option with speculative gradients. There is also overlap with the mode override approach used with certain optimizers to combine individual value, gradient, and Hessian requests.

evaluation_cache

- Keywords Area
- interface
- deactivate
- evaluation_cache

Do not retain function evaluation history in memory

Specification

Alias: none

Argument(s): none

Description

Do not retain the complete function evaluation history in memory.

This can be important for reducing memory requirements in large-scale applications (i.e., applications with a large number of variables or response functions) and for eliminating the overhead of searching for duplicates within the function evaluation cache prior to each new function evaluation (e.g., for improving speed in problems with 1000's of inexpensive function evaluations or for eliminating overhead when performing timing studies).

However, the downside is that unnecessary computations may be performed since duplication in function evaluation requests may not be detected. For this reason, this option is not recommended when function evaluations are costly.

Note: duplication detection within Dakota can be deactivated, but duplication detection features within specific optimizers may still be active.

strict_cache_equality

- Keywords Area
- interface
- deactivate
- strict_cache_equality

Do not require strict cache equality when finding duplicates

Specification

Alias: none

Argument(s): none
<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional Optional</td>
<td>Group</td>
<td>cache_tolerance</td>
<td>Specify tolerance when identifying duplicate function evaluations</td>
</tr>
</tbody>
</table>

**Description**

By default, Dakota’s evaluation cache and restart capabilities are based on strict binary equality. This provides a performance advantage, as it permits a hash-based data structure to be used to search the evaluation cache. However, deactivating strict equality may prevent cache misses, which can occur when attempting to use a restart file on a machine different from the one on which it was generated.

**cache_tolerance**

- Keywords Area
- interface
- deactivate
- strict_cache_equality
- cache_tolerance

Specify tolerance when identifying duplicate function evaluations

**Specification**

**Alias:** none

**Argument(s):** REAL

**Description**

Described on parent page

**Restart_file**

- Keywords Area
- interface
- deactivate
- restart_file

Deactivate writing to the restart file

**Specification**

**Alias:** none

**Argument(s):** none
Description

Eliminate the output of each new function evaluation to the binary restart file. This can increase speed and reduce disk storage requirements, but at the expense of a loss in the ability to recover and continue a run that terminates prematurely (e.g., due to a system crash or network problem).

Usage Tips

• This option is not recommended when function evaluations are costly or prone to failure.

• Using the `deactivate restart_file` specification will result in a zero length restart file with the default name `dakota.rst`.

6.5.6 asynchronous

• Keywords Area

• interface

• asynchronous

Specify local evaluation or analysis concurrency

Topics

This keyword is related to the topics:

• concurrency_and_parallelism

Specification

Alias: none

Argument(s): none

Default: synchronous interface usage

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>Evaluation_concurrency</td>
<td>local_evaluation_scheduling</td>
<td>Determine how many concurrent evaluations Dakota will schedule. Control how local asynchronous jobs are scheduled.</td>
</tr>
<tr>
<td>Optional</td>
<td>Analysis_concurrency</td>
<td>analysis_concurrency</td>
<td>Limit the number of analysis drivers within an evaluation that Dakota will schedule.</td>
</tr>
</tbody>
</table>
CHAPTER 6. KEYWORDS AREA

Description

The optional asynchronous keyword specifies use of asynchronous protocols (i.e., background system calls, nonblocking forks, POSIX threads) when evaluations or analyses are invoked. Evaluation and analysis concurrency can be independently controlled, as can the scheduling mode (static vs. dynamic) of the local evaluations.

Default Behavior

- when running Dakota on a single processor in asynchronous mode, the default concurrency of evaluations and analyses is all concurrency that is available. The evaluation_concurrency and analysis_concurrency specifications can be used to limit this concurrency in order to avoid machine overload or usage policy violation.

- when running Dakota on multiple processors in message passing mode, the default concurrency of evaluations and analyses on each of the servers is one (i.e., the parallelism is exclusively that of the message passing). With the evaluation_concurrency and analysis_concurrency specifications, a hybrid parallelism can be selected through combination of message passing parallelism with asynchronous parallelism on each server.

evaluation_concurrency

- Keywords Area

- interface

- asynchronous

- evaluation_concurrency

Determine how many concurrent evaluations Dakota will schedule

Topics

This keyword is related to the topics:

- concurrency_and_parallelism

Specification

Alias: none

Argument(s): INTEGER

Default: local: unlimited concurrency, hybrid: no concurrency

Description

When asynchronous execution is enabled, the default behavior is to launch all available evaluations simultaneously. The evaluation_concurrency keyword can be used to limit the number of concurrent evaluations.
6.5. INTERFACE

local_evaluation_scheduling

- **Keywords Area**
- interface
- asynchronous
- local_evaluation_scheduling

Control how local asynchronous jobs are scheduled

**Topics**

This keyword is related to the topics:

- concurrency_and_parallelism

**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** dynamic

| Required/- | Description of Group Scheduling Mode (Group 1) | Dakota Keyword | Dakota Keyword Description |
| Optional | dynamic | static | Static local scheduling (tiled) |

| Required/- | Description of Group Scheduling Mode (Group 1) | Dakota Keyword | Dakota Keyword Description |
| Optional | dynamic | static | Static local scheduling (tiled) |

**Description**

When performing asynchronous local evaluations, the local_evaluation_scheduling keyword controls how new evaluation jobs are dispatched when one completes.

The two options are:

- dynamic
- static

If the local_evaluation_scheduling is specified as dynamic (the default), each completed evaluation will be replaced by the next in the local evaluation queue.

If local_evaluation_scheduling is specified as static, each completed evaluation will be replaced by an evaluation number that is congruent modulo the evaluation_concurrency. This is helpful for relative node scheduling as described in dakota/examples/parallelism. For example, assuming only asynchronous local concurrency (no MPI), if the local concurrency is 6 and job 2 completes, it will be replaced with job 8.

For the case of hybrid parallelism, static local scheduling results in evaluation replacements that are modulo the total capacity, defined as the product of the evaluation concurrency and the number of evaluation servers. Both of these cases can result in idle processors if runtimes are non-uniform, so the default dynamic scheduling is preferred when relative node scheduling is not required.
Dynamic local scheduling (sequential)

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

If the local_evaluation_scheduling is specified as dynamic (the default), each completed evaluation will be replaced by the next in the local evaluation queue.

Static local scheduling (tiled)

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

If local_evaluation_scheduling is specified as static, each completed evaluation will be replaced by an evaluation number that is congruent modulo the evaluation_concurrency. This is helpful for relative node scheduling as described in Dakota/examples/parallelism. For example, assuming only asynchronous local concurrency (no M-P)I, if the local concurrency is 6 and job 2 completes, it will be replaced with job 8.

For the case of hybrid parallelism, static local scheduling results in evaluation replacements that are modulo the total capacity, defined as the product of the evaluation concurrency and the number of evaluation servers. Both of these cases can result in idle processors if runtimes are non-uniform, so the default dynamic scheduling is preferred when relative node scheduling is not required.
6.5. INTERFACE

analysis_concurrency

- Keywords Area
- interface
- asynchronous
- analysis_concurrency

Limit the number of analysis drivers within an evaluation that Dakota will schedule

Topics
This keyword is related to the topics:
- concurrency_and_parallelism

Specification
Alias: none
Argument(s): INTEGER
Default: local: unlimited concurrency, hybrid: no concurrency

Description
When asynchronous execution is enabled and each evaluation involves multiple analysis drivers, then the default behavior is to launch all drivers simultaneously. The analysis_concurrency keyword can be used to limit the number of concurrently run drivers.

6.5.7 evaluation_servers

- Keywords Area
- interface
- evaluation_servers

Specify the number of evaluation servers when Dakota is run in parallel

Topics
This keyword is related to the topics:
- concurrency_and_parallelism

Specification
Alias: none
Argument(s): INTEGER
Default: automatic (see discussion)
Description

The optional `evaluation_servers` specification supports user override of the automatic parallel configuration for the number of evaluation servers. That is, if the automatic configuration is undesirable for some reason, the user can enforce a desired number of partitions at the evaluation parallelism level. Refer to ParallelLibrary and the Parallel Computing chapter of the Users Manual [4] for additional information.

6.5.8 `evaluation_scheduling`

- Keywords Area
- interface
- `evaluation_scheduling`

Specify the scheduling of concurrent evaluations when Dakota is run in parallel

Specification

Alias: none

*Argument(s)*: none

*Default*: automatic (see discussion)

<table>
<thead>
<tr>
<th>Required/-Optional Required (Choose One)</th>
<th>Description of Group Server Mode (Group 1)</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>master</td>
<td>Specify a dedicated master partition for parallel evaluation scheduling</td>
</tr>
<tr>
<td></td>
<td></td>
<td>peer</td>
<td>Specify a peer partition for parallel evaluation scheduling</td>
</tr>
</tbody>
</table>

Description

When Dakota is run in parallel, the partition type and scheduling for the evaluation servers are determined automatically. If these settings are undesirable, they may be overridden by the user using the `evaluation_scheduling` keyword.

`master`

- Keywords Area
- interface
- `evaluation_scheduling`
- `master`

Specify a dedicated master partition for parallel evaluation scheduling
6.5. INTERFACE

**Topics**

This keyword is related to the topics:

- concurrency_and_parallelism

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

This option overrides the Dakota parallel automatic configuration, forcing the use of a dedicated master partition. In a dedicated master partition, one processor (the "master") dynamically schedules work on the evaluation servers. This reduces the number of processors available to create servers by 1.

peer

- **Keywords Area**
- interface
- evaluation_scheduling
- peer

Specify a peer partition for parallel evaluation scheduling

**Topics**

This keyword is related to the topics:

- concurrency_and_parallelism

**Specification**

**Alias:** none

**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/-Optional Required</th>
<th>Description of Group Scheduling Mode (Group 1)</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>dynamic</td>
<td>Specify dynamic scheduling in a peer partition when Dakota is run in parallel.</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Specify static scheduling in a peer partition when Dakota is run in parallel.

**Description**

This option overrides the Dakota parallel automatic configuration, forcing the use of a peer partition. In a peer partition, all processors are available to be assigned to evaluation servers. The scheduling, static or dynamic, must also be specified.

**dynamic**

- **Keywords Area**
- **interface**
- **evaluation_scheduling**
- **peer**
- **dynamic**

Specify dynamic scheduling in a peer partition when Dakota is run in parallel.

**Topics**

This keyword is related to the topics:

- concurrency_and_parallelism

**Specification**

Alias: none

**Argument(s):** none

**Default:** dynamic (see discussion)

**Description**

In dynamic scheduling, evaluations are assigned to servers as earlier evaluations complete. Dynamic scheduling is advantageous when evaluations are of uneven duration.

**static**

- **Keywords Area**
- **interface**
- **evaluation_scheduling**
- **peer**
- **static**

Specify static scheduling in a peer partition when Dakota is run in parallel.
6.5. INTERFACE

**Topics**
This keyword is related to the topics:

- concurrency_and_parallelism

**Specification**

**Alias:** none

**Argument(s):** none

**Description**
In static scheduling, all available evaluations are assigned to servers in a predetermined fashion. Each completed evaluation is replaced with one congruent modulo the evaluation concurrency. For example, with 6 servers, eval number 2 will be replaced by eval number 8.

### 6.5.9 processors_per_evaluation

- Keywords Area
- interface
- processors_per_evaluation

Specify the number of processors per evaluation server when Dakota is run in parallel

**Topics**
This keyword is related to the topics:

- concurrency_and_parallelism

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** automatic (see discussion)

**Description**
The optional `processors_per_evaluation` specification supports user override of the automatic parallel configuration for the number of processors in each evaluation server. That is, if the automatic configuration is undesirable for some reason, the user can enforce a desired server size at the evaluation parallelism level. Refer to ParallelLibrary and the Parallel Computing chapter of the Users Manual [4] for additional information.

### 6.5.10 analysis_servers

- Keywords Area
- interface
- analysis_servers

Specify the number of analysis servers when Dakota is run in parallel
Topics
This keyword is related to the topics:

- `concurrency_and_parallelism`

Specification
Alias: none
Argument(s): INTEGER
Default: automatic (see discussion)

Description
The optional `analysis_servers` specification supports user override of the automatic parallel configuration for the number of analysis servers. That is, if the automatic configuration is undesirable for some reason, the user can enforce a desired number of partitions at the analysis parallelism level. Refer to ParallelLibrary and the Parallel Computing chapter of the Users Manual [4] for additional information.

6.5.11  analysis_scheduling

- Keywords Area
- interface
- `analysis_scheduling`

Specify the scheduling of concurrent analyses when Dakota is run in parallel.

Topics
This keyword is related to the topics:

- `concurrency_and_parallelism`

Specification
Alias: none
Argument(s): none
Default: automatic (see discussion)

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group Scheduling Mode (Group 1)</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required</td>
<td>master</td>
<td>Specify a dedicated master partition for parallel analysis scheduling</td>
</tr>
</tbody>
</table>
**6.5. INTERFACE**

| peer          | Specify a peer partition for parallel analysis scheduling |

**Description**

When Dakota is run in parallel, the partition type for the analysis servers is determined automatically. If this setting is undesirable, it may be overridden by the user using the `analysis_scheduling` keyword.

**master**

- Keywords Area
- interface
- analysis_scheduling
- master

Specify a dedicated master partition for parallel analysis scheduling

**Topics**

This keyword is related to the topics:

- concurrency_and_parallelism

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

This option overrides the Dakota parallel automatic configuration, forcing the use of a dedicated master partition. In a dedicated master partition, one processor (the "master") dynamically schedules work on the analysis servers. This reduces the number of processors available to create servers by 1.

**peer**

- Keywords Area
- interface
- analysis_scheduling
- peer

Specify a peer partition for parallel analysis scheduling
CHAPTER 6. KEYWORDS AREA

Topics
This keyword is related to the topics:

- concurrency and parallelism

Specification
Alias: none
Argument(s): none

Description
This option overrides the Dakota parallel automatic configuration, forcing the use of a peer partition. In a peer partition, all processors are available to be assigned to analysis servers. Note that unlike the case of evaluation-scheduling, it is not possible to specify static or dynamic.

6.6 responses

- Keywords Area
- responses

Description of the model output data returned to Dakota upon evaluation of an interface.

Topics
This keyword is related to the topics:

- block

Specification
Alias: none
Argument(s): none

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>Group</td>
<td>id_responses</td>
<td>Description</td>
</tr>
</tbody>
</table>

Name the responses block; helpful when there are multiple.
<table>
<thead>
<tr>
<th>Optional</th>
<th>Required (Choose One)</th>
<th>response type (Group 1)</th>
<th>descriptors</th>
<th>Labels for the responses</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>objective_functions</td>
<td>Response type suitable for optimization</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>calibration_terms</td>
<td>Response type suitable for calibration or least squares</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>response_functions</td>
<td>Generic response type</td>
</tr>
<tr>
<td></td>
<td>Required (Choose One)</td>
<td>gradient type (Group 2)</td>
<td>no_gradients</td>
<td>Gradients will not be used</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>analytic_gradients</td>
<td>Analysis driver will return gradients</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>mixed_gradients</td>
<td>Gradients are needed and will be obtained from a mix of numerical and analytic sources</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>numerical_gradients</td>
<td>Gradients are needed and will be approximated by finite differences</td>
</tr>
<tr>
<td></td>
<td>Required (Choose One)</td>
<td>Hessian type (Group 3)</td>
<td>no_hessians</td>
<td>Hessians will not be used</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>numerical_hessians</td>
<td>Hessians are needed and will be approximated by finite differences</td>
</tr>
</tbody>
</table>
CHAPTER 6. KEYWORDS AREA

| quasi_hessians | Hessians are needed and will be approximated by secant updates (BFGS or SR1) from a series of gradient evaluations |
| analytic_hessians | Hessians are needed and are available directly from the analysis driver |
| mixed_hessians | Hessians are needed and will be obtained from a mix of numerical, analytic, and “quasi” sources |

Description

The responses specification in a Dakota input file indicates the types of data that can be returned by an interface when invoked during Dakota’s execution. The specification includes three groups and two optional keywords.

**The response type group** indicates the type and number of responses expected by Dakota. It must be one of three types:

1. Optimization: objective and constraint functions
2. Calibration: calibration (least squares) terms and constraint functions
3. Uncertainty Quantification: generic response functions

The response type specified should be consistent with the iterative technique called for in the method specification. Certain general-purpose iterative techniques, such as parameter studies and design of experiments methods, can be used with any of these response types.

**The gradient type group** indicates the availability of first derivatives (gradient vectors) for the response functions.

The gradient specification also links back to the iterative method used. Gradients commonly are needed when the iterative study involves gradient-based optimization, local reliability analysis for uncertainty quantification, or local sensitivity analysis. They can optionally be used to build some types of surrogate models.

**The Hessian type group** specifies the availability of second derivatives (Hessian matrices) for the response functions.

Hessian availability for the response functions is similar to the gradient availability specifications, with the addition of support for “quasi-Hessians”. The Hessian specification also links back to the iterative method in use; Hessians commonly would be used in gradient-based optimization by full Newton methods or in reliability analysis with second-order limit state approximations or second-order probability integrations.
6.6. RESPONSES

Examples

Several examples follow. The first example shows an optimization data set containing an objective function and two nonlinear inequality constraints. These three functions have analytic gradient availability and no Hessian availability.

```
responses
    objective_functions = 1
    nonlinear_inequality_constraints = 2
    analytic_gradients
    no_hessians
```

The next example shows a typical specification for a calibration data set. The six residual functions will have numerical gradients computed using the dakota finite differencing routine with central differences of 0.1% (plus/minus delta relative to current variables value = .001*value).

```
responses
    calibration_terms = 6
    numerical_gradients
    method_source dakota
    interval_type central
    fd_gradient_step_size = .001
    no_hessians
```

The last example shows a generic specification that could be used with a nondeterministic sampling iterator. The three response functions have no gradient or Hessian availability; therefore, only function values will be used by the iterator.

```
responses
    response_functions = 3
    no_gradients
    no_hessians
```

Parameter study and design of experiments iterators are not restricted in terms of the response data sets which may be catalogued; they may be used with any of the function specification examples shown above.

Theory

Responses specify the total data set that is available for use by the method over the course of iteration. This is distinguished from the data subset described by an active set vector (see Dakota File Data Formats in the Users Manual [Adams et al., 2010]) indicating the particular subset of the response data needed for a particular function evaluation. Thus, the responses specification is a broad description of the data to be used during a study whereas the active set vector indicates the subset currently needed.

6.6.1 id_responses

- Keywords Area
- responses
- id_responses

Name the responses block; helpful when there are multiple
CHAPTER 6. KEYWORDS AREA

Topics
This keyword is related to the topics:

- block_identifier

Specification
Alias: none
Argument(s): STRING
Default: use of last responses parsed

Description
The optional id_responses keyword accepts a string that uniquely identifies this responses block. A model can then use these responses by specifying the same string in its responses_pointer specification.

Default Behavior
If the id_responses specification is omitted, a particular responses specification will be used by a model only if that model does not include an responses_pointer and the responses block was the last (or only) one parsed.

Usage Tips
- It is a best practice to always use explicit responses IDs and pointers to avoid confusion.
- If only one responses block exists, then id_responses can be safely omitted from the responses block (and responses_pointer omitted from the model specification(s)), since there is no ambiguity.

Examples
For example, a model specification including

model
  responses_pointer = 'R1'

will link to a response set with

  id_responses = 'R1'

6.6.2 descriptors

- Keywords Area
- responses
- descriptors

Labels for the responses

Specification
Alias: response_descriptors
Argument(s): STRINGLIST
Default: root strings plus numeric identifiers
6.6. RESPONSES

Description
A list of strings which identify the responses. These are used in console and tabular output. Response descriptors are ordered by primary response functions (objective, calibration, or response functions), followed by inequality, then equality constraints, if present.

Default Behavior
The default descriptor strings use a response type-dependent root string plus a one-based numeric identifier:

- Objective functions: obj_fn_i
- Calibration terms: least_sq_term_i
- Nonlinear inequality constraints: nln_ineq_con_i
- Nonlinear equality constraints: nln_eq_con_i
- Response functions: response_fn

Expected Output
Dakota will label the various response functions in console and tabular output.

Usage Tips
When specifying descriptors for scalar and/or field responses, include as many descriptors as top-level scalar + field responses, e.g.,

responses
descriptors 'scalar1' 'scalar2' 'scalar3' 'field1' 'field2'
response_functions 5
scalar_responses 3
field_responses 2
field_lengths 42 24

Dakota will append a numeric identifier for each field entry, for a total of 42 field1_j and 24 field2_k in this example.

Examples

responses
descriptors 'cost' 'impact' 'safety'
ojective_functions 2
nonlinear_inequality_constraints 1

6.6.3 objective_functions

- Keywords Area
- responses
- objective_functions

Response type suitable for optimization

Specification
Alias: num_objective_functions
Argument(s): INTEGER
### Description

Specifies the number (1 or more) of objective functions returned to Dakota.

### Constraints

The keywords `nonlinear_inequality_constraints` and `nonlinear_equality_constraints` specify the number of nonlinear inequality constraints, and nonlinear equality constraints, respectively. When interfacing to external applications, the responses must be returned to Dakota in this order: objective functions, nonlinear_inequality_constraints, then nonlinear_equality_constraints.

Any linear constraints present in an application need only be input to an optimizer at start up and do not need to be part of the data returned on every function evaluation. These are therefore specified in the `method` block.

Bounds on the design variables are specified in the `variables` block.

### Optional Keywords

The optional keywords relate to scaling the objective functions (for better numerical results), formulating the problem as minimization or maximization, and dealing with multiple objective functions. If scaling is used, it is applied before multi-objective weighted sums are formed.

| Required/-  
<table>
<thead>
<tr>
<th>Optional</th>
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<tbody>
<tr>
<td>Optional</td>
</tr>
<tr>
<td>Definition of</td>
</tr>
<tr>
<td>Group</td>
</tr>
<tr>
<td>sense</td>
</tr>
<tr>
<td>primary_scale_types</td>
</tr>
<tr>
<td>primary_scales</td>
</tr>
<tr>
<td>weights</td>
</tr>
<tr>
<td>nonlinear_inequality_constraints</td>
</tr>
<tr>
<td>nonlinear_equality_constraints</td>
</tr>
<tr>
<td>scalar_objectives</td>
</tr>
<tr>
<td>field_objectives</td>
</tr>
</tbody>
</table>
6.6. RESPONSES

See Also

These keywords may also be of interest:

- calibration_terms
- response_functions
- method
- variables

**sense**

- Keywords Area
- responses
- objective_functions
- sense

Whether to minimize or maximize each objective function

**Specification**

**Alias:** none

**Argument(s):** STRINGLIST

**Default:** vector values = 'minimize'

**Description**

The `sense` keyword is used to declare whether each objective function should be minimized or maximized. The argument options are:

- "minimization" (can be abbreviated to "min")
- "maximization" (can be abbreviated to "max")

The number of strings should either be equal to the number of objective functions, or one. If a single string is specified it will apply to each objective function.

**primary_scale_types**

- Keywords Area
- responses
- objective_functions
- primary_scale_types

Choose a scaling type for each response
CHAPTER 6. KEYWORDS AREA

Specification

Alias: objective_function_scale_types
Argument(s): STRINGLIST
Default: no scaling

Description

The primary_scale_types keyword specifies one or number of primary functions strings indicating the scaling type for each response value in methods that support scaling, when scaling is enabled. If only one type is specified, it will apply to each primary response function.

See the scaling information under specific methods, e.g., method-+-scaling for details on how to use this keyword.

Note that primary response functions (objective, calibration, or response functions) cannot be automatically scaled due to lack of bounds, so valid scale types are ‘none’ ‘value’ and ‘log’.

If scaling is specified, it is applied before multi-objective weighted sums are formed.

primary_scales
- Keywords Area
- responses
- objective_functions
- primary_scales

Supply a characteristic value to scale each response

Specification

Alias: objective_function_scales
Argument(s): REALLIST
Default: 1.0 (no scaling)

Description

Each entry in primary_scales is a user-specified nonzero characteristic value to scale each response. The argument may be of length 1 or the number of primary response functions. If only one scale is specified, it will apply to each primary response function.

See the scaling information under specific methods, e.g., method-+-scaling for details on how to use this keyword.

If scaling is specified, it is applied before multi-objective weighted sums are formed.

weights
- Keywords Area
- responses
- objective_functions
- weights

Specify weights for each objective function
6.6. RESPONSES

**Specification**

*Alias:* multi_objective_weights
  
  **Argument(s):** REALLIST
  
  **Default:** equal weights

**Description**

For multi-objective optimization problems (where the number of objective functions is greater than 1), then a weights specification provides a simple weighted-sum approach to combining multiple objectives into a single objective:

\[ f = \sum_{i=1}^{n} w_i f_i \]

**Default Behavior** If weights are not specified, then each response is given equal weighting:

\[ f = \sum_{i=1}^{n} \frac{f_i}{n} \]

where, in both of these cases, a "minimization" sense will retain a positive weighting for a minimizer and a "maximization" sense will apply a negative weighting.

If scaling is specified, it is applied before multi-objective weighted sums are formed.

**nonlinear_inequality_constraints**

- **Keywords Area**
- responses
- objective_functions
- nonlinear_inequality_constraints

Group to specify nonlinear inequality constraints

**Topics**

This keyword is related to the topics:

- nonlinear_constraints

**Specification**

*Alias:* num_nonlinear_inequality_constraints
  
  **Argument(s):** INTEGER
  
  **Default:** 0

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<td>Optional</td>
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</table>
CHAPTER 6. KEYWORDS AREA

| Optional   | lower_bounds   | Specify minimum values |
| Optional   | upper_bounds   | Specify maximum values |
| Optional   | scale_types    | Choose how each constraint is scaled |
| Optional   | scales         | Characteristic values for scaling |

### Description

Specifies the number of nonlinear inequality constraint functions returned by the interface.

The `lower_bounds` and `upper_bounds` specifications provide the lower and upper bounds for 2-sided nonlinear inequalities of the form

\[ g_l \leq g(x) \leq g_u \]

The defaults for the inequality constraint bounds are selected so that one-sided inequalities of the form

\[ g(x) \leq 0.0 \]

result when there are no user constraint bounds specifications (this provides backwards compatibility with previous Dakota versions).

In a user bounds specification, any upper bound values greater than `+bigRealBoundSize` (1.e+30, as defined in Minimizer) are treated as `+infinity` and any lower bound values less than `-bigRealBoundSize` are treated as `-infinity`. This feature is commonly used to drop one of the bounds in order to specify a 1-sided constraint (just as the default lower bounds drop out since `-DBL_MAX < -bigRealBoundSize`). The same approach is used for nonexistent linear inequality bounds and for nonexistent design variable bounds.

The `scale_types` and `scales` keywords are related to scaling of `g(x)`. See the scaling information under specific methods, e.g., method-**scaling** for details on how to use this keyword.

### lower_bounds

- Keywords Area
- responses
- objective_functions
- nonlinear_inequality_constraints
- lower_bounds

Specify minimum values

### Specification

**Alias:** nonlinear_inequality_lower_bounds

**Argument(s):** REALLIST

**Default:** vector values = `-infinity`
6.6. RESPONSES

**Description**
Specify minimum values

**upper_bounds**
- Keywords Area
- responses
- objective_functions
- nonlinear_inequality_constraints
- upper_bounds
Specify maximum values

**Specification**
**Alias:** nonlinear_inequality_upper_bounds
**Argument(s):** REALLIST
**Default:** vector values = 0.

**Description**
Specify maximum values

**scale_types**
- Keywords Area
- responses
- objective_functions
- nonlinear_inequality_constraints
- scale_types
Choose how each constraint is scaled

**Specification**
**Alias:** nonlinear_inequality_scale_types
**Argument(s):** STRINGLIST
**Default:** no scaling

**Description**
Type of scaling to apply to nonlinear constraints: ‘none’, ‘value’, ‘auto’ or ‘log’. If a single string is specified it will apply to all components of the relevant nonlinear constraint vector.
See the scaling information under specific methods, e.g., method-*scaling for details on how to use this keyword.
scales

- Keywords Area
- responses
- objective_functions
- nonlinear_inequality_constraints
- scales

Characteristic values for scaling

**Specification**

**Alias:** nonlinear_inequality_scales  
**Argument(s):** REALLIST  
**Default:** 1.0 (no scaling)

**Description**

See the scaling information under specific methods, e.g., method-**-scaling for details on how to use this keyword.

**nonlinear_inequality_constraints**

- Keywords Area
- responses
- objective_functions
- nonlinear_inequality_constraints

Group to specify nonlinear equality constraints

**Topics**

This keyword is related to the topics:

- nonlinear_constraints

**Specification**

**Alias:** num_nonlinear_inequality_constraints  
**Argument(s):** INTEGER  
**Default:** 0

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<tr>
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<td></td>
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</tr>
</tbody>
</table>
6.6. RESPONSES

| Optional | targets | Target values for the nonlinear equality constraint |
| Optional | scale_types | Choose how each constraint is scaled |
| Optional | scales | Characteristic values for scaling |

**Description**

Specifies the number of nonlinear equality constraint functions returned by the interface.

The `targets` specification provides the targets for nonlinear equalities of the form

\[ h(x) = h_t \]

and the defaults for the equality targets enforce a value of 0.0 for each constraint:

\[ h(x) = 0.0 \]

The `scale_types` and `scales` keywords are related to scaling of \( h(x) \). See the scaling information under specific methods, e.g., method-\*\-scaling for details on how to use this keyword.

**targets**

- Keywords Area
- responses
- objective_functions
- nonlinear_equality_constraints
- targets

Target values for the nonlinear equality constraint

**Specification**

**Alias:** nonlinear_equality_targets

**Argument(s):** REALLIST

**Default:** vector values = 0.

**Description**

The `targets` specification provides the targets for nonlinear equalities of the form

\[ g(x) = g_t \]

and the defaults for the equality targets enforce a value of 0.0 for each constraint:

\[ g(x) = 0.0 \]
scale_types

- Keywords Area
- responses
- objective_functions
- nonlinear_equality_constraints
- scale_types

Choose how each constraint is scaled

**Specification**

**Alias:** nonlinear_equality_scale_types  
**Argument(s):** STRINGLIST  
**Default:** no scaling

**Description**

Type of scaling to apply to nonlinear constraints: ‘none’, ‘value’, ‘auto’ or ‘log’. If a single string is specified it will apply to all components of the relevant nonlinear constraint vector.

See the scaling information under specific methods, e.g., method-<symbol>-scaling for details on how to use this keyword.

scales

- Keywords Area
- responses
- objective_functions
- nonlinear_equality_constraints
- scales

Characteristic values for scaling

**Specification**

**Alias:** nonlinear_equality_scales  
**Argument(s):** REALLIST  
**Default:** 1.0 (no scaling)

**Description**

See the scaling information under specific methods, e.g., method-*-scaling for details on how to use this keyword.
6.6. RESPONSES

scalar_objectives

- Keywords Area
- responses
- objective_functions
- scalar_objectives

Number of scalar objective functions

Specification

Alias: num_scalar_objectives

Argument(s): INTEGER

Description

This keyword describes the number of scalar objective functions. It is meant to be used in conjunction with field_objectives, which describes the number of field objectives functions. The total number of objective functions, both scalar and field, is given by objective_functions. If only scalar objective functions are specified, it is not necessary to specify the number of scalar terms explicitly: one can simply say objective_functions = 5 and get 5 scalar objectives. However, if there are three scalar objectives and 2 field objectives, then objective_functions = 5 but scalar_objectives = 3 and field_objectives = 2.

Objective functions are responses that are used with optimization methods in Dakota. Currently, each term in a field objective is added to the total objective function presented to the optimizer. For example, if you have one field objective with 100 terms (e.g. a time-temperature trace with 100 time points and 100 corresponding temperature points), the 100 temperature values will be added to create the overall objective.

See Also

These keywords may also be of interest:

- field_objectives

field_objectives

- Keywords Area
- responses
- objective_functions
- field_objectives

Number of field objective functions

Specification

Alias: num_field_objectives

Argument(s): INTEGER
### Description

This keyword describes the number of field objective functions. A field function is a set of related response values collected over a range of independent coordinate values which may or may not be specified by the user. For example, voltage over time would be a field function, where voltage is the field objective and time is the independent coordinate. Similarly, temperature over time and space would be a field response, where the independent coordinates would be both time and spatial coordinates such as (x,y) or (x,y,z), depending on the application. The main difference between scalar objectives and field objectives is that for field data, we plan to implement methods that take advantage of the correlation or relationship between the field values.

Note that if there is one field objective, and it has length 100 (meaning 100 values), then the user’s simulation code must return 100 values. Also, if there are both scalar and field objectives, the user should specify the number of scalar objectives as scalar_objectives. If there are only field objectives, it still is necessary to specify both objective_functions = NN and field_objectives = NN, where NN is the number of field objectives.

Objective functions are responses that are used with optimization methods in Dakota. Currently, each term in a field objective is added to the total objective function presented to the optimizer. For example, if you have one field objective with 100 terms (e.g. a time-temperature trace with 100 time points and 100 corresponding temperature points), the 100 temperature values will be added to create the overall objective.

### See Also
These keywords may also be of interest:

- scalar_objectives
- lengths

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Description</th>
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<tr>
<td>Optional</td>
<td>length</td>
<td>lengths</td>
<td>Lengths of field responses</td>
</tr>
<tr>
<td>Optional</td>
<td>num_coordinates_per_field</td>
<td></td>
<td>Number of independent coordinates for field responses</td>
</tr>
<tr>
<td>Optional</td>
<td>read_field_coordinates</td>
<td></td>
<td>Add context to data: flag to indicate that field coordinates should be read</td>
</tr>
</tbody>
</table>
6.6. RESPONSES

Specification

Alias: none
Argument(s): INTEGERLIST

Description

This keyword describes the lengths of each field response. It is an integer vector of length field_responses. For example, if the field_responses = 2, an example would be lengths = 50 200, indicating that the first field response has 50 field elements but the second one has 200. The coordinate values (e.g. the independent variables) corresponding to these field responses are read in files labeled response_descriptor.coords.

See Also

These keywords may also be of interest:
- field_responses

num_coordinates_per_field

- Keywords Area
- responses
- objective_functions
- field_objectives
- num_coordinates_per_field

Number of independent coordinates for field responses

Specification

Alias: none
Argument(s): INTEGERLIST

Description

This keyword describes the number of independent coordinates for each field response. It is an integer vector of length field_responses. For example, if the field_responses = 2, an example would be num_coordinates_per_field = 2 1 means that the first field response has two sets of independent coordinates (perhaps x, y locations), but the second response only has one (for example, time where the field response is only dependent upon time). The actual coordinate values (e.g. the independent variables) corresponding to these field responses are defined in a file call response_descriptor.coords, where response_descriptor is the name of the individual field.

See Also

These keywords may also be of interest:
- field_responses
read_field_coordinates

- Keywords Area
- responses
- objective_functions
- field_objectives
- read_field_coordinates

Add context to data: flag to indicate that field coordinates should be read

**Specification**

**Alias:** none  
**Argument(s):** none

**Description**

Field coordinates specify independent variables (e.g. spatial or temporal coordinates) upon which the field depends. For example, the voltage level above might be a function of time, so time is the field coordinate. If the user has field coordinates to read, they need to specify `read_field_coordinates`. The field coordinates will then be read from a file named `response_descriptor.coords`, where `response_descriptor` is the user-provided descriptor for the field response. The number of columns in the coords file should be equal to the number of field coordinates.

### 6.6.4 calibration_terms

- Keywords Area
- responses
- calibration_terms

Response type suitable for calibration or least squares

**Specification**

**Alias:** least_squares_terms num_least_squares_terms  
**Argument(s):** INTEGER

<p>| Required/- | Description of | Dakota Keyword                          | Dakota Keyword                        |</p>
<table>
<thead>
<tr>
<th>Optional/Optional</th>
<th>Group</th>
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</thead>
<tbody>
<tr>
<td>Optional</td>
<td>scalar_calibration_terms</td>
<td>field_calibration_terms</td>
<td>Number of scalar calibration terms</td>
</tr>
<tr>
<td></td>
<td>number of scalar calibration terms</td>
<td>number of field calibration terms</td>
<td>Number of field calibration terms</td>
</tr>
</tbody>
</table>
### Description

Responses for a calibration study are specified using `calibration_terms` and optional keywords for weighting/scaling, data, and constraints. In general when calibrating, Dakota automatically tunes parameters $\theta$ to minimize discrepancies or residuals between the model and the data:

$$R_i = y_{i}^{\text{Model}}(\theta) - y_{i}^{\text{Data}}.$$

There are two use cases:

- If calibration data is not specified, then each of the calibration terms returned to Dakota through the interface is a residual $R_i$ to be driven toward zero.

- If calibration data is specified, then each of the calibration terms returned to Dakota must be a response $y_{i}^{\text{Model}}(\theta)$, which Dakota will difference with the data in the specified data file.

### Constraints

The keywords `nonlinear_inequality_constraints`, and `nonlinear_equality_constraints` specify the number of nonlinear inequality constraints, and nonlinear equality constraints, respectively. When interfacing to external applications, the responses must be returned to Dakota in this order: calibration terms, nonlinear_inequality_constraints, then nonlinear_equality_constraints.

<table>
<thead>
<tr>
<th>Optional</th>
<th>primary_scale_types</th>
<th>Choose a scaling type for each response</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>primary_scales</td>
<td>Supply a characteristic value to scale each response</td>
</tr>
<tr>
<td>Optional</td>
<td>weights</td>
<td>Apply different weights to each response</td>
</tr>
<tr>
<td>Optional (Choose One)</td>
<td>calibration_data</td>
<td>Supply field or mixed field/scalar calibration data</td>
</tr>
<tr>
<td>Optional (Group 1)</td>
<td>calibration_data_file</td>
<td>Supply scalar calibration data only</td>
</tr>
<tr>
<td>Optional</td>
<td>nonlinear_inequality_constraints</td>
<td>Group to specify nonlinear inequality constraints</td>
</tr>
<tr>
<td>Optional</td>
<td>nonlinear_equality_constraints</td>
<td>Group to specify nonlinear equality constraints</td>
</tr>
</tbody>
</table>
Any linear constraints present in an application need only be input to an optimizer at start up and do not need to be part of the data returned on every function evaluation. These are therefore specified in the method block.

**Optional Keywords**

The optional keywords relate to scaling responses (for better numerical results), dealing with multiple residuals, and importing data.

See the `scaling` keyword in the method section for more details on scaling. If scaling is specified, then it is applied to each residual prior to squaring:

\[ f = \sum_{i=1}^{n} w_i \left( \frac{y_{Model}^i - y_{Data}^i}{s_i} \right)^2 \]

In the case where experimental data uncertainties are supplied, then the weights are automatically defined to be the inverse of the experimental variance:

\[ f = \sum_{i=1}^{n} \frac{1}{\sigma_i^2} \left( \frac{y_{Model}^i - y_{Data}^i}{s_i} \right)^2 \]

**Theory**

Dakota calibration terms are typically used to solve problems of parameter estimation, system identification, and model calibration/inversion. Local least squares calibration problems are most efficiently solved using special-purpose least squares solvers such as Gauss-Newton or Levenberg-Marquardt; however, they may also be solved using any general-purpose optimization algorithm in Dakota. While Dakota can solve these problems with either least squares or optimization algorithms, the response data sets to be returned from the simulator are different when using objective functions versus calibration terms.

Least squares calibration involves a set of residual functions, whereas optimization involves a single objective function (sum of the squares of the residuals), i.e.,

\[ f = \sum_{i=1}^{n} R_i^2 = \sum_{i=1}^{n} \left( y_{Model}^i(\theta) - y_{Data}^i \right)^2 \]

where \( f \) is the objective function and the set of \( R_i \) are the residual functions, most commonly defined as the difference between a model response and data. Therefore, function values and derivative data in the least squares case involve the values and derivatives of the residual functions, whereas the optimization case involves values and derivatives of the sum of squares objective function. This means that in the least squares calibration case, the user must return each of \( n \) residuals separately as a separate calibration term. Switching between the two approaches sometimes requires different simulation interfaces capable of returning the different granularity of response data required, although Dakota supports automatic recasting of residuals into a sum of squares for presentation to an optimization method. Typically, the user must compute the difference between the model results and the observations when computing the residuals. However, the user has the option of specifying the observational data (e.g. from physical experiments or other sources) in a file.

**See Also**

These keywords may also be of interest:

- `objective_functions`
- `response_functions`
6.6. RESPONSES

scalar_calibration_terms

- **Keywords Area**
- responses
- calibration_terms
- scalar_calibration_terms

Number of scalar calibration terms

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Description**

This keyword describes the number of scalar calibration terms. It is meant to be used in conjunction with field_calibration_terms, which describes the number of field calibration terms. The total number of calibration terms, both scalar and field, is given by calibration_terms. If only scalar calibration terms are specified, it is not necessary to specify the number of scalar terms explicitly: one can simply say calibration_terms = 5 and get 5 scalar terms. However, if there are three scalar terms and 2 field terms, then calibration_terms = 5 but scalar_calibration_terms = 3 and field_calibration_terms = 2.

Calibration terms are responses that are used with calibration methods in Dakota, such as least squares optimizers. Currently, each scalar term is added to the total sum-of-squares error function presented to the optimizer. However, each individual field value is added as well. For example, if you have one field calibration term with length 100 (e.g. a time-temperature trace with 100 time points and 100 temperature points), the 100 temperature values will be added to create the overall sum-of-squares error function used in calibration.

**See Also**

These keywords may also be of interest:

- field_calibration_terms

field_calibration_terms

- **Keywords Area**
- responses
- calibration_terms
- field_calibration_terms

Number of field calibration terms

**Specification**

**Alias:** none

**Argument(s):** INTEGER
<table>
<thead>
<tr>
<th>Required/Optional Group</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required</td>
<td></td>
<td>lengths</td>
<td>Lengths of field responses</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>num_coordinates_per_field</td>
<td>Number of independent coordinates for field responses</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>read_field_coordinates</td>
<td>Add context to data: flag to indicate that field coordinates should be read</td>
</tr>
</tbody>
</table>

### Description

This keyword describes the number of field calibration terms. A set of field calibration terms is a set of related response values collected over a range of independent coordinate values which may or may not be specified by the user. For example, voltage over time would be a field function, where voltage is the field objective and time is the independent coordinate. Similarly, temperature over time and space would be a field response, where the independent coordinates would be both time and spatial coordinates such as (x,y) or (x,y,z), depending on the application. The main difference between scalar calibration terms and field calibration terms is that for field data, we plan to implement methods that take advantage of the correlation or relationship between the field values. For example, with calibration, if we want to calibrate parameters that result in a good model fit to a time-temperature curve, we may have to do some interpolation between the experimental data and the simulation data. That capability requires knowledge of the independent coordinates.

Note that if there is one field_calibration_terms, and it has length 100 (meaning 100 values), then the user’s simulation code must return 100 values. Also, if there are both scalar and field calibration, the user should specify the number of scalar terms as scalar_calibration_terms. If there are only field calibration terms, it still is necessary to specify both field_calibration_terms = NN and calibration_terms = NN, where NN is the number of field calibration terms.

Calibration terms are responses that are used with calibration methods in Dakota, such as least squares optimizers. Currently, each scalar term is added to the total sum-of-squares error function presented to the optimizer. However, each individual field value is added as well. For example, if you have one field calibration term with length 100 (e.g. a time-temperature trace with 100 time points and 100 temperature points), the 100 temperature values will be added to create the overall sum-of-squares error function used in calibration. We have an initial capability to interpolate the field data from the user’s simulation to the experimental data. For example, if the user has thermocouple readings at 20 time points, it will be an experimental field response with 20 time points and 20 temperature values. Dakota takes the 100 simulation time-temperature values (from the example above) and interpolates those to the 20 experimental points, to create 20 residual terms (simulation minus experimental data points) that will be used in calibration.

### See Also

These keywords may also be of interest:

- scalar_calibration_terms
- lengths

- Keywords Area
6.6. RESPONSES

- responses
- calibration_terms
- field_calibration_terms
- lengths

Lengths of field responses

**Specification**

**Alias:** none

**Argument(s):** INTEGERLIST

**Description**

This keyword describes the lengths of each field response. It is an integer vector of length `field_responses`. For example, if the `field_responses = 2`, an example would be `lengths = 50 200`, indicating that the first field response has 50 field elements but the second one has 200. The coordinate values (e.g., the independent variables) corresponding to these field responses are read in files labeled `response_descriptor.coords`.

**See Also**

These keywords may also be of interest:

- field_responses

**num_coordinates_per_field**

- **Keywords Area**
- responses
- calibration_terms
- field_calibration_terms
- `num_coordinates_per_field`

Number of independent coordinates for field responses

**Specification**

**Alias:** none

**Argument(s):** INTEGERLIST

**Description**

This keyword describes the number of independent coordinates for each field response. It is an integer vector of length `field_responses`. For example, if the `field_responses = 2`, an example would be `num_coordinates_per_field = 2 1` means that the first field response has two sets of independent coordinates (perhaps x, y locations), but the second response only has one (for example, time where the field response is only dependent upon time). The actual coordinate values (e.g., the independent variables) corresponding to these field responses are defined in a file call `response_descriptor.coords`, where `response_descriptor` is the name of the individual field.
See Also

These keywords may also be of interest:

- field_responses

read_field_coordinates

- Keywords Area
- responses
- calibration_terms
- field_calibration_terms
- read_field_coordinates

Add context to data: flag to indicate that field coordinates should be read

Specification

Alias: none
Argument(s): none

Description

Field coordinates specify independent variables (e.g. spatial or temporal coordinates) upon which the field depends. For example, the voltage level above might be a function of time, so time is the field coordinate. If the user has field coordinates to read, they need to specify read_field_coordinates. The field coordinates will then be read from a file named response_descriptor.coords, where response_descriptor is the user-provided descriptor for the field response. The number of columns in the coords file should be equal to the number of field coordinates.

primary_scale_types

- Keywords Area
- responses
- calibration_terms
- primary_scale_types

Choose a scaling type for each response

Specification

Alias: calibration_term_scale_types least_squares_term_scale_types
Argument(s): STRINGLIST
Default: no scaling
6.6. RESPONSES

Description

The primary_scale_types keyword specifies one or number of primary functions strings indicating the scaling type for each response value in methods that support scaling, when scaling is enabled. If only one type is specified, it will apply to each primary response function.

See the scaling information under specific methods, e.g., method-*-scaling for details on how to use this keyword.

Note that primary response functions (objective, calibration, or response functions) cannot be automatically scaled due to lack of bounds, so valid scale types are 'none' 'value' and 'log'.

If scaling is specified, it is applied before multi-objective weighted sums are formed.

primary_scales

- Keywords Area
- responses
- calibration_terms
- primary_scales

Supply a characteristic value to scale each response

 Specification

Alias: calibration_term_scales least_squares_term_scales

Argument(s): REALLIST

Default: 1.0 (no scaling)

Description

Each entry in primary_scales is a user-specified nonzero characteristic value to scale each response. The argument may be of length 1 or the number of primary response functions. If only one scale is specified, it will apply to each primary response function.

See the scaling information under specific methods, e.g., method-*-scaling for details on how to use this keyword.

If scaling is specified, it is applied before multi-objective weighted sums are formed.

weights

- Keywords Area
- responses
- calibration_terms
- weights

Apply different weights to each response
**Specification**

**Alias:** calibration_weights least_squares_weights  
**Argument(s):** REALLIST  
**Default:** equal weights

**Description**

The `weights` specification provides a means to specify a relative emphasis among the vector of squared residuals through multiplication of these squared residuals by a vector of weights:

\[ f = \sum_{i=1}^{n} w_i R_i^2 = \sum_{i=1}^{n} w_i (y_i^M - y_i^O)^2 \]

**calibration_data**

- **Keywords Area**
- **responses**
- **calibration_terms**
- **calibration_data**

Supply field or mixed field/scalar calibration data

**Specification**

**Alias:** none  
**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>num_experiments</td>
<td>num_config_variables</td>
<td>Add context to data: number of different experiments Add context to data: number of configuration variables.</td>
</tr>
</tbody>
</table>
### Description

calibration.data specifies a keyword block that indicates that Dakota should read in experimental data for calibration. This block is primarily to support the reading of field calibration data. For simpler, scalar-only response cases, see calibration_data_file. The user will typically specify the number of experiments, num_experiments. If this is not specified, it is assumed there is only one experiment.

Up to four types of data may be read. They are read from a collection of files, one per response descriptor, per experiment. In this discussion, DESC refers to the response descriptor and NUM to the experiment number.

1. **Values:** The scalar or field-valued response function values, e.g., temperature values, voltage levels. These are read from files named DESC.NUM.dat (one per response descriptor, per experiment), e.g., volts-1.dat, volts.2.dat. Scalar files will contain a single value, while field files will each contain a column of field response values with length indicated in lengths.

2. **Coordinates:** Field coordinates specify independent variables (e.g., spatial or temporal coordinates) upon which the field depends. For example, the voltage might be a function of time, so time is the field coordinate. These are read from files named DESC.NUM.coords, each containing num_coordinates_per_field columns and 1 (scalar) or field length (lengths).

3. **Variances:** If variance_type is specified, variance values are read from files DESC.NUM.sigma. Note that a single variance_type may be specified, or a unique variance_type per response descriptor (per scalar or field). If the variance_type is:
   - 'scalar': a single variance value will be read from the file.
   - 'diagonal' (field responses only): a column vector of variance values (length equal to length of the field) will be read from the file. The values are the variances of each field value for this descriptor.
   - 'matrix' (field responses only): a matrix of covariance values (square with size the length of the field) will be read from the file. The matrix is a full covariance matrix for the components of this field response. While covariance among entries in a field response may be specified, covariance among experiments is not permitted.

4. **Configuration variables:** specify the conditions corresponding to different experiments. When responses-calibration_terms-calibration_data-num_config_variables is specified, the configuration variable values for each experiment should be placed in a file named experiment.NUM.config, where the number of items in that config file are the num_config_variables. These variables are used as auxiliary state variables for the simulation (for example) and are not calibrated.
Aggregating scalar data: The above description is primarily relevant for field data (with files for field values, field coordinates, field variances). If the user also has scalar experimental data, it may be entered as described above, i.e., one file named DESC.NUM.dat per scalar response. However, an alternative is to provide the data for all scalar responses in aggregate in the simpler scalar data file format, with the number of rows of that file equal to the number of experiments. The scalar data file may be used in combination with the separate field files described above.

Interpolation: One important feature of field data is the capability to interpolate between points in the field. For example, we may have simulation data at a set of responses \( y \) at time points \( t \): ( \( t_s^1, y_{s^1} \), ( \( t_s^2, y_{s^2} \), etc. In this example, \( t \) is the independent coordinate for the simulation, and the simulation time and response points are denoted with subscripts \( s_1, s_2, s_3, \). If the user has experimental data that is taken at different time points: ( \( t_e^1, y_{e^1} \), ( \( t_e^2, y_{e^2} \), ..., it is necessary to interpolate the simulation data to provide estimates of the simulation response at the experimental time points to construct the residual terms (model - experiment) at the experimental time points. Dakota can perform 1-D interpolation. The user must specify the keyword `interpolate`, and also provide the field coordinates as well as field values for the experimental data.

If the `interpolate` keyword is not specified, Dakota will assume that the simulation field data and the experiment field data is taken at the same set of independent coordinate values and simply construct the difference between these field terms to create the set of residuals for the sum-of-squares calculation. When `interpolate` is specified, the simulation coordinates are assumed fixed and the same for each simulation. These simulation coordinates are provided in DESC.coords. However, the experiment coordinates for each experiment can be different, and are provided in the files numbered by experiment with the file names given by DESC.NUM.coords, as indicated above.

Examples

Consider this field example with three field-valued responses (volts as a function of 7 time points, amps as a function of 3 time points, and power as a function of 5 time points). The experiments each have one coordinate (time) per field. The experiments were conducted given values of two configuration variables. There are four experiments (note that there often is only one experiment).

```plaintext
responses
descriptors = 'volts' 'amps' 'power'
calibration_terms = 3

#define field terms
field_calibration_terms = 3
lengths = 7 3 5
num_coordinates_per_field = 1 1 1
read_field_coordinates

# specify the data
calibration_data
num_experiments = 4
num_config_variables = 2
variance_type 'diagonal' 'scalar' 'matrix'
```

The field data will be read from separate files:

1. **Values:** 7 values for voltage as a function of time will be read from each of `volts.1.dat ... volts.-4.dat`, while the 3 values of amperage come from `amps.1.dat`, ..., `amps.4.dat` and the 5 values of power will come from `power.1.dat`, ..., `power.4.dat`.

2. **Coordinates:** The corresponding time values will be read from a single column vector in each of the files `volts.*.coords`, `amps.*.coords`, and `power.*.coords`. 


3. **Variances:** Will be read per-experiment (no covariance among experiments is permitted). The variance information is depicted graphically in `variance_type`.

   - Volts specifies 'diagonal' covariance, so a column vector of length 7 with the diagonal variances will be read from each of `volts.1.sigma`, ..., `volts.4.sigma`.
   - Amps specifies 'scalar' covariance, so a single variance value will read from each of `amps.1.-sigma`, ..., `amps.4.sigma`.
   - Power specifies 'matrix' covariance, so a square 5 x 5 covariance matrix will be read from each of `power.1.sigma`, ..., `power.4.sigma`.

4. **Configuration variables:** Will be read from a set of files named `experiment.1.config`, ..., `experiment.-4.config`.

**num_experiments**

- Keywords Area
- responses
- calibration_terms
- calibration_data
- num_experiments

Add context to data: number of different experiments

**Specification**

**Alias:** none  
**Argument(s):** INTEGER  
**Default:** 1

**Description**

The number of different experiments. Dakota will expand the total number of residual terms based on the number of calibration terms and the number of experiments. For example, if the number of calibration terms are five scalars, and there are three experiments, the total number of residuals in the least squares formulation will be 15. See `calibration_data` or `calibration_data_file`.

**num_config_variables**

- Keywords Area
- responses
- calibration_terms
- calibration_data
- num_config_variables

Add context to data: number of configuration variables.
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none
Argument(s): INTEGER
Default: 0

Description

If there are multiple experiments, there can be different configuration variables (e.g. experimental settings, boundary conditions, etc.) per experiment. See calibration data or calibration data file.

During calibration, configuration variables are state variables which will be passed to the simulation, and are not treated as calibration parameters.

variance_type

- Keywords Area
- responses
- calibration_terms
- calibration_data
- variance_type

Add context to data: specify the type of experimental error

Specification

Alias: none
Argument(s): STRINGLIST
Default: none

Description

There are four options for specifying the experimental error (e.g. the measurement error in the data you provide for calibration purposes): 'none' (default), 'scalar', 'diagonal', or 'matrix'.

If the user specifies scalar, they can provide a scalar variance per calibration term. Note that for scalar calibration terms, only 'none' or 'scalar' are options for the measurement variance. However, for field calibration terms, there are two additional options. 'diagonal' allows the user to provide a vector of measurement variances (one for each term in the calibration field). This vector corresponds to the diagonal of the full covariance matrix of measurement errors. If the user specifies 'matrix', they can provide a full covariance matrix (not just the diagonal terms), where each element (i,j) of the covariance matrix represents the covariance of the measurement error between the i-th and j-th field values.

Usage Tips

Variance information is specified on a per-response group (descriptor), per-experiment basis. Off-diagonal covariance between response groups or between experiments is not supported.
Examples

The figure below shows an observation vector with 5 responses; 2 scalar + 3 field (each field of length > 1). The corresponding covariance matrix has scalar variances $\sigma_1^2, \sigma_2^2$ for each of the scalars $s1, s2$, diagonal covariance $D_3$ for field $f3$, scalar covariance $\sigma_4^2$ for field $f4$, and full matrix covariance $C_5$ for field $f5$. In total, Dakota supports block diagonal covariance $\Sigma$ across the responses, with blocks $\Sigma_i$, which could be fully dense within a given field response group. Covariance across the highest-level responses (off-diagonal blocks) is not supported, nor is covariance between experiments.

**scalar_data_file**

- Keywords Area
- responses
- calibration_terms
- calibration_data
- scalar_data_file

Specify a scalar data file to complement field data files (mixed case)

**Specification**

Alias: none  
Argument(s): STRING

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Required/-Optional/Choose One</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<tbody>
<tr>
<td>Optional</td>
<td>Tabular Format (Group 1)</td>
<td></td>
<td>annotated</td>
<td>Selects annotated tabular file format for experiment data</td>
</tr>
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<td>custom_annotated</td>
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<td>Selects custom-annotated tabular file format for experiment data</td>
</tr>
<tr>
<td>freeform</td>
<td></td>
<td></td>
<td></td>
<td>Selects free-form tabular file format for experiment data</td>
</tr>
</tbody>
</table>

**Description**

When calibrating both scalar and field calibration terms, to associated experimental data, the scalar data may be provided in the file named by scalar_data_file. This file follows the same format as: calibration_data_file.

**Default Behavior**

If scalar_data_file is omitted, all calibration data, including for scalar responses, will be read from the generic field calibration_data format.
annotated

- Keywords Area
- responses
- calibration_terms
- calibration_data
- scalar_data_file
- annotated

Selects annotated tabular file format for experiment data

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none

Argument(s): none

Default: annotated format

Description

An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. For experiment data files, each subsequent row contains an experiment ID, followed by data for configuration variables, observations, and/or observation errors, depending on context.

Default Behavior

By default, Dakota imports tabular experiment data files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips

- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

Examples

Import an annotated experimental data file containing a header row, leading exp_id column, and experiment data in a calibration study

```plaintext
responses

scalar_data_file 'shock_experiment.dat' annotated
```

Example data file with two measured quantities, three experiments:
6.6. RESPONSES

%exp_id   velocity   stress
1   18.23       83.21
2   34.14       93.24
3   22.41       88.92

custom_annotated

• Keywords Area
• responses
• calibration_terms
• calibration_data
• scalar_data_file
• custom_annotated

Selects custom-annotated tabular file format for experiment data

Topics

This keyword is related to the topics:
• file_formats

Specification

Alias: none
Argument(s): none

Default: annotated format

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
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<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>header</td>
<td>Enable header row in custom-annotated tabular file</td>
</tr>
<tr>
<td></td>
<td></td>
<td>exp_id</td>
<td>Enable experiment ID column in custom-annotated tabular file</td>
</tr>
</tbody>
</table>

Description

A custom-annotated tabular file is a whitespace-separated text file containing experiment data, including configuration variables, observations, and/or observation errors, depending on context. For experiment import, custom-annotated allows user options for whether header row and exp_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

Default Behavior

By default, Dakota imports tabular experiment data files in annotated format. The custom_annotated keyword, followed by options can be used to select other formats.

Usage Tips
Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

Examples

Import an experimental data file containing a header row, no leading exp_id column, and experiment data in a calibration study

```
responses
...
scalar_data_file 'shock_experiment.dat'
custom_annotated header
```

Example data file with two measured quantities, three experiments:

```
% velocity  stress
18.23  83.21
34.14  93.24
22.41  88.92
```

header

- Keywords Area
- responses
- calibration_terms
- calibration_data
- scalar_data_file
- custom_annotated
- header

Enable header row in custom-annotated tabular file

Specification

Alias: none  
Argument(s): none  
Default: no header

Description

See description of parent custom_annotated
6.6. RESPONSES

exp_id

- Keywords Area
- responses
- calibration_terms
- calibration_data
- scalar_data_file
- custom_annotated
- exp_id

Enable experiment ID column in custom-annotated tabular file

Specification

Alias: none
Argument(s): none
Default: no exp_id column

Description

See description of parent custom_annotated

freeform

- Keywords Area
- responses
- calibration_terms
- calibration_data
- scalar_data_file
- freeform

Selects free-form tabular file format for experiment data

Topics

This keyword is related to the topics:

- file_formats

Specification

Alias: none
Argument(s): none
Default: annotated format
CHAPTER 6. KEYWORDS AREA

Description
A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. For experiment data files, each row contains data for configuration variables, observations, and/or observation errors, depending on context.

Default Behavior
By default, Dakota imports tabular experiment data files in annotated format. Specify freeform to instead select this format.

Usage Tips
- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

Examples
Import a free-form experimental data file containing raw experiment data in a calibration study

```
responses
    ... scalar_data_file 'shock_experiment.dat' freeform
```
Example data file with two measured quantities, three experiments:

```
18.23  83.21
34.14  93.24
22.41  88.92
```

interpolate
- Keywords Area
- responses
- calibration_terms
- calibration_data
- interpolate

Flag to indicate interpolation of simulation values.

Specification
Alias: none
Argument(s): none

Description
If interpolate is specified, Dakota will interpolate between the simulation data and the experiment data to calculate the residuals for calibration methods. Specifically, the simulation data is interpolated onto the experimental data points. So, if the simulation data is a field of length 100 with one independent coordinate, and the experiment data is of length 5 with one independent coordinate, the interpolation is done between the 100 (t,f) simulation points (where t is the independent coordinate and f is the simulation field value) onto the five (t,e, f,e) points to obtain the residual differences between the simulation and experiment. See calibration_data.
6.6. RESPONSES

**calibration_data_file**
- **Keywords Area**
- responses
- calibration_terms
- calibration_data_file

Supply scalar calibration data only

**Specification**

**Alias:** least_squares.data_file  
**Argument(s):** STRING  
**Default:** none

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group Tabular Format (Group 1)</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<td>custom_annotated</td>
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<tr>
<td>Optional</td>
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<td>freeform</td>
<td>Selects free-form tabular file format for experiment data</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>num_experiments</td>
<td>Add context to data: number of different experiments</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>num_config_variables</td>
<td>Add context to data: number of configuration variables.</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>variance_type</td>
<td>Add context to data: specify the type of experimental error</td>
</tr>
</tbody>
</table>

**Description**

Enables text file import of experimental observations for use in calibration, for scalar responses only, with optional scalar variance information. For more complex data import cases see **calibration_data** Dakota will calibrate model variables to best match these data.
Key options include:

- **format**: whether the data file is in annotated, custom_annotated, or freeform format
- **content**: where `num_experiments`, `num_config_variables`, and `variance_type` indicate which columns appear in the data.

In the most general case, the content of the data file is described by the arguments of three optional parameters.

- **num_experiments** ($N_{exp}$)
  
  Default: $N_{exp} = 1$
  
  This indicates that the data represent multiple experiments, where each experiment might be conducted with different values of configuration variables. An experiment can also be thought of as a replicate, where the experiments are run at the same values of the configuration variables.

- **num_config_variables** ($N_{cfg}$)
  
  Configuration variables specify the values of experimental conditions at which data were collected. The variables in these columns must correspond to state variables in the calibration study. The simulation model will be run at each configuration and compared to the appropriate experiment data.

- **variance_type** (‘none’ or ‘scalar’)
  
  This indicates if the data file contains variances for measurement error of the experimental data. The default is ‘none’.

While some components may be omitted, the most complete version of a an annotated calibration data file could include columns corresponding to experiment ID, configuration variables, function value observations, and variances (observation errors), shown here in annotated format:

<table>
<thead>
<tr>
<th>exp_id</th>
<th>configuration xvars</th>
<th>y data observations</th>
<th>y data variances</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>7.8 7</td>
<td>21.9372 1.8687</td>
<td>0.25 0.04</td>
</tr>
<tr>
<td>2</td>
<td>8.6 2</td>
<td>19.0779 4.8976</td>
<td>0.25 0.04</td>
</tr>
<tr>
<td>3</td>
<td>8.4 8</td>
<td>38.2758 4.4559</td>
<td>0.25 0.04</td>
</tr>
<tr>
<td>4</td>
<td>4.2 1</td>
<td>39.7600 6.4631</td>
<td>0.25 0.04</td>
</tr>
</tbody>
</table>

Each row in the file corresponds to an experiment or replicate observation of an experiment to be compared to the model output. This example shows 4 experiments, governed by two configuration variables (one real-valued and one integer-valued), two responses (QOIs), and corresponding observation errors with standard deviation 0.5 and 0.2.

**Usage Tips**

- The `calibration_data_file` keyword is used when *only* scalar calibration terms are present. If there are field calibration terms, instead use `calibration_data`. For mixed scalar and field calibration terms, one may use the `scalar_data_file` specification, which uses the format described on this page.

**Examples**

**Simple Case**: In the simplest case, no data content descriptors are specified:

```plaintext
responses
calibration_terms = 2
descriptors = 'volts' 'amps'
calibration_data_file = 'circuit.dat'
annotated
```
And the data file `circuit.dat` must contain only the \( y^{\text{Data}} \) observations which represent a single experimental observation. In this case, the data file should have \( N_{\text{terms}} = 2 \) columns (for volts, amps) and 1 row, where \( N_{\text{terms}} \) is the value of `calibration_terms`. The data file is shown here in annotated format:

```
%exp_id | y data observations
1       21.9372  1.8687
```

For each function evaluation, Dakota will run the analysis driver, which must return \( N_{\text{terms}} = 2 \) model responses. Then the residuals are computed as:

\[
R_i = y_i^{\text{Model}} - y_i^{\text{Data}}.
\]

These residuals can be weighted using weights.

**Multiple experiments:** One might specify `num_experiments \( N_E \)` indicating that there are multiple experiments. When multiple experiments are present, Dakota will expand the number of residuals for the repeat measurement data and difference with the data accordingly. For example, if the user has \( N_E = 4 \) experiments in the example above with 2 calibration terms, the input file would contain

```python
responses
calibration_terms = 2
descriptors = 'volts' 'amps'
calibration_data_file = 'circuit.dat'
annotated
num_experiments = 4
```

And the `calibration_data_file` would need to contain 2 rows (one for each experiment), and each row should contain 2 experimental data values that will be differenced with respect to the appropriate model response:

```
%exp_id | y data observations
1       21.9372  1.8687
2       19.0779  4.8976
3       38.2758  4.4559
4       39.7600  6.4631
```

To summarize, Dakota will calculate the sum of the squared residuals as:

\[
f = \sum_{i=1}^{N_E} R_i^2
\]

where the residuals now are calculated as:

\[
R_i = y_i^{\text{Model}}(\theta) - y_i^{\text{Data}}.
\]

**With experimental variances:** If information is known about the measurement error and the uncertainty in the measurement, that can be specified by sending the measurement error variance to Dakota. In this case, the keyword `variance_type` is added, followed by a string of variance types of length one or of length \( N_{\text{terms}} \), where \( N_{\text{terms}} \) is the value of `calibration_terms`. The `variance_type` for each response can be 'none' or 'scalar'. NOTE: you must specify the same `variance_type` for all scalar terms. That is, they will all be 'none' or all be 'scalar.'

```python
responses
calibration_terms = 2
descriptors = 'volts' 'amps'
calibration_data_file = 'circuit.dat'
annotated
variance_type 'scalar'
```
For each response that has a 'scalar' variance type, each row of the datafile will now have \( N_{\text{terms}} = 2 \) of \( y \) data values (volts, amps) followed by \( N_{\text{terms}} = 2 \) columns that specify the measurement error (in units of variance, not standard deviation) for volts, amps. An example with two experiments in annotated format:

%exp_id | y data observations | y data variances  
1       | 21.9372 1.8687 | 0.25 0.04  

Dakota will run the analysis driver, which must return \( N_{\text{terms}} \) responses. Then the residuals are computed as:

\[
R_i = \frac{y_i^{\text{Model}} - y_i^{\text{Data}}}{\sqrt{\text{var}_i}}
\]

for \( i = 1 \ldots N_{\text{terms}} \).

**Putting all the options together:** Specifying all these options together might look like

```python
responses
calibration_terms = 2
descriptors = 'volts' 'amps'
calibration_data_file = 'circuit.dat'
annotated
num_experiments = 4
variance_type 'scalar'
```

Dakota will expect a data file

%exp_id | configuration xvars | y data observations | y data variances  
1       | 7.8 7 | 21.9372 1.8687 | 0.25 0.04  
2       | 8.6 2 | 19.0779 4.8976 | 0.25 0.04  
3       | 8.4 8 | 38.2758 4.4559 | 0.25 0.04  
4       | 4.2 1 | 39.7600 6.4631 | 0.25 0.04  

To compute residuals for each experiment, e.g., exp_id = 4, Dakota will

1. Evaluate the computational model at the specified configuration (state variables = [4.2, 1]).
2. Difference the resulting 2 function values with the data [39.7600 volts, 6.4631 amps]
3. Weight by the standard deviation = sqrt([0.25 0.04])

**See Also**

These keywords may also be of interest:

- `calibration_data`

`annotated`

- Keywords Area
- responses
- calibration_terms
- calibration_data_file
- annotated

Selects annotated tabular file format for experiment data
6.6. RESPONSES

Topics
This keyword is related to the topics:

- file_formats

Specification
Alias: none

  Argument(s): none
  Default: annotated format

Description
An annotated tabular file is a whitespace-separated text file with one leading header row of comments/column labels. For experiment data files, each subsequent row contains an experiment ID, followed by data for configuration variables, observations, and/or observation errors, depending on context.

Default Behavior
By default, Dakota imports tabular experiment data files in annotated format. The annotated keyword can be used to explicitly specify this.

Usage Tips
- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

Examples
Import an annotated experimental data file containing a header row, leading exp_id column, and experiment data in a calibration study

  responses
  ...
  scalar_data_file 'shock_experiment.dat'
  annotated

  Example data file with two measured quantities, three experiments:

<table>
<thead>
<tr>
<th>exp_id</th>
<th>velocity</th>
<th>stress</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>18.23</td>
<td>83.21</td>
</tr>
<tr>
<td>2</td>
<td>34.14</td>
<td>93.24</td>
</tr>
<tr>
<td>3</td>
<td>22.41</td>
<td>88.92</td>
</tr>
</tbody>
</table>

custom_annotated

- Keywords Area
- responses
- calibration_terms
- calibration_data_file
- custom_annotated

Selects custom-annotated tabular file format for experiment data
CHAPTER 6. KEYWORDS AREA

Topics
This keyword is related to the topics:

• file formats

Specification
Alias: none
Argument(s): none
Default: annotated format

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>header</td>
<td>Enable header row in custom-annotated tabular file</td>
</tr>
<tr>
<td></td>
<td></td>
<td>exp_id</td>
<td>Enable experiment ID column in custom-annotated tabular file</td>
</tr>
</tbody>
</table>

Description
A custom-annotated tabular file is a whitespace-separated text file containing experiment data, including configuration variables, observations, and/or observation errors, depending on context. For experiment import, custom-annotated allows user options for whether header row and exp_id column appear in the tabular file, thus bridging freeform and (fully) annotated.

Default Behavior
By default, Dakota imports tabular experiment data files in annotated format. The custom_annotated keyword, followed by options can be used to select other formats.

Usage Tips

• Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.

• When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

Examples
Import an experimental data file containing a header row, no leading exp_id column, and experiment data in a calibration study

responses

    scalar_data_file 'shock_experiment.dat'
    custom_annotated header

Example data file with two measured quantities, three experiments:
% velocity stress
18.23 83.21
34.14 93.24
22.41 88.92

header
- Keywords Area
- responses
- calibration_terms
- calibration_data_file
- custom_annotated
- header

Enable header row in custom-annotated tabular file

**Specification**

**Alias:** none
**Argument(s):** none
**Default:** no header

**Description**

See description of parent `custom_annotated`

**exp_id**
- Keywords Area
- responses
- calibration_terms
- calibration_data_file
- custom_annotated
- exp_id

Enable experiment ID column in custom-annotated tabular file

**Specification**

**Alias:** none
**Argument(s):** none
**Default:** no exp_id column

**Description**

See description of parent `custom_annotated`
freeform
- Keywords Area
- responses
- calibration_terms
- calibration_data_file
- freeform

Selects free-form tabular file format for experiment data.

Topics
This keyword is related to the topics:
- file_formats

Specification
Alias: none
Argument(s): none
Default: annotated format

Description
A freeform tabular file is whitespace-separated text file with no leading header row and no leading columns. For experiment data files, each row contains data for configuration variables, observations, and/or observation errors, depending on context.

Default Behavior
By default, Dakota imports tabular experiment data files in annotated format. Specify freeform to instead select this format.

Usage Tips
- Prior to October 2011, calibration and surrogate data files were in free-form format. They now default to annotated format, though freeform remains an option.
- When importing tabular data, a warning will be generated if a specific number of data are expected, but extra is found and an error generated when there is insufficient data.

Examples
Import a free-form experimental data file containing raw experiment data in a calibration study

```
responses
...
scalar_data_file 'shock_experiment.dat'
  freeform
```

Example data file with two measured quantities, three experiments:

```
18.23  83.21
34.14  93.24
22.41  88.92
```
6.6. RESPONSES

num_experiments

- Keywords Area
- responses
- calibration_terms
- calibration_data_file
- num_experiments

Add context to data: number of different experiments

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** 1

**Description**

The number of different experiments. Dakota will expand the total number of residual terms based on the number of calibration terms and the number of experiments. For example, if the number of calibration terms are five scalars, and there are three experiments, the total number of residuals in the least squares formulation will be 15. See calibration_data or calibration_data_file.

num_config_variables

- Keywords Area
- responses
- calibration_terms
- calibration_data_file
- num_config_variables

Add context to data: number of configuration variables.

**Specification**

**Alias:** none

**Argument(s):** INTEGER

**Default:** 0

**Description**

If there are multiple experiments, there can be different configuration variables (e.g. experimental settings, boundary conditions, etc.) per experiment. See calibration_data or calibration_data_file.

During calibration, configuration variables are state variables which will be passed to the simulation, and are not treated as calibration parameters.
variance_type
  - Keywords Area
  - responses
  - calibration_terms
  - calibration_data_file
  - variance_type

Add context to data: specify the type of experimental error

**Specification**

**Alias:** none

**Argument(s):** STRINGLIST

**Default:** none

**Description**

There are four options for specifying the experimental error (e.g. the measurement error in the data you provide for calibration purposes): 'none' (default), 'scalar', 'diagonal', or 'matrix.'

If the user specifies scalar, they can provide a scalar variance per calibration term. Note that for scalar calibration terms, only 'none' or 'scalar' are options for the measurement variance. However, for field calibration terms, there are two additional options. 'diagonal' allows the user to provide a vector of measurement variances (one for each term in the calibration field). This vector corresponds to the diagonal of the full covariance matrix of measurement errors. If the user specifies 'matrix', they can provide a full covariance matrix (not just the diagonal terms), where each element (i,j) of the covariance matrix represents the covariance of the measurement error between the i-th and j-th field values.

**Usage Tips**

Variance information is specified on a per-response group (descriptor), per-experiment basis. Off-diagonal covariance between response groups or between experiments is not supported.

**Examples**

The figure below shows an observation vector with 5 responses; 2 scalar + 3 field (each field of length > 1). The corresponding covariance matrix has scalar variances $\sigma_1^2, \sigma_2^2$ for each of the scalars $s1, s2$, diagonal covariance $D_3$ for field $f3$, scalar covariance $\sigma_4^2$ for field $f4$, and full matrix covariance $C_5$ for field $f5$. In total, Dakota supports block diagonal covariance $\Sigma$ across the responses, with blocks $\Sigma_i$, which could be fully dense within a given field response group. Covariance across the highest-level responses (off-diagonal blocks) is not supported, nor is covariance between experiments.

nonlinear_inequality_constraints
  - Keywords Area
  - responses
  - calibration_terms
  - nonlinear_inequality_constraints

Group to specify nonlinear inequality constraints
### Topics

This keyword is related to the topics:

- nonlinear_constraints

### Specification

**Alias:** num_nonlinear_inequality_constraints  
**Argument(s):** INTEGER  
**Default:** 0

<table>
<thead>
<tr>
<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword Description</th>
<th>Dakota Keyword</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>lower_bounds</td>
<td>Specify minimum values</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>upper_bounds</td>
<td>Specify maximum values</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>scale_types</td>
<td>Choose how each constraint is scaled</td>
<td></td>
</tr>
<tr>
<td>Optional</td>
<td>scales</td>
<td>Characteristic values for scaling</td>
<td></td>
</tr>
</tbody>
</table>

### Description

Specifies the number of nonlinear inequality constraint functions returned by the interface.

The lower_bounds and upper_bounds specifications provide the lower and upper bounds for 2-sided nonlinear inequalities of the form

$$g_l \leq g(x) \leq g_u$$

The defaults for the inequality constraint bounds are selected so that one-sided inequalities of the form

$$g(x) \leq 0.0$$

result when there are no user constraint bounds specifications (this provides backwards compatibility with previous Dakota versions).

In a user bounds specification, any upper bound values greater than +bigRealBoundSize (1.e+30, as defined in Minimizer) are treated as +infinity and any lower bound values less than -bigRealBoundSize are treated as -infinity. This feature is commonly used to drop one of the bounds in order to specify a 1-sided constraint (just as the default lower bounds drop out since -DBL_MAX < -bigRealBoundSize). The same approach is used for nonexistent linear inequality bounds and for nonexistent design variable bounds.

The scale_types and scales keywords are related to scaling of $g(x)$. See the scaling information under specific methods, e.g., method-+-scaling for details on how to use this keyword.

**lower_bounds**

- Keywords Area
- responses
- calibration_terms
• nonlinear_inequality_constraints
• lower_bounds

Specify minimum values

**Specification**

Alias: nonlinear_inequality_lower_bounds
Argument(s): REALLIST
Default: vector values = -infinity

**Description**

Specify minimum values

**upper_bounds**

• Keywords Area
• responses
• calibration_terms
• nonlinear_inequality_constraints
• upper_bounds

Specify maximum values

**Specification**

Alias: nonlinear_inequality_upper_bounds
Argument(s): REALLIST
Default: vector values = 0.

**Description**

Specify maximum values

**scale_types**

• Keywords Area
• responses
• calibration_terms
• nonlinear_inequality_constraints
• scale_types

Choose how each constraint is scaled
6.6. RESPONSES

**Specification**

**Alias:** nonlinear_inequality_scale_types  
**Argument(s):** STRINGLIST  
**Default:** no scaling

**Description**

Type of scaling to apply to nonlinear constraints: 'none', 'value', 'auto' or 'log'. If a single string is specified it will apply to all components of the relevant nonlinear constraint vector.

See the scaling information under specific methods, e.g., method-*scaling for details on how to use this keyword.

**scales**

- Keywords Area  
- responses  
- calibration_terms  
- nonlinear_inequality_constraints  
- scales

Characteristic values for scaling

**Specification**

**Alias:** nonlinear_inequality_scales  
**Argument(s):** REALLIST  
**Default:** 1.0 (no scaling)

**Description**

See the scaling information under specific methods, e.g., method-*scaling for details on how to use this keyword.

**nonlinear_inequality_constraints**

- Keywords Area  
- responses  
- calibration_terms  
- nonlinear_inequality_constraints

Group to specify nonlinear equality constraints

**Topics**

This keyword is related to the topics:

- nonlinear_constraints
**Specification**

**Alias:** num_nonlinear_equality_constraints  
**Argument(s):** INTEGER  
**Default:** 0

<p>| Required/- | Description of | Dakota Keyword | Dakota Keyword Description |</p>
<table>
<thead>
<tr>
<th>Optional</th>
<th>Group</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td></td>
<td>targets</td>
<td>Target values for the nonlinear equality constraint</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>scale_types</td>
<td>Choose how each constraint is scaled</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>scales</td>
<td>Characteristic values for scaling</td>
</tr>
</tbody>
</table>

**Description**

Specifies the number of nonlinear equality constraint functions returned by the interface.

The **targets** specification provides the targets for nonlinear equalities of the form

\[ h(x) = h_t \]

and the defaults for the equality targets enforce a value of 0. for each constraint

\[ h(x) = 0.0 \]

The **scale_types** and **scales** keywords are related to scaling of \( h(x) \). See the scaling information under specific methods, e.g., method-*scaling for details on how to use this keyword.

**targets**

- Keywords Area
- responses
- calibration_terms
- nonlinear_equality_constraints
- targets

Target values for the nonlinear equality constraint

**Specification**

**Alias:** nonlinear_equality_targets  
**Argument(s):** REALLIST  
**Default:** vector values = 0.
Description

The targets specification provides the targets for nonlinear equalities of the form

\[ g(x) = g_t \]

and the defaults for the equality targets enforce a value of 0.0 for each constraint:

\[ g(x) = 0.0 \]

scale_types

- Keywords Area
- responses
- calibration_terms
- nonlinear_equality_constraints
- scale_types

Choose how each constraint is scaled

Specification

Alias: nonlinear_equality_scale_types

Argument(s): STRINGLIST

Default: no scaling

Description

Type of scaling to apply to nonlinear constraints: 'none', 'value', 'auto' or 'log'. If a single string is specified it will apply to all components of the relevant nonlinear constraint vector.

See the scaling information under specific methods, e.g., method-**-scaling for details on how to use this keyword.

scales

- Keywords Area
- responses
- calibration_terms
- nonlinear_equality_constraints
- scales

Characteristic values for scaling
### Specification

**Alias:** nonlinear_equality_scales  
**Argument(s):** REALLIST  
**Default:** 1.0 (no scaling)

### Description

See the scaling information under specific methods, e.g., method-*-scaling for details on how to use this keyword.

#### 6.6.5 response_functions

- **Keywords Area**
- **responses**
- **response_functions**

Generic response type

### Specification

**Alias:** num_response_functions  
**Argument(s):** INTEGER

<table>
<thead>
<tr>
<th>Required/-</th>
<th>Description of</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>Group</td>
<td>scalar_responses</td>
<td>Description</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td>field_responses</td>
<td>Number of scalar</td>
</tr>
<tr>
<td>Optional</td>
<td></td>
<td></td>
<td>response functions</td>
</tr>
</tbody>
</table>

### Description

A generic response data set is specified using `response_functions`. Each of these functions is simply a response quantity of interest with no special interpretation taken by the method in use.

Whereas objective, constraint, and residual functions have special meanings for optimization and least squares algorithms, the generic response function data set need not have a specific interpretation and the user is free to define whatever functional form is convenient.

### Theory

This type of data set is used by uncertainty quantification methods, in which the effect of parameter uncertainty on response functions is quantified, and can also be used in parameter study and design of experiments methods (although these methods are not restricted to this data set), in which the effect of parameter variations on response functions is evaluated.
6.6. RESPONSES

See Also
These keywords may also be of interest:

- objective_functions
- calibration_terms

scalar_responses

- Keywords Area
- responses
- response_functions
- scalar_responses

Number of scalar response functions

Specification

Alias: num_scalar_responses
Argument(s): INTEGER

Description
This keyword describes the number of scalar response functions. It is meant to be used in conjunction with fieldResponses, which describes the number of field response functions. The total number of response functions, both scalar and field, is given by responseFunctions. If only scalar response functions are specified, it is not necessary to specify the number of scalar terms explicitly: one can simply say responseFunctions = 5 and get 5 scalar responses. However, if there are three scalar responses and 2 field responses, then responseFunctions = 5 but scalarResponses = 3 and fieldResponses = 2.

This type of data set is used by uncertainty quantification methods, in which the effect of parameter uncertainty on response functions is quantified, and can also be used in parameter study and design of experiments methods (although these methods are not restricted to this data set), in which the effect of parameter variations on response functions is evaluated.

See Also
These keywords may also be of interest:

- field_responses

field_responses

- Keywords Area
- responses
- response_functions
- field_responses

Number of field responses functions
CHAPTER 6. KEYWORDS AREA

Specifying the Number of Field Response Functions

**Specification**

**Alias:** num_field_responses

**Argument(s):** INTEGER

| Required/- | Description of | Dakota Keyword | Dakota Keyword Description |
| Optional/ | Group | | |
| Optional | lengths | lengths | Lengths of field responses |
| Optional | num_coordinates_per_field | num_coordinates_per_field | Number of independent coordinates for field responses |
| Optional | read_field_coordinates | read_field_coordinates | Add context to data: flag to indicate that field coordinates should be read |

**Description**

This keyword describes the number of field response functions. A field function is a set of related response values collected over a range of independent coordinate values which may or may not be specified by the user. For example, voltage over time would be a field function, where voltage is the field of interest and time is the independent coordinate. Similarly, temperature over time and space would be a field response, where the independent coordinates would be both time and spatial coordinates such as (x,y) or (x,y,z), depending on the application. The main difference between scalar responses and field responses is that for field data, we plan to implement methods that take advantage of the correlation or relationship between the field values.

Note that if there is one field_response, and it has length 100 (meaning 100 values), then the user's simulation code must return 100 values. Also, if there are both scalar and field responses, the user should specify the number of scalar responses as scalar_responses. If there are only field responses, it still is necessary to specify both response_functions = NN and field_responses = NN, where NN is the number of field responses.

This type of data set is used by uncertainty quantification methods, in which the effect of parameter uncertainty on response functions is quantified, and can also be used in parameter study and design of experiments methods (although these methods are not restricted to this data set), in which the effect of parameter variations on response functions is evaluated. Currently, field response functions will be translated back to scalar responses. So, a field of length 100 will be treated as 100 separate scalar responses. However, in future versions of Dakota, we plan to implement methods which can exploit the nature of field data.

**See Also**

These keywords may also be of interest:

- scalar_responses
- lengths
- Keywords Area
- responses
- response_functions
6.6. RESPONSES

- field_responses
- lengths

Lengths of field responses

Specification

Alias: none

Argument(s): INTEGERLIST

Description

This keyword describes the lengths of each field response. It is an integer vector of length field_responses. For example, if the field_responses = 2, an example would be lengths = 50 200, indicating that the first field response has 50 field elements but the second one has 200. The coordinate values (e.g. the independent variables) corresponding to these field responses are read in files labeled response_descriptor.coords.

See Also

These keywords may also be of interest:

- field_responses
- num_coordinates_per_field

num_coordinates_per_field

- Keywords Area
- responses
- response_functions
- field_responses
- num_coordinates_per_field

Number of independent coordinates for field responses

Specification

Alias: none

Argument(s): INTEGERLIST

Description

This keyword describes the number of independent coordinates for each field response. It is an integer vector of length field_responses. For example, if the field_responses = 2, an example would be num_coordinates_per_field = 2 1 means that the first field response has two sets of independent coordinates (perhaps x, y locations), but the second response only has one (for example, time where the field response is only dependent upon time). The actual coordinate values (e.g. the independent variables) corresponding to these field responses are defined in a file call response_descriptor.coords, where response_descriptor is the name of the individual field.
See Also
These keywords may also be of interest:

- field_responds

read_field_coordinates

- Keywords Area
- responses
- response_functions
- field_responds
- read_field_coordinates

Add context to data: flag to indicate that field coordinates should be read

Specification
Alias: none
  Argument(s): none

Description
Field coordinates specify independent variables (e.g. spatial or temporal coordinates) upon which the field depends. For example, the voltage level above might be a function of time, so time is the field coordinate. If the user has field coordinates to read, they need to specify read_field_coordinates. The field coordinates will then be read from a file named response_descriptor.coords, where response_descriptor is the user-provided descriptor for the field response. The number of columns in the coords file should be equal to the number of field coordinates.

6.6.6 no_gradients

- Keywords Area
- responses
- no_gradients

Gradients will not be used

Specification
Alias: none
  Argument(s): none

Description
The no_gradients specification means that gradient information is not needed in the study. Therefore, it will neither be retrieved from the simulation nor computed with finite differences. The no_gradients keyword is a complete specification for this case.
See Also
These keywords may also be of interest:
- numerical_gradients
- analytic_gradients
- mixed_gradients

6.6.7 analytic_gradients

- Keywords Area
- responses
- analytic_gradients

Analysis driver will return gradients

Specification
Alias: none
Argument(s): none

Description
The analytic_gradients specification means that gradient information is available directly from the simulation (finite differencing is not required). The simulation must return the gradient data in the Dakota format (enclosed in single brackets; see Dakota File Data Formats in the Users Manual[4]) for the case of file transfer of data. The analytic_gradients keyword is a complete specification for this case.

See Also
These keywords may also be of interest:
- numerical_gradients
- no_gradients
- mixed_gradients

6.6.8 mixed_gradients

- Keywords Area
- responses
- mixed_gradients

Gradients are needed and will be obtained from a mix of numerical and analytic sources

Specification
Alias: none
Argument(s): none
### Description

The `mixed_gradients` specification means that some gradient information is available directly from the simulation (analytic) whereas the rest will have to be finite differenced (numerical). This specification allows the user to make use of as much analytic gradient information as is available and then finite difference for the rest.

The `method_source`, `interval_type`, and `fd_gradient_step_size` specifications pertain to those functions listed by the `id_numerical_gradients` list.

### Examples

For example, the objective function may be a simple analytic function of the design variables (e.g., weight) whereas the constraints are nonlinear implicit functions of complex analyses (e.g., maximum stress).
See Also

These keywords may also be of interest:

- numerical_gradients
- no_gradients
- analytic_gradients

id_numerical_gradients

- Keywords Area
- responses
- mixed_gradients
- id_numerical_gradients

Identify which numerical gradient corresponds to which response

Topics

This keyword is related to the topics:

- objective_function_pointer

Specification

Alias: none

Argument(s): INTEGERLIST

Description

The id_analytic_gradients list specifies by number the functions which have analytic gradients, and the id_numerical_gradients list specifies by number the functions which must use numerical gradients. Each function identifier, from 1 through the total number of functions, must appear once and only once within the union of the id_analytic_gradients and id_numerical_gradients lists.

See Also

These keywords may also be of interest:

- id_analytic_gradients

id_analytic_gradients

- Keywords Area
- responses
- mixed_gradients
- id_analytic_gradients

Identify which analytical gradient corresponds to which response
**Topics**
This keyword is related to the topics:
- `objective_function_pointer`

**Specification**
Alias: none
Argument(s): INTEGERLIST

**Description**
The `id_analytic_gradients` list specifies by number the functions which have analytic gradients, and the `id_numerical_gradients` list specifies by number the functions which must use numerical gradients. Each function identifier, from 1 through the total number of functions, must appear once and only once within the union of the `id_analytic_gradients` and `id_numerical_gradients` lists.

**See Also**
These keywords may also be of interest:
- `id_numerical_gradients`

**method_source**
- `Keywords Area`
- `responses`
- `mixed_gradients`
- `method_source`

Specify which finite difference routine is used

**Specification**
Alias: none
Argument(s): none
Default: dakota

**Description**
The `method_source` setting specifies the source of the finite differencing routine that will be used to compute the numerical gradients:
- `dakota` (default)
- `vendor`
dakota denotes Dakota’s internal finite differencing algorithm and vendor denotes the finite differencing algorithm supplied by the iterator package in use (DOT, CONMIN, NPSOL, NL2SOL, NLSSOL, and OPT++ each have their own internal finite differencing routines). The dakota routine is the default since it can execute in parallel and exploit the concurrency in finite difference evaluations (see Exploiting Parallelism in the Users Manual [4]).

However, the vendor setting can be desirable in some cases since certain libraries will modify their algorithm when the finite differencing is performed internally. Since the selection of the dakota routine hides the use of finite differencing from the optimizers (the optimizers are configured to accept user-supplied gradients, which some algorithms assume to be of analytic accuracy), the potential exists for the vendor setting to trigger the use of an algorithm more optimized for the higher expense and/or lower accuracy of finite-differencing. For example, NPSOL uses gradients in its line search when in user-supplied gradient mode (since it assumes they are inexpensive), but uses a value-based line search procedure when internally finite differencing. The use of a value-based line search will often reduce total expense in serial operations. However, in parallel operations, the use of gradients in the NPSOL line search (user-supplied gradient mode) provides excellent load balancing without need to resort to speculative optimization approaches.

In summary, then, the dakota routine is preferred for parallel optimization, and the vendor routine may be preferred for serial optimization in special cases.

dakota

- Keywords Area
- responses
- mixed_gradients
- dakota

((Default) Use internal Dakota finite differences algorithm)

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** relative

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CHAPTER 6. KEYWORDS AREA

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<tr>
<th>absolute</th>
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</tr>
</thead>
<tbody>
<tr>
<td>bounds</td>
<td>Scale step-size by the domain of the parameter</td>
</tr>
</tbody>
</table>

### Description

The dakota routine is the default since it can execute in parallel and exploit the concurrency in finite difference evaluations (see Exploiting Parallelism in the Users Manual [4]).

When the method_source is dakota, the user may also specify the type of scaling desired when determining the finite difference step size. The choices are absolute, bounds, and relative. For absolute, the step size will be applied as is. For bounds, it will be scaled by the range of each parameter. For relative, it will be scaled by the parameter value.

**ignore_bounds**

- Keywords Area
- responses
- mixed_gradients
- dakota
- ignore_bounds

Do not respect bounds when computing gradients or Hessians

### Specification

**Alias:** none  
**Argument(s):** none  
**Default:** bounds respected

### Description

When Dakota computes gradients or Hessians by finite differences and the variables in question have bounds, it by default chooses finite-differencing steps that keep the variables within their specified bounds. Older versions of Dakota generally ignored bounds when computing finite differences. To restore the older behavior, one can add keyword ignore_bounds to the response specification when method_source dakota (or just dakota) is also specified.

In forward difference or backward difference computations, honoring bounds is straightforward.

To honor bounds when approximating $\partial f / \partial x_i$, i.e., component $i$ of the gradient of $f$, by central differences, Dakota chooses two steps $h_1$ and $h_2$ with $h_1 \neq h_2$, such that $x + h_1 e_i$ and $x + h_2 e_i$ both satisfy the bounds, and then computes

$$\frac{\partial f}{\partial x_i} \approx \frac{h_2^2(f_2 - f_0) - h_1^2(f_2 - f_0)}{h_1 h_2 (h_2 - h_1)},$$

with $f_0 = f(x)$, $f_1 = f(x + h_1 e_i)$, and $f_2 = f(x + h_2 e_i)$. 
6.6. RESPONSES

relative
- Keywords Area
- responses
- mixed_gradients
- dakota
- relative

( Default) Scale step size by the parameter value

**Specification**

Alias: none

Argument(s): none

**Description**

Scale step size by the parameter value

absolute
- Keywords Area
- responses
- mixed_gradients
- dakota
- absolute

Do not scale step-size

**Specification**

Alias: none

Argument(s): none

Default: relative

**Description**

Do not scale step-size

**bounds**
- Keywords Area
- responses
- mixed_gradients
- dakota
- bounds

Scale step-size by the domain of the parameter
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none
Argument(s): none

Description

Scale step-size by the domain of the parameter

vendor

- Keywords Area
- responses
- mixed_gradients
- vendor

Use non-Dakota fd algorithm

Specification

Alias: none
Argument(s): none

Description

See parent page for usage notes.

interval_type

- Keywords Area
- responses
- mixed_gradients
- interval_type

Specify how to compute gradients and hessians

Specification

Alias: none
Argument(s): none
Default: forward
Description
The interval type setting is used to select between forward and central differences in the numerical gradient calculations. The dakota, DOT vendor, and OPT++ vendor routines have both forward and central differences available, the CONMIN and NL2SOL vendor routines support forward differences only, and the NP-SOL and NLSSOL vendor routines start with forward differences and automatically switch to central differences as the iteration progresses (the user has no control over this). The following forward difference expression

$$\nabla f(x) \approx \frac{f(x + he_i) - f(x)}{h}$$

and the following central difference expression

$$\nabla f(x) \approx \frac{f(x + he_i) - f(x - he_i)}{2h}$$

are used to estimate the $i^{th}$ component of the gradient vector.

forward
- Keywords Area
- responses
- mixed_gradients
- forward

(Default) Use forward differences

Specification
Alias: none
Argument(s): none
Default: forward

Description
See parent page for usage notes.

central
- Keywords Area
- responses
- mixed_gradients
- central

Use central differences

Specification
Alias: none
Argument(s): none
Description

See parent page for usage notes.

fd_step_size

- Keywords Area
- responses
- mixed_gradients
- fd_step_size

Step size used when computing gradients and Hessians

Specification

Alias: fd_gradient_step_size
Argument(s): REALLIST
Default: 0.001

Description

fd_step_size specifies the relative finite difference step size to be used in the computations. Either a single value may be entered for use with all parameters, or a list of step sizes may be entered, one for each parameter.

The latter option of a list of step sizes is only valid for use with the Dakota finite differencing routine. For Dakota with an interval scaling type of absolute, the differencing interval will be fd_step_size.

For Dakota with an interval scaling type of bounds, the differencing intervals are computed by multiplying fd_step_size with the range of the parameter. For Dakota (with an interval scaling type of relative), DOT, CONMIN, and OPT++, the differencing intervals are computed by multiplying the fd_step_size with the current parameter value. In this case, a minimum absolute differencing interval is needed when the current parameter value is close to zero. This prevents finite difference intervals for the parameter which are too small to distinguish differences in the response quantities being computed. Dakota, DOT, CONMIN, and OPT++ all use $0.01 \times \text{fd\_step\_size}$ as their minimum absolute differencing interval. With a fd_step_size = 0.001, for example, Dakota, DOT, CONMIN, and OPT++ will use intervals of $0.01 \times \text{current parameter value}$ with a minimum interval of 1e-5. NPSOL and NLSSOL use a different formula for their finite difference intervals: $\text{fd\_step\_size} \times (1+|\text{current parameter value}|)$. This definition has the advantage of eliminating the need for a minimum absolute differencing interval since the interval no longer goes to zero as the current parameter value goes to zero.

6.6.9 numerical_gradients

- Keywords Area
- responses
- numerical_gradients

Gradients are needed and will be approximated by finite differences
6.6. RESPONSES

Specification

Alias: none
  Argument(s): none
### Required/Optional

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<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<tr>
<td>Optional <em>(Choose One)</em></td>
<td>method_source</td>
<td>Specify which finite difference routine is used</td>
</tr>
<tr>
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<td>dakota</td>
<td><em>(Default)</em> Use internal Dakota finite differences algorithm</td>
</tr>
<tr>
<td>Optional</td>
<td>vendor</td>
<td>Use non-Dakota fd algorithm</td>
</tr>
<tr>
<td>Optional <em>(Choose One)</em></td>
<td>interval_type</td>
<td>Specify how to compute gradients and hessians</td>
</tr>
<tr>
<td></td>
<td>forward</td>
<td><em>(Default)</em> Use forward differences</td>
</tr>
<tr>
<td>Optional</td>
<td>central</td>
<td>Use central differences</td>
</tr>
<tr>
<td>Optional</td>
<td>fd_step_size</td>
<td>Step size used when computing gradients and Hessians</td>
</tr>
</tbody>
</table>

### Description

The `numerical_gradients` specification means that gradient information is needed and will be computed with finite differences using either the native or one of the vendor finite differencing routines.

### See Also

These keywords may also be of interest:

- `no_gradients`
- `analytic_gradients`
- `mixed_gradients`

### method_source

- `Keywords Area`
- `responses`
- `numerical_gradients`
- `method_source`

Specify which finite difference routine is used.
6.6. RESPONSES

Specification

Alias: none

Argument(s): none

Default: dakota

Description

The method_source setting specifies the source of the finite differencing routine that will be used to compute the numerical gradients:

- dakota (default)
- vendor

_dakota_ denotes Dakota’s internal finite differencing algorithm and _vendor_ denotes the finite differencing algorithm supplied by the iterator package in use (DOT, CONMIN, NPSOL, NL2SOL, NLSSOL, and OPT++ each have their own internal finite differencing routines). The _dakota_ routine is the default since it can execute in parallel and exploit the concurrency in finite difference evaluations (see Exploiting Parallelism in the Users Manual [4]).

However, the _vendor_ setting can be desirable in some cases since certain libraries will modify their algorithm when the finite differencing is performed internally. Since the selection of the _dakota_ routine hides the use of finite differencing from the optimizers (the optimizers are configured to accept user-supplied gradients, which some algorithms assume to be of analytic accuracy), the potential exists for the _vendor_ setting to trigger the use of an algorithm more optimized for the higher expense and/or lower accuracy of finite-differencing. For example, NPSOL uses gradients in its line search when in user-supplied gradient mode (since it assumes they are inexpensive), but uses a value-based line search procedure when internally finite differencing. The use of a value-based line search will often reduce total expense in serial operations. However, in parallel operations, the use of gradients in the NPSOL line search (user-supplied gradient mode) provides excellent load balancing without need to resort to speculative optimization approaches.

In summary, then, the _dakota_ routine is preferred for parallel optimization, and the _vendor_ routine may be preferred for serial optimization in special cases.

dakota

- Keywords Area
- responses
- numerical_gradients
- dakota

(Default) Use internal Dakota finite differences algorithm

Specification

Alias: none

Argument(s): none

Default: relative
### Description

The **dakota** routine is the default since it can execute in parallel and exploit the concurrency in finite difference evaluations (see Exploiting Parallelism in the Users Manual [4]).

When the method_source is **dakota**, the user may also specify the type of scaling desired when determining the finite difference step size. The choices are **absolute**, **bounds**, and **relative**. For **absolute**, the step size will be applied as is. For **bounds**, it will be scaled by the range of each parameter. For **relative**, it will be scaled by the parameter value.

### ignore_bounds

- **Keywords Area**
- **responses**
- **numerical_gradients**
- **dakota**
- **ignore_bounds**

Do not respect bounds when computing gradients or Hessians

### Specification

**Alias:** none  
**Argument(s):** none  
**Default:** bounds respected

### Description

When Dakota computes gradients or Hessians by finite differences and the variables in question have bounds, it by default chooses finite-differencing steps that keep the variables within their specified bounds. Older versions of Dakota generally ignored bounds when computing finite differences. To restore the older behavior, one

<table>
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<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Description</th>
</tr>
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<td>Optional (Choose One)</td>
<td>step scaling (Group 1)</td>
<td><strong>ignore_bounds</strong></td>
<td>Do not respect bounds when computing gradients or Hessians (Default) Scale step size by the parameter value</td>
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<tr>
<td></td>
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<td><strong>relative</strong></td>
<td>Scale step-size by the domain of the parameter</td>
</tr>
<tr>
<td></td>
<td></td>
<td><strong>absolute</strong></td>
<td>Do not scale step-size</td>
</tr>
<tr>
<td></td>
<td></td>
<td><strong>bounds</strong></td>
<td>Scale step-size by the domain of the parameter</td>
</tr>
</tbody>
</table>
can add keyword *ignore_bounds* to the response specification when *method_source* dakota (or just dakota) is also specified.

In forward difference or backward difference computations, honoring bounds is straightforward.

To honor bounds when approximating \( \frac{\partial f}{\partial x_i} \), i.e., component \( i \) of the gradient of \( f \), by central differences, Dakota chooses two steps \( h_1 \) and \( h_2 \) with \( h_1 \neq h_2 \), such that \( x + h_1 e_i \) and \( x + h_2 e_i \) both satisfy the bounds, and then computes

\[
\frac{\partial f}{\partial x_i} \approx \frac{h_2^2 (f_1 - f_0) - h_1^2 (f_2 - f_0)}{h_1 h_2 (h_2 - h_1)},
\]

with \( f_0 = f(x) \), \( f_1 = f(x + h_1 e_i) \), and \( f_2 = f(x + h_2 e_i) \).

**relative**

- **Keywords Area**
- **responses**
- **numerical_gradients**
- **dakota**
- **relative**

(DefaultValue) Scale step size by the parameter value

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

Scale step size by the parameter value

**absolute**

- **Keywords Area**
- **responses**
- **numerical_gradients**
- **dakota**
- **absolute**

Do not scale step-size

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** relative
**Description**

Do not scale step-size

**bounds**

- Keywords Area
- responses
- numerical_gradients
- dakota
- bounds

Scale step-size by the domain of the parameter

**Specification**

**Alias**: none

**Argument(s)**: none

**Description**

Scale step-size by the domain of the parameter

**vendor**

- Keywords Area
- responses
- numerical_gradients
- vendor

Use non-Dakota fd algorithm

**Specification**

**Alias**: none

**Argument(s)**: none

**Description**

See parent page for usage notes.
6.6. RESPONSES

interval_type

- Keywords Area
- responses
- numerical_gradients
- interval_type

Specify how to compute gradients and hessians

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** forward

**Description**

The `interval_type` setting is used to select between forward and central differences in the numerical gradient calculations. The dakota, DOT vendor, and OPT++ vendor routines have both forward and central differences available, the CONMIN and NL2SOL vendor routines support forward differences only, and the NP-SOL and NLSSOL vendor routines start with forward differences and automatically switch to central differences as the iteration progresses (the user has no control over this). The following forward difference expression

\[ \nabla f(x) \approx \frac{f(x + h e_i) - f(x)}{h} \]

and the following central difference expression

\[ \nabla f(x) \approx \frac{f(x + h e_i) - f(x - h e_i)}{2h} \]

are used to estimate the \( i^{th} \) component of the gradient vector.

**forward**

- Keywords Area
- responses
- numerical_gradients
- forward

( Default) Use forward differences

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** forward
**Description**
See parent page for usage notes.

**central**
- Keywords Area
- responses
- numerical_gradients
- central

Use central differences

**Specification**
Alias: none
Argument(s): none

**FD_STEP_SIZE**
See parent page for usage notes.

**FD_STEP_SIZE**
- Keywords Area
- responses
- numerical_gradients
- fd_step_size

Step size used when computing gradients and Hessians

**Specification**
Alias: fd_gradient_step_size
Argument(s): REALLIST
Default: 0.001

**Description**

*fd_step_size* specifies the relative finite difference step size to be used in the computations. Either a single value may be entered for use with all parameters, or a list of step sizes may be entered, one for each parameter.

The latter option of a list of step sizes is only valid for use with the Dakota finite differencing routine. For Dakota with an interval scaling type of *absolute*, the differencing interval will be *fd_step_size*.

For Dakota with and interval scaling type of *bounds*, the differencing intervals are computed by multiplying *fd_step_size* with the range of the parameter. For Dakota (with an interval scaling type of *relative*), DOT, CONMIN, and OPT++, the differencing intervals are computed by multiplying the *fd_step_size* with the current parameter value. In this case, a minimum absolute differencing interval is needed when the current
parameter value is close to zero. This prevents finite difference intervals for the parameter which are too small
to distinguish differences in the response quantities being computed. Dakota, DOT, CONMIN, and OPT++ all use .01*fd_step_size as their minimum absolute differencing interval. With a fd_step_size = .001,
for example, Dakota, DOT, CONMIN, and OPT++ will use intervals of .001*current value with a minimum
interval of 1.e-5. NPSOL and NLSSOL use a different formula for their finite difference intervals: fd_step_size*(1+|current parameter value|). This definition has the advantage of eliminating the need for a
minimum absolute differencing interval since the interval no longer goes to zero as the current parameter value
goes to zero.

### 6.6.10 no_hessians

- **Keywords Area**
- **responses**
- **no_hessians**

Hessians will not be used

**Specification**

**Alias:** none  
**Argument(s):** none

**Description**

The no_hessians specification means that the method does not require Dakota to manage the computation of
any Hessian information. Therefore, it will neither be retrieved from the simulation nor computed by Dakota. The
no_hessians keyword is a complete specification for this case. Note that, in some cases, Hessian information
may still be being approximated internal to an algorithm (e.g., within a quasi-Newton optimizer such as optpp-
_q_newton); however, Dakota has no direct involvement in this process and the responses specification need not
include it.

**See Also**

These keywords may also be of interest:

- **numerical_hessians**
- **quasi_hessians**
- **analytic_hessians**
- **mixed_hessians**

### 6.6.11 numerical_hessians

- **Keywords Area**
- **responses**
- **numerical_hessians**

Hessians are needed and will be approximated by finite differences
CHAPTER 6. KEYWORDS AREA

Specification

Alias: none
Argument(s): none

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<th>Required/-Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<td>Step size used when computing gradients and Hessians</td>
</tr>
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<td>absolute</td>
<td>Do not scale step-size</td>
</tr>
<tr>
<td></td>
<td></td>
<td>bounds</td>
<td>Scale step-size by the domain of the parameter</td>
</tr>
<tr>
<td></td>
<td></td>
<td>forward</td>
<td>(Default) Use forward differences</td>
</tr>
<tr>
<td></td>
<td></td>
<td>central</td>
<td>Use central differences</td>
</tr>
</tbody>
</table>

Description

The numerical_hessians specification means that Hessian information is needed and will be computed with finite differences using either first-order gradient differencing (for the cases of analytic_gradients or for the functions identified by id_analytic_gradients in the case of mixed_gradients) or first- or second-order function value differencing (all other gradient specifications). In the former case, the following expression

$$\nabla^2 f(x)_i \approx \frac{\nabla f(x + he_i) - \nabla f(x)}{h}$$

estimates the $i^{th}$ Hessian column, and in the latter case, the following expressions

$$\nabla^2 f(x)_{i,j} \approx \frac{f(x + he_i + he_j) - f(x + he_i) - f(x - h e_j) + f(x)}{h_i h_j}$$

and

$$\nabla^2 f(x)_{i,j} \approx \frac{f(x + he_i + he_j) - f(x + he_i - he_j) - f(x - he_i + he_j) + f(x - he_i - he_j)}{4h^2}$$

provide first- and second-order estimates of the $ij^{th}$ Hessian term. Prior to Dakota 5.0, Dakota always used second-order estimates. In Dakota 5.0 and newer, the default is to use first-order estimates (which honor bounds on the variables and require only about a quarter as many function evaluations as do the second-order estimates), but specifying central after numerical_hessians causes Dakota to use the old second-order estimates, which do not honor bounds. In optimization algorithms that use Hessians, there is little reason to use second-order differences in computing Hessian approximations.
See Also

These keywords may also be of interest:

- no_hessians
- quasi_hessians
- analytic_hessians
- mixed_hessians

**fd_step_size**

- Keywords Area
- responses
- numerical_hessians
- fd_step_size

Step size used when computing gradients and Hessians

**Specification**

**Alias:** fd_hessian_step_size

**Argument(s):** REALLIST

**Default:** 0.001 (forward), 0.002 (central)

**Description**

*fd_step_size* specifies the relative finite difference step size to be used in the computations. Either a single value may be entered for use with all parameters, or a list of step sizes may be entered, one for each parameter.

The latter option of a list of step sizes is only valid for use with the Dakota finite differencing routine. For Dakota with an interval scaling type of `absolute`, the differencing interval will be *fd_step_size*.

For Dakota with and interval scaling type of `bounds`, the differencing intervals are computed by multiplying *fd_step_size* with the range of the parameter. For Dakota (with an interval scaling type of `relative`), DOT, CONMIN, and OPT++, the differencing intervals are computed by multiplying the *fd_step_size* with the current parameter value. In this case, a minimum absolute differencing interval is needed when the current parameter value is close to zero. This prevents finite difference intervals for the parameter which are too small to distinguish differences in the response quantities being computed. Dakota, DOT, CONMIN, and OPT++ all use `.01*fd_step_size` as their minimum absolute differencing interval. With a *fd_step_size* = .001, for example, Dakota, DOT, CONMIN, and OPT++ will use intervals of .001*current value* with a minimum interval of 1.e-5. NPSOL and NLSSOL use a different formula for their finite difference intervals: *fd_step_size*(1+|current parameter value|). This definition has the advantage of eliminating the need for a minimum absolute differencing interval since the interval no longer goes to zero as the current parameter value goes to zero.
relative

- Keywords Area
- responses
- numerical_hessians
- relative

(Default) Scale step size by the parameter value

**Specification**

Alias: none

Argument(s): none

**Description**

Scale step size by the parameter value

absolute

- Keywords Area
- responses
- numerical_hessians
- absolute

Do not scale step-size

**Specification**

Alias: none

Argument(s): none

Default: relative

**Description**

Do not scale step-size

bounds

- Keywords Area
- responses
- numerical_hessians
- bounds

Scale step-size by the domain of the parameter
6.6. **RESPONSES**

**Specification**

Alias: none  
Argument(s): none

**Description**

Scale step-size by the domain of the parameter

*forward*

- **Keywords Area**
- responses  
- numerical_hessians 
- forward

(Default) Use forward differences

**Specification**

Alias: none  
Argument(s): none  
Default: forward

**Description**

See parent page for usage notes.

*central*

- **Keywords Area**
- responses  
- numerical_hessians 
- central

Use central differences

**Specification**

Alias: none  
Argument(s): none

**Description**

See parent page for usage notes.
6.6.12 quasi_hessians

- Keywords Area
- responses
- quasi_hessians

Hessians are needed and will be approximated by secant updates (BFGS or SR1) from a series of gradient evaluations.

**Specification**

**Alias:** none

**Argument(s):** none

<table>
<thead>
<tr>
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<th>Description of Group Group 1</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword Description</th>
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<tbody>
<tr>
<td></td>
<td></td>
<td>bfgs</td>
<td>Use BFGS method to compute quasi-hessians</td>
</tr>
<tr>
<td></td>
<td></td>
<td>srl</td>
<td>Use the Symmetric Rank 1 update method to compute quasi-Hessians</td>
</tr>
</tbody>
</table>

**Description**

The `quasi_hessians` specification means that Hessian information is needed and will be approximated using secant updates (sometimes called "quasi-Newton updates", though any algorithm that approximates Newton’s method is a quasi-Newton method).

Compared to finite difference numerical Hessians, secant approximations do not expend additional function evaluations in estimating all of the second-order information for every point of interest. Rather, they accumulate approximate curvature information over time using the existing gradient evaluations.

The supported secant approximations include the Broyden-Fletcher-Goldfarb-Shanno (BFGS) update (specified with the keyword `bfgs`) and the Symmetric Rank 1 (SR1) update (specified with the keyword `srl`).

**See Also**

These keywords may also be of interest:

- `no_hessians`
- `numerical_hessians`
- `analytic_hessians`
- `mixed_hessians`
Use BFGS method to compute quasi-hessians

**Specification**

**Alias:** none

**Argument(s):** none

<p>| Required/- | Description of | Dakota Keyword | Dakota Keyword |</p>
<table>
<thead>
<tr>
<th>Optional</th>
<th>Group</th>
<th></th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>damped</td>
<td>Numerical safeguarding for BFGS updates</td>
</tr>
</tbody>
</table>

**Description**

Broyden-Fletcher-Goldfarb-Shanno (BFGS) update will be used to compute quasi-Hessians.

\[ B_{k+1} = B_k - \frac{B_k s_k s_k^T B_k}{s_k^T B_k s_k} + \frac{y_k y_k^T}{y_k^T s_k} \]

where \( B_k \) is the \( k \text{th} \) approximation to the Hessian, \( s_k = x_{k+1} - x_k \) is the step and \( y_k = \nabla f_{k+1} - \nabla f_k \) is the corresponding yield in the gradients.

**Notes**

- Initial scaling of \( \frac{y_k^T s_k}{y_k^T y_k} I \) is used for \( B_0 \) prior to the first update.
- Numerical safeguarding is used to protect against numerically small denominators within the updates.
- This safeguarding skips the update if \( |y_k^T s_k| < 10^{-6} s_k^T B_k s_k \)
- Additional safeguarding can be added using the **damped** option, which utilizes an alternative damped BFGS update when the curvature condition \( y_k^T s_k > 0 \) is nearly violated.
**Specification**

**Alias:** none  
**Argument(s):** none  
**Default:** undamped BFGS

**Description**

See parent page.

**sr1**

- **Keywords Area**
- responses
- quasi_hessians
- sr1

Use the Symmetric Rank 1 update method to compute quasi-Hessians

**Specification**

**Alias:** none  
**Argument(s):** none

**Description**

The Symmetric Rank 1 (SR1) update (specified with the keyword sr1) will be used to compute quasi-Hessians.

\[ B_{k+1} = B_k + \frac{(y_k - B_k s_k)(y_k - B_k s_k)^T}{(y_k - B_k s_k)^T s_k} \]

where \( B_k \) is the \( k^{th} \) approximation to the Hessian, \( s_k = x_{k+1} - x_k \) is the step and \( y_k = \nabla f_{k+1} - \nabla f_k \) is the corresponding yield in the gradients.

**Notes**

- Initial scaling of \( \frac{y_k^T y_k}{y_k^T s_k} I \) is used for \( B_0 \) prior to the first update.
- Numerical safeguarding is used to protect against numerically small denominators within the updates.
- This safeguarding skips the update if \( |(y_k - B_k s_k)^T s_k| < 10^{-6} \| s_k \|_2 \| y_k - B_k s_k \|_2 \)

**6.6.13 analytic_hessians**

- **Keywords Area**
- responses
- analytic_hessians

Hessians are needed and are available directly from the analysis driver
6.6. RESPONSES

Specification

Alias: none
  Argument(s): none

Description

The *analytic_hessians* specification means that Hessian information is available directly from the simulation. The simulation must return the Hessian data in the Dakota format (enclosed in double brackets; see Dakota File Data Formats in Users Manual[4]) for the case of file transfer of data. The *analytic_hessians* keyword is a complete specification for this case.

See Also

These keywords may also be of interest:

- *no_hessians*
- *numerical_hessians*
- *quasi_hessians*
- *mixed_hessians*

6.6.14 mixed_hessians

- Keywords Area
- responses
- mixed_hessians

Hessians are needed and will be obtained from a mix of numerical, analytic, and "quasi" sources

Specification

Alias: none
  Argument(s): none

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<th>Dakota Keyword Description</th>
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<td>Identify which numerical-Hessian corresponds to which response (Default) Scale step size by the parameter value</td>
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<td>relative</td>
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CHAPTER 6. KEYWORDS AREA

<table>
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<tr>
<th>absolute</th>
<th>Do not scale step-size</th>
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<tbody>
<tr>
<td>bounds</td>
<td>Scale step-size by the domain of the parameter</td>
</tr>
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<td>forward</td>
<td>(Default) Use forward differences</td>
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</table>

<table>
<thead>
<tr>
<th>Optional</th>
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<tr>
<td>central</td>
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</tbody>
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<table>
<thead>
<tr>
<th>Optional</th>
</tr>
</thead>
<tbody>
<tr>
<td>id_quasi_hessians</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Optional</th>
</tr>
</thead>
<tbody>
<tr>
<td>id_analytic_hessians</td>
</tr>
</tbody>
</table>

**Description**

The `mixed_hessians` specification means that some Hessian information is available directly from the simulation (analytic) whereas the rest will have to be estimated by finite differences (numerical) or approximated by secant updating. As for mixed gradients, this specification allows the user to make use of as much analytic information as is available and then estimate/approximate the rest.

The `id_analytic_hessians` list specifies by number the functions which have analytic Hessians, and the `id_numerical_hessians` and `id_quasi_hessians` lists specify by number the functions which must use numerical Hessians and secant Hessian updates, respectively. Each function identifier, from 1 through the total number of functions, must appear once and only once within the union of the `id_analytic_hessians`, `id_numerical_hessians`, and `id_quasi_hessians` lists.

The `fd_hessian_step_size` and `bfgs`, `damped bfgs`, or `sr1` secant update selections are as described previously in `responses` and pertain to those functions listed by the `id_numerical_hessians` and `id_quasi_hessians` lists.

**See Also**

These keywords may also be of interest:

- `no_hessians`
- `numerical_hessians`
- `quasi_hessians`
- `analytic_hessians`

**id_numerical_hessians**

- Keywords Area
- `responses`
6.6. RESPONSES

- mixed_hessians
- id_numerical_hessians

Identify which numerical-Hessian corresponds to which response

Topics

This keyword is related to the topics:

- objective_function_pointer

Specification

Alias: none

<table>
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<th>Dakota Keyword Description</th>
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<td>Optional</td>
<td>fd_step_size</td>
<td></td>
<td>Step size used when computing gradients and Hessians</td>
</tr>
</tbody>
</table>

Description

The id_analytic_hessians list specifies by number the functions which have analytic Hessians, and the id_numerical_hessians and id_quasi_hessians lists specify by number the functions which must use numerical Hessians and secant Hessian updates, respectively. Each function identifier, from 1 through the total number of functions, must appear once and only once within the union of the id_analytic_hessians, id_numerical_hessians, and id_quasi_hessians lists.

See Also

These keywords may also be of interest:

- id_analytic_hessians
- id_quasi_hessians

fd_step_size

- Keywords Area
- responses
- mixed_hessians
- id_numerical_hessians
- fd_step_size

Step size used when computing gradients and Hessians
CHAPTER 6. KEYWORDS AREA

**Specification**

**Alias:** fd_hessian_step_size

**Argument(s):** REALLIST

**Default:** 0.001 (forward), 0.002 (central)

**Description**

`fd_step_size` specifies the relative finite difference step size to be used in the computations. Either a single value may be entered for use with all parameters, or a list of step sizes may be entered, one for each parameter.

The latter option of a list of step sizes is only valid for use with the Dakota finite differencing routine. For Dakota with an interval scaling type of `absolute`, the differencing interval will be `fd_step_size`.

For Dakota with an interval scaling type of `bounds`, the differencing intervals are computed by multiplying `fd_step_size` with the range of the parameter. For Dakota (with an interval scaling type of `relative`), DOT, CONMIN, and OPT++, the differencing intervals are computed by multiplying the `fd_step_size` with the current parameter value. In this case, a minimum absolute differencing interval is needed when the current parameter value is close to zero. This prevents finite difference intervals for the parameter which are too small to distinguish differences in the response quantities being computed. Dakota, DOT, CONMIN, and OPT++ all use `.01*fd_step_size` as their minimum absolute differencing interval. With a `fd_step_size = .001`, for example, Dakota, DOT, CONMIN, and OPT++ will use intervals of `.001*current_value` with a minimum interval of 1.e-5. NPSOL and NLSSOL use a different formula for their finite difference intervals: `fd_step_size*(1+|current parameter value|)`. This definition has the advantage of eliminating the need for a minimum absolute differencing interval since the interval no longer goes to zero as the current parameter value goes to zero.

**relative**

- Keywords Area
- responses
- mixed_hessians
- relative

(Default) Scale step size by the parameter value

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

Scale step size by the parameter value

**absolute**

- Keywords Area
- responses
- mixed_hessians
6.6. RESPONSES

- **absolute**

  Do not scale step-size

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** relative

**Description**

Do not scale step-size

**bounds**

- **Keywords Area**
- **responses**
- **mixed_hessians**
- **bounds**

  Scale step-size by the domain of the parameter

**Specification**

**Alias:** none

**Argument(s):** none

**Description**

Scale step-size by the domain of the parameter

**forward**

- **Keywords Area**
- **responses**
- **mixed_hessians**
- **forward**

  (Default) Use forward differences

**Specification**

**Alias:** none

**Argument(s):** none

**Default:** forward
CHAPTER 6. KEYWORDS AREA

Description
See parent page for usage notes.

central
- Keywords Area
- responses
- mixed_hessians
- central

Use central differences

Specification
Alias: none
Argument(s): none

Description
See parent page for usage notes.

id_quasi_hessians
- Keywords Area
- responses
- mixed_hessians
- id_quasi_hessians

Identify which quasi-Hessian corresponds to which response

Topics
This keyword is related to the topics:
- objective_function_pointer

Specification
Alias: none
Argument(s): INTEGERLIST

<table>
<thead>
<tr>
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<th>Description of</th>
<th>Dakota Keyword</th>
<th>Dakota Keyword</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optional</td>
<td>Group</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>


### Description

The `id_analytic_hessians` list specifies by number the functions which have analytic Hessians, and the `id_numerical_hessians` and `id_quasi_hessians` lists specify by number the functions which must use numerical Hessians and secant Hessian updates, respectively. Each function identifier, from 1 through the total number of functions, must appear once and only once within the union of the `id_analytic_hessians`, `id_numerical_hessians`, and `id_quasi_hessians` lists.

### See Also

These keywords may also be of interest:

- `id_numerical_hessians`
- `id_analytic_hessians`

### bfgs

- Keywords Area
- `responses`
- `mixed_hessians`
- `id_quasi_hessians`
- `bfgs`

Use BFGS method to compute quasi-hessians

### Specification

**Alias:** none

**Argument(s):** none

<table>
<thead>
<tr>
<th>Required/Optional</th>
<th>Description of Group</th>
<th>Dakota Keyword</th>
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</thead>
<tbody>
<tr>
<td><strong>bfgs</strong></td>
<td></td>
<td></td>
<td>Numerical safeguarding for BFGS updates</td>
</tr>
</tbody>
</table>
CHAPTER 6. KEYWORDS AREA

Description

Broyden-Fletcher-Goldfarb-Shanno (BFGS) update will be used to compute quasi-Hessians.

\[ B_{k+1} = B_k - \frac{B_k s_k s_k^T B_k}{s_k^T B_k s_k} + \frac{y_k y_k^T}{y_k^T s_k} \]

where \( B_k \) is the \( k^{th} \) approximation to the Hessian, \( s_k = x_{k+1} - x_k \) is the step and \( y_k = \nabla f_{k+1} - \nabla f_k \) is the corresponding yield in the gradients.

Notes

- Initial scaling of \( \frac{y_k^T y_k}{y_k^T s_k} I \) is used for \( B_0 \) prior to the first update.
- Numerical safeguarding is used to protect against numerically small denominators within the updates.
- This safeguarding skips the update if \( |y_k^T s_k| < 10^{-6} s_k^T B_k s_k \)
- Additional safeguarding can be added using the damped option, which utilizes an alternative damped BFGS update when the curvature condition \( y_k^T s_k > 0 \) is nearly violated.

damped

- Keywords Area
- responses
- mixed_hessians
- id_quasi_hessians
- bfgs
- damped

Numerical safeguarding for BFGS updates

Specification

Alias: none

Argument(s): none

Default: undamped BFGS

Description

See parent page.

sr1

- Keywords Area
- responses
- mixed_hessians
- id_quasi_hessians
- sr1

Use the Symmetric Rank 1 update method to compute quasi-Hessians
6.6. RESPONSES

Specification

Alias: none
Argument(s): none

Description

The Symmetric Rank 1 (SR1) update (specified with the keyword \texttt{sr1}) will be used to compute quasi-Hessians.

\begin{equation}
B_{k+1} = B_k + \frac{(y_k - B_k s_k)(y_k - B_k s_k)^T}{(y_k - B_k s_k)^T s_k}
\end{equation}

where $B_k$ is the $k^{th}$ approximation to the Hessian, $s_k = x_{k+1} - x_k$ is the step and $y_k = \nabla f_{k+1} - \nabla f_k$ is the corresponding yield in the gradients.

Notes

- Initial scaling of $\frac{y_k^T y_k}{y_k^T s_k} I$ is used for $B_0$ prior to the first update.
- Numerical safeguarding is used to protect against numerically small denominators within the updates.
- This safeguarding skips the update if $|(y_k - B_k s_k)^T s_k| < 10^{-6}||s_k||_2||y_k - B_k s_k||_2$

\texttt{id\_analytic\_hessians}

- Keywords Area
- responses
- mixed\_hessians
- \texttt{id\_analytic\_hessians}

Identify which analytical Hessian corresponds to which response

Topics

This keyword is related to the topics:

- \texttt{objective\_function\_pointer}

Specification

Alias: none
Argument(s): INTEGERLIST

Description

The \texttt{id\_analytic\_hessians} list specifies by number the functions which have analytic Hessians, and the \texttt{id\_numerical\_hessians} and \texttt{id\_quasi\_hessians} lists specify by number the functions which must use numerical Hessians and secant Hessian updates, respectively. Each function identifier, from 1 through the total number of functions, must appear once and only once within the union of the \texttt{id\_analytic\_hessians}, \texttt{id\_numerical\_hessians}, and \texttt{id\_quasi\_hessians} lists.
See Also
These keywords may also be of interest:

- `id_numerical_hessians`
- `id_quasi_hessians`
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