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DAKOTA 101: Calibration

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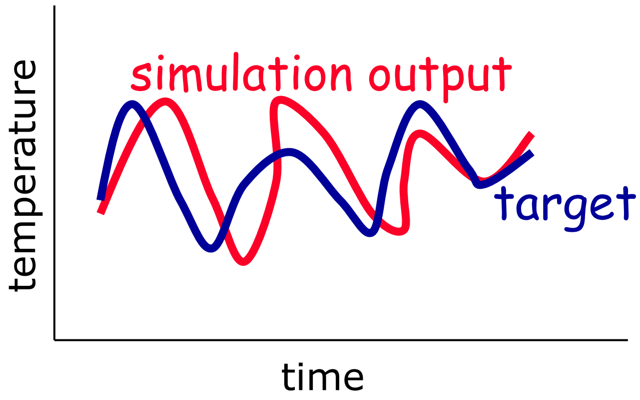
Learning Goals - Calibration

- Define a calibration/parameter estimation problem
- Understand relationship to optimization
- Recognize differences in DAKOTA interface
- Identify problems in your field
- Calibrate cantilever beam model to synthetic data
- Become cognizant of potential challenges

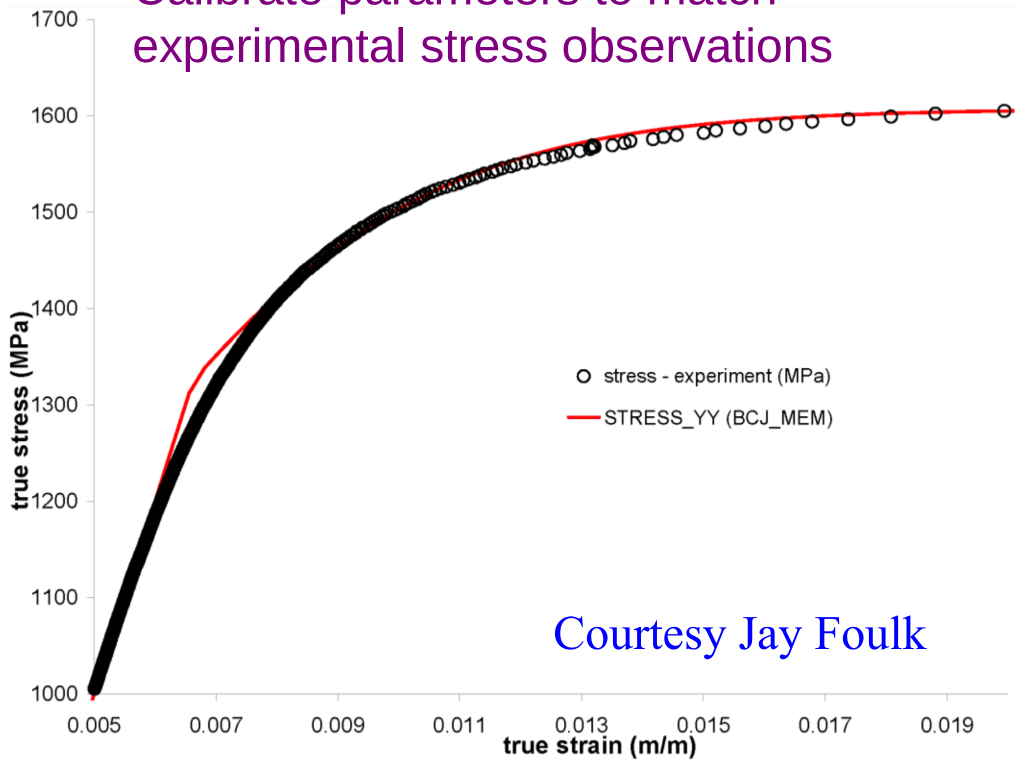
Why Use Calibration?



- **What: Determine parameter values that maximize agreement between simulation response and target response**
  - **A.K.A. parameter estimation, parameter identification, systems identification, nonlinear least-squares, inverse problem.**
  - **Calibration is not validation! Separate data should be used to assess whether a calibrated model is valid.**
- **Why?**
  - **Fit a model to data**
    - **E.g., determine material model parameters such that predicted stress-strain curve matches one generated experimentally**
  - **Find control settings that enable a system to achieve a prescribed performance profile**
    - **E.g., determine thermostat settings the yield uniform building temperature across multiple control zones**
  - **Determine source terms for an observed phenomenon**
    - **E.g., determine the size and location of a chemical release**

Parameter estimation for a material plasticity model

Calibrate parameters to match experimental stress observations



f – yields rate dependence (fit)
Y – the yield stress (chosen)
n – exponent in flow rule (fit)
H – hardening in evolution of κ (fit)
R_d – recovery in evolution of κ (fit)

f	*4.52 x 10^4*
Y	*1325 MPa*
n	*0.386*
H	*1.10 x 10^5 MPa*
R_d	*389*

NOTE: Experimental data taken from a representative test, ph13-8-h950-test-3

Flow rule concentrating the effective stress

$$\dot{\epsilon_p} = f\{\sinh[\frac{\bar{\sigma}}{(1-\phi)(\kappa+Y)} - 1]\}^n$$

evolution of isotropic hardening

$$\dot{\kappa} = [H - R_d\kappa]\dot{\epsilon_p}$$

*Large values of f make the formulation rate independent. I did not need to fit f.

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Brief Group Discussion: Calibration Practice

5-10 min discussion

- **In what settings do you have desired model responses or data?**
- **How do you measure differences between target and model response?**
- **How do you go about identifying parameter values that maximize agreement?**
- **What makes your problems challenging?**

Recall the Optimization Problem

Minimize:	$f(x_1,\ldots,x_N)$	***Objective function(s)***
Subject to:	$g_{LB} \le g(x) \le g_{UB}$	***Nonlinear inequality constraints***
	$h(x) = h_E$	***Nonlinear equality constraints***
	$A_I x \le b_I$	***Linear inequality constraints***
	$A_E x = b_E$	***Linear equality constraints***
	$x_{LB} \le x \le x_{UB}$	***Bound constraints***

Calibration: Optimization Problem with Special Structure and Goals

Simulation-generated response

Target response

Minimize: $f(x_1,\ldots,x_N) = \boxed{\sum_{i=1}^{m} [s_i(x_1,\ldots,x_N) - d_i]^2}$ *Objective function(s)*

Subject to: $g_{LB} \leq g(x) \leq g_{UB}$ *Nonlinear inequality constraints*

$h(x) = h_E$ *Nonlinear equality constraints*

$A_I x \leq b_I$ *Linear inequality constraints*

$A_E x = b_E$ *Linear equality constraints*

$x_{LB} \leq x \leq x_{UB}$ *Bound constraints*

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DAKOTA Calibration Interface Accommodates Special Structure

Responses Option1: Compute list of these differences (residuals) and return it to DAKOTA. It will square and sum them.

OR

$$\sum_{i=1}^{m} [s_i(x_1,\ldots,x_N) - d_i]^2$$

Responses Option 2: Compute list of simulation responses and…

AND

…tell DAKOTA where to find a data file with a list of the target responses. It will put the pieces together.

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Local Least-squares Methods Take Advantage of Special Structure

Alternate objective formulation: $f(x) = \frac{1}{2} r(x)^T r(x) = \frac{1}{2}[s(x) - d]^T [s(x) - d]$

Derivative formulations:

$$\nabla f(x) = J(x)^T r(x); \quad J_{ij} = \frac{\partial r_i}{\partial x_j} \qquad \nabla^2 f(x) = J^T J + \sum_{i=1}^{n} r_i(x) \nabla^2 r_i(x)$$

Methods vary in second derivative approximation:

Gauss-Newton: $J(x)^T J(x)$

Levenberg-Marquardt: $J(x)^T J(x) + \mu I$, with $\mu \geq 0$

$NL2SOL : J(x)^T J(x) + S,$

with $S = 0$ or $S =$ Quasi-Newton approximation to $\sum_{i=1}^{n} f_i(x) \nabla^2 f_i(x)$

Exercise: Calibrate Cantilever to Experimental Data

- **Calibrate design variables *E, w, t* to data from all 3 responses**
- ***X, Y, R* fixed (state) at nominal values**
- **Use NL2SOL or OPT++ Gauss-Newton**
- **Key DAKOTA specs:**
  - **num_least_squares_terms = 3**
  - **no constraints**
  - **least_squares_datafile**
- **Possible template: Calib. Local Data File**

DATA	clean	with error
area	7.5	7.772
stress	2667	2658
displacement	0.309	0.320

```
cantilever_clean.dat
cantilever_witherror.dat
```

- ***For least-squares methods, application normally must return residuals $r_i(x) = s_i(x) - d_i$ to DAKOTA***
- ***Here we return the usual area, stress, displacement and specify a datafile and DAKOTA computes the residuals***

Potential Solution: Cantilever Least-Squares

```
# Calibrate to area, stress, and displacement data generated with
# E = 2.85e7, w = 2.5, t = 3.0

method
  nl2sol
    convergence_tolerance = 1.0e-6

variables
  continuous_design = 3
    upper_bounds  3.1e7 10.0 10.0
    initial_point 2.9e7 4.0  4.0
    lower_bounds  2.7e7 1.0  1.0
    descriptors   'E' 'beam_width' 'beam_thickness'
  # Fix at nominal
  continuous_state = 3
    initial_state 40000 500 1000
    descriptors 'R' 'X' 'Y'

interface
  direct
    analysis_driver = 'mod_cantilever'

responses
  calibration_terms = 3
#    calibration_data_file = 'cantilever_clean.dat'
    calibration_data_file = 'cantilever_witherror.dat'
    descriptors = 'area' 'stress' 'displacement'
  analytic_gradients
  no_hessians
```

```
CIs without error:
E: [ 2.850e+07, 2.850e+07 ]
w: [ 2.500e+00, 2.500e+00 ]
t: [ 3.000e+00, 3.000e+00 ]
```

```
CIs with error:
E: [ 1.992e+07, 4.190e+07 ]
w: [ 1.962e+00, 3.918e+00 ]
t: [ 1.954e+00, 3.309e+00 ]
```

Brief Group Discussion: Cantilever Problem and Solution

5-10 min discussion

- **How do the calibrated parameter values differ with clean vs. noisy data?**
- **How do the confidence intervals differ?**
- **What would you do if you wanted to calibrate against multiple sets of data?**
- **What would you do if agreement was more important in some regions than others?**
- **Do you expect that desired target responses always give rise to unique matching parameters?**

Quick Guide for Calibration Method Selection

Category	DAKOTA method names	Continuous Variables	Categorical/ Discrete Variables	Bound Constraints	General Constraints
Gradient-Based Local (Smooth Response)	`nl2sol`	x		x	
	`nlssol_sqp, optpp_g_newton`	x		x	x
Gradient-Based Global (Smooth Response)	`hybrid strategy, multi_start strategy`	x		x	x
Derivative-Free Local (Nonsmooth Response)					
Derivative-Free Global (Nonsmooth Response)	`efficient_global, surrogate_based_global`	x		x	x

See Usage Guidelines in DAKOTA User's Manual. Also, can apply any optimizer when doing derivative-free local or global calibration.

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Calibration References

- G. A. F. Seber and C. J. Wilde, "Nonlinear Regression", John Wiley and Sons, Inc., Hoboken, New Jersey, 2003.

- M. C. Hill and C. R. Tiedeman, "Effective Groundwater Model Calibration: With Analysis of Data, Sensitivities, Predictions, and Uncertainty", John Wiley and Sons, Inc., Hoboken, New Jersey, 2007.

- R. C. Aster, B. Borchers, and C. H. Thurber, "Parameter Estimation and Inverse Problems", Elsevier, Inc., Oxford, UK, 2005.

- DAKOTA User's Manual
  - Nonlinear Least Squares Capabilities
  - Surrogate-Based Minimization
- DAKOTA Reference Manual

Learning Goals Revisited: Did we meet them?

- **Define a calibration/parameter estimation problem**
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