SAND2015-6868 TR

Center for Computing Research

Dakota Software Training

Characterizing Your Model: Performing Initial Dakota Studies

http://dakota.sandia.gov

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Module Learning Goals

- See how Dakota can automate what you are already doing
- Know what model characteristics will affect how you use Dakota
- Be able to run a basic study to characterize a model

Module Outline

- Introduce cantilever beam example

- Explore the cantilever beam model
  - What does it mean to explore a model?
  - How would you do it now? (discussion and example)
  - How can it be done with Dakota? (including exercise)

- Model characteristics relevant for Dakota use
  - Definitions and illustrations
  - Exercises: Use Dakota to identify characteristics of multiple example problems

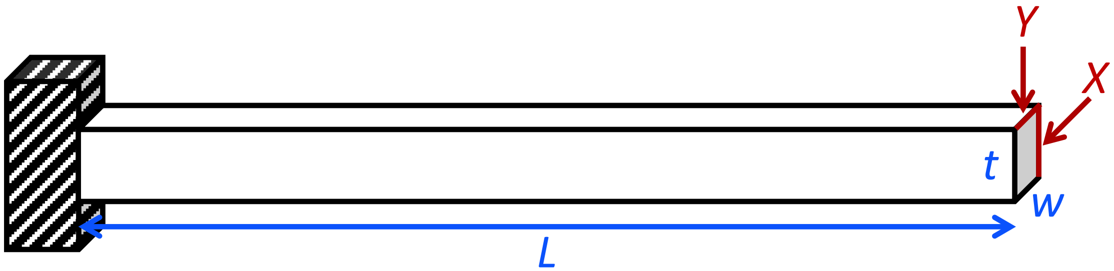
Model Characterization

THE CANTILEVER BEAM MODEL

Your first week on the job…

- **Scenario:** Your company believes the latest version (12.1.4) of *Cantilever Physics*, an advanced cantilever beam simulation tool developed by Sandia National Laboratories, may be useful in performing mission-relevant simulation based analyses. You are asked to evaluate the tool, so you download the software and put together a simple cantilever beam model that is representative of many of your problems.

Cantilever Physics



Parameters:

L: length (in)

w: width (in)

t: thickness (in.)

ρ: density (lb/ft^3)

E: Young's modulus (lb/in^2)

X: horizontal load (lb)

Y: vertical load (lb)

Responses:

M: mass (lb)

S: stress (lb/in^2)

D: displacement (in)

$$M = \rho * wt * \frac{L}{12^3}$$

$$S = \frac{600}{wt^2} Y + \frac{600}{w^2 t} X$$

$$D = \frac{4L^3}{Ewt} \sqrt{\left(\frac{Y}{t^2}\right)^2 + \left(\frac{X}{w^2}\right)^2}$$

Cantilever Physics

SNL's *Cantilever Physics* simulator has several characteristics typical of engineering and science codes:

- Text-based input file/deck and text-based output
- Each run of *Cantilever Physics* simulator "maps" one set of inputs to one set of outputs
- Command-line driven

```
cantilever cantilever.i
```

- *Demo materials are in ~/exercises/characterization/1*

Model Characterization

EXPLORE THE MODEL

Characterizing model behavior enables model and software assessment

- Is the model behaving as you would expect based on your physics knowledge?
- Is the model/software robust across the range of model parameters you might expect to see?
- What tools or methods would you be able to use to perform more sophisticated design/reliability/safety analyses? (I.e., what methods in Dakota would be applicable?)
- Discussion: What are other motivations for model characterization?

How would you go about exploring *Cantilever Physics*?

- Basic Idea: Vary model inputs (parameters/variables) and observe how model outputs (responses/quantities of interest) are affected
- Discussion: What are some approaches to varying model parameters you might use?

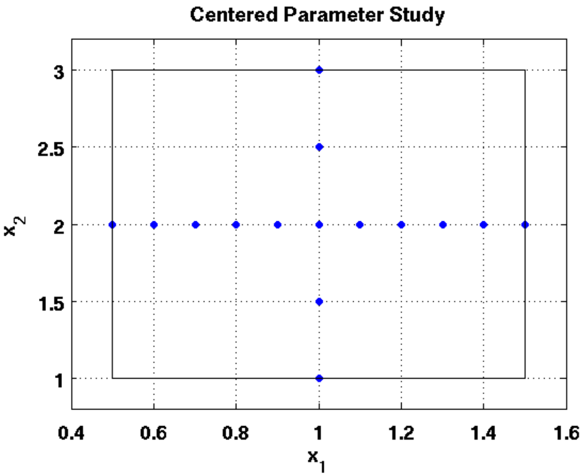
Demo: Exploring *Cantilever Physics*

- See how responses vary as we change parameter values
- *Demo (Exercise 1) materials are in* *~/exercises/characterization/1*

- Discussion: What are some shortcomings of this approach?

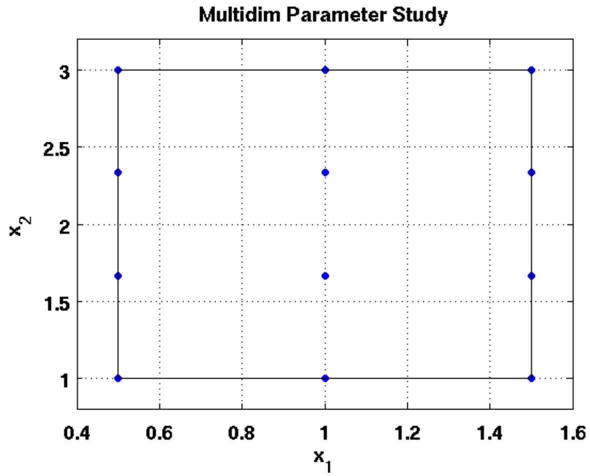
Model exploration using Dakota

Centered Parameter Study



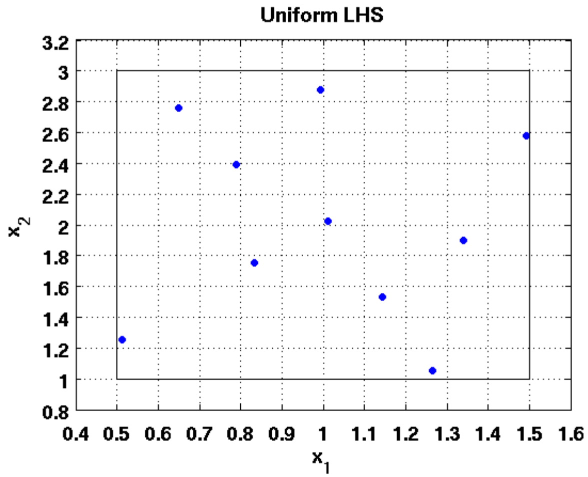
- Vary parameters along coordinate axes
- Least computationally expensive
- Only get univariate effects

Multi-Dimensional (Grid) Parameter Study



- Vary parameters according to a grid pattern
- High computational cost
- Multi-purpose use (e.g., multivariate effects, sensitivities, surrogates)

Latin Hypercube Sampling (LHS)



- Vary parameters according to a space filling statistical design
- Low cost for univariate effects; moderate to high for multivariate
- Multi-purpose use

Exercise 2: Explore the cantilever model using Dakota

- Exercise materials are in `~/exercises/characterization/2`
- Along with the cantilever files, you will find three Dakota input files
  - `dakota_cantilever_centered.in` – Centered parameter study
  - `dakota_cantilever_grid.in` – Grid parameter study *(long run time)*
  - `dakota_cantilever_lhs.in` – Latin hypercube sampling
- Run the Dakota studies

```
dakota -i <dakota_input_file> -o <dakota_output_file>
```

  - A .dat file will be produced for each
- Plot the results
  - Use `plot_dakota_centered` for the centered parameter study and `plot_dakota_scatter` for the grid and LHS studies

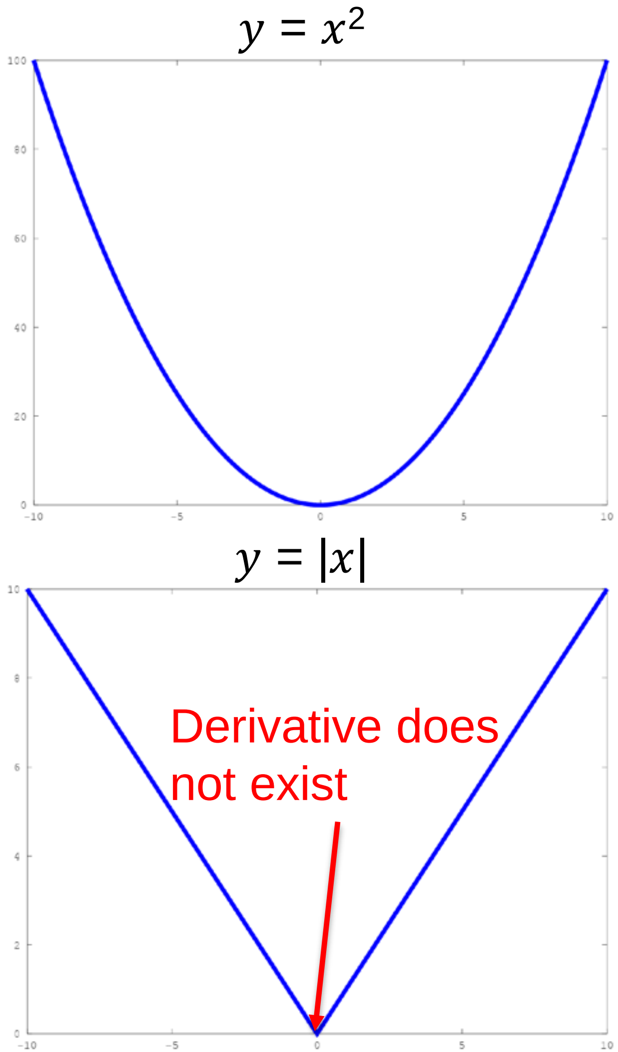
```
plot_dakota_scatter cantilever_grid_tabular.dat L,p,E mass,stress,displacement
```

- Let's take a quick look at the Dakota output…

Model Characterization

RELEVANT MODEL CHARACTERISTICS

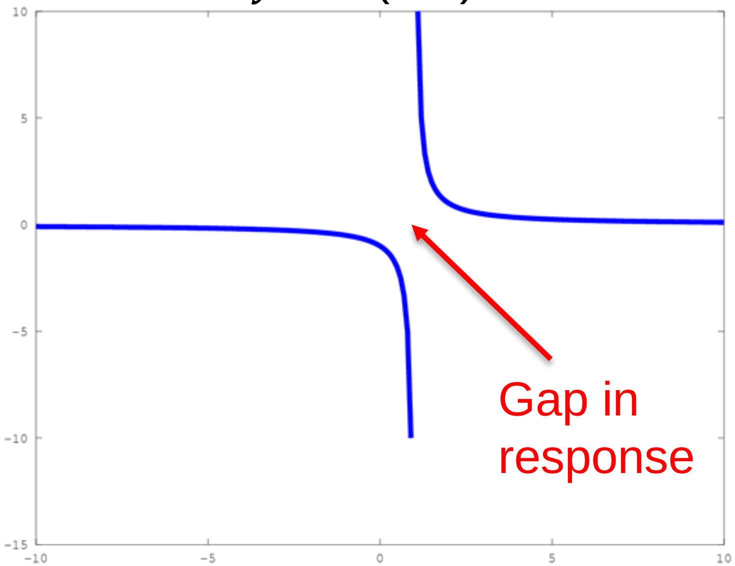
Model characteristics relevant for Dakota use (1)



- **Smooth**: derivatives exist and are continuous everywhere
- **Non-smooth**: has "kinks" in it

Model characteristics relevant for Dakota use (2)

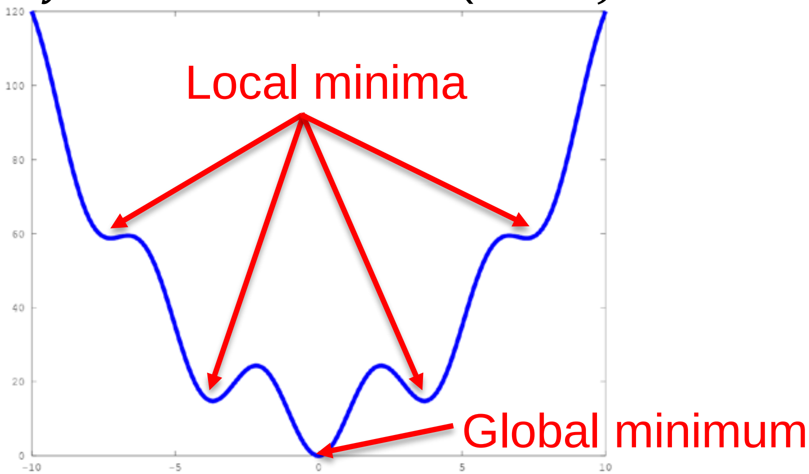
$y = 1/(x-1)$



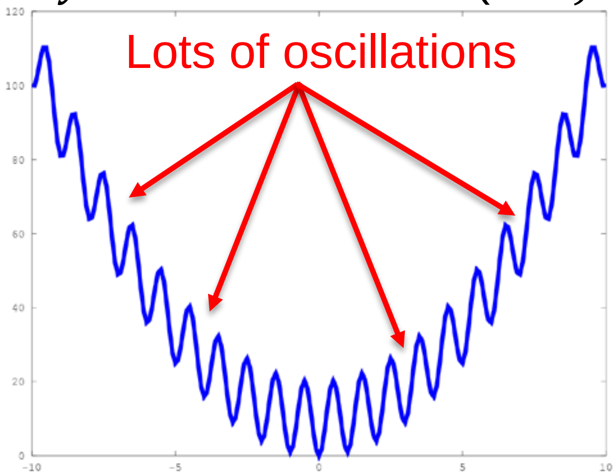
- Discontinuous: cannot be drawn without lifting your pencil
  - i.e., has “gaps” in the response
- Note that robustness of simulation can be a factor here
  - i.e., crashes or fails for particular parameter value combinations

Model characteristics relevant for Dakota use (3)

$y = 10 + x^2 - 10\cos(0.5\pi x)$



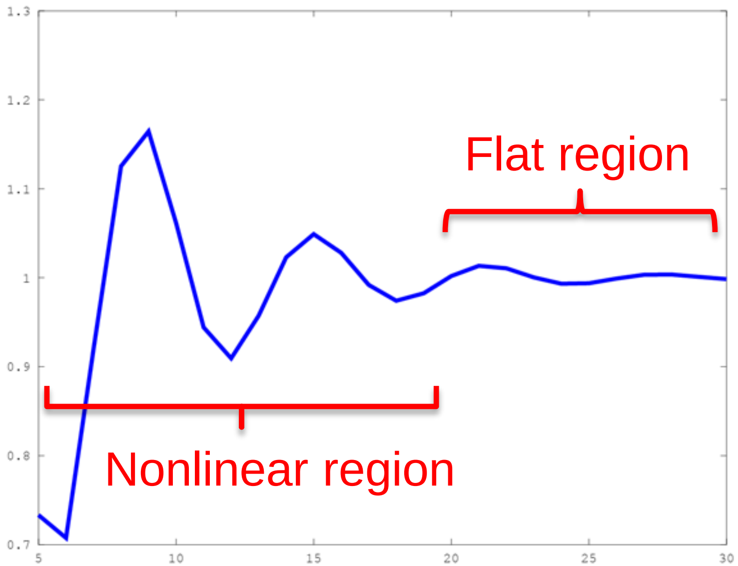
$y = 10 + x^2 - 10\cos(2\pi x)$



- Multi-modal: having multiple local minima
- Noisy: multi-modal "on steroids"
  - Often has some underlying trend

Model characteristics relevant for Dakota use (4)

$$y = 1 + \sin(x - \pi/3) * e^{-0.2x}$$



- Range with multiple "regimes": response behavior is notably different over different intervals of parameters

Exercise 3: Explore additional examples and identify characteristics

- Discussion: But first, what relevant characteristics just discussed did the cantilever model exhibit?
- Exercise materials are in `~/exercises/characterization/3`
- For any or all of the following, run Dakota and plotting tools
  - `dakota_herbie_grid.in, dakota_quasi-sine_centered.in, dakota_shubert_centered.in, dakota_genz_grid.in`
  - Note: use `plot_dakota_centered` for the centered studies and `plot_dakota_scatter` for the grid studies
    - For herbie, quasi-sine, and genz: parameters are x1, x2.
    - For shubert: parameters are x1, x2, x3, x4.
    - For all: response is f1.
- Discussion: Which examples exhibit which characteristics? Are there any for which it is not entirely clear?