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Dakota Software Training

Characterizing Your Model: Performing
Initial Dakota Studies

<http://dakota.sandia.gov>



Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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

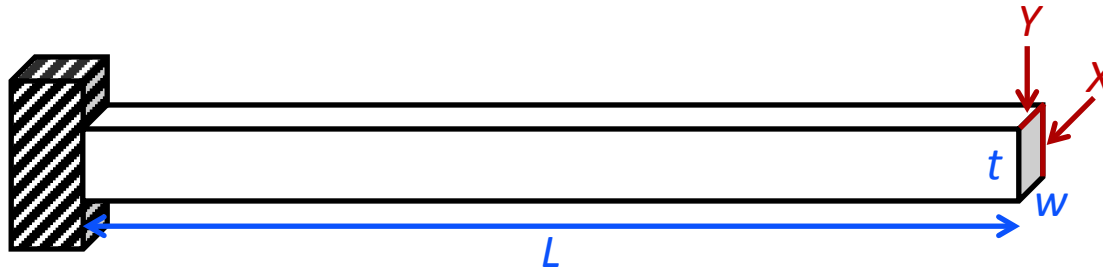
THE CANTILEVER BEAM MODEL

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/ft³)

E : Young's modulus (lb/in²)

X : horizontal load (lb)

Y : vertical load (lb)

Responses:

M : mass (lb)

S : stress (lb/in²)

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*



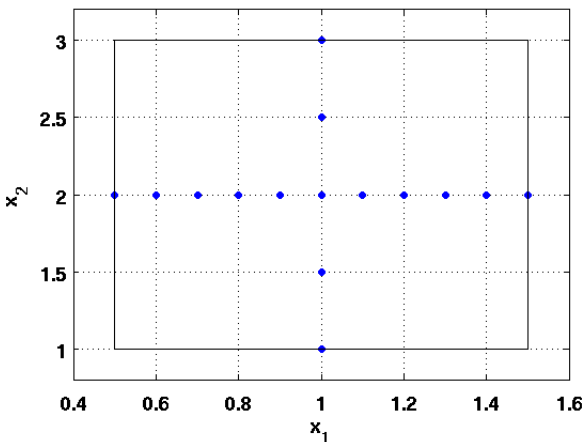
- See how responses vary as we change parameter values
- *Demo (Exercise 1) materials are in
~/exercises/characterization/1*
- Discussion: What are some shortcomings of this approach?

Model exploration using Dakota



Centered Parameter Study

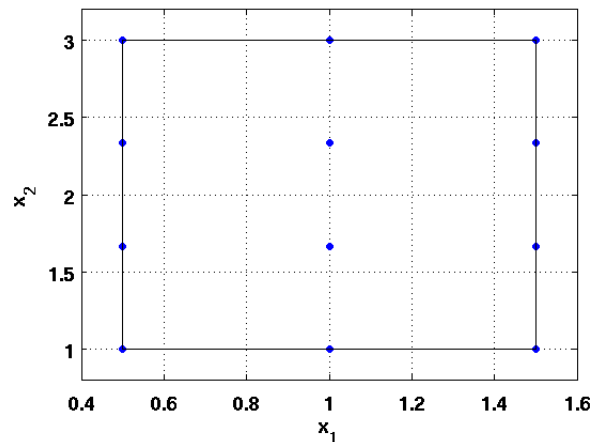
Centered Parameter Study



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

Multi-Dimensional (Grid) Parameter Study

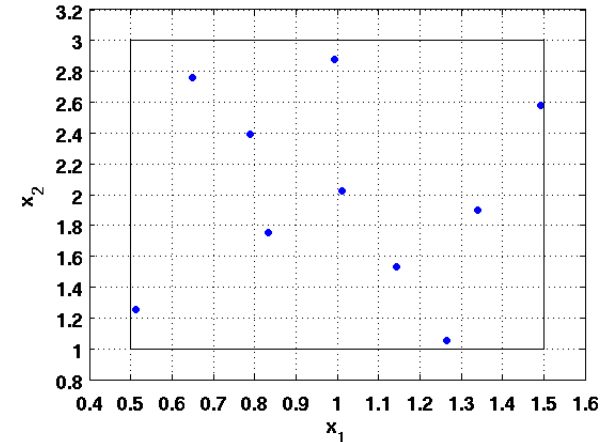
Multidim Parameter Study



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

Latin Hypercube Sampling (LHS)

Uniform 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
```

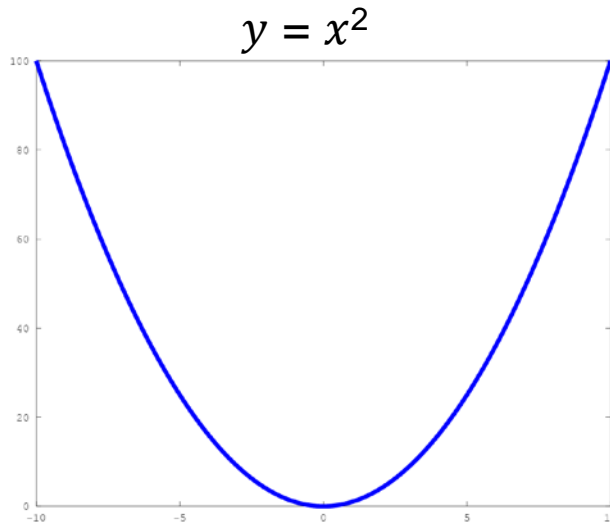
- Let's take a quick look at the Dakota output...



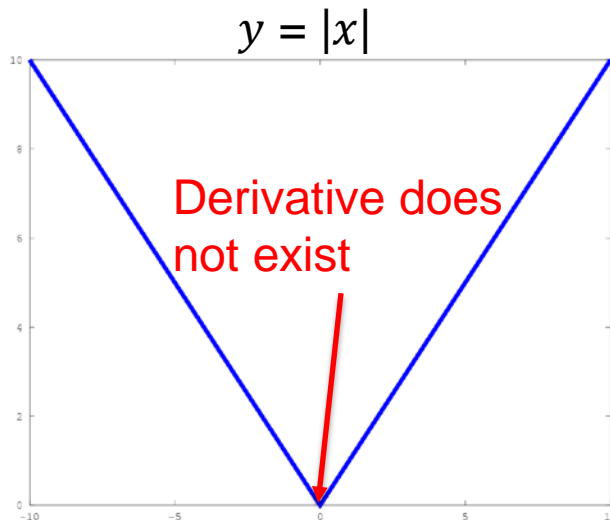
Model Characterization

RELEVANT MODEL CHARACTERISTICS

Model characteristics relevant for Dakota use (1)

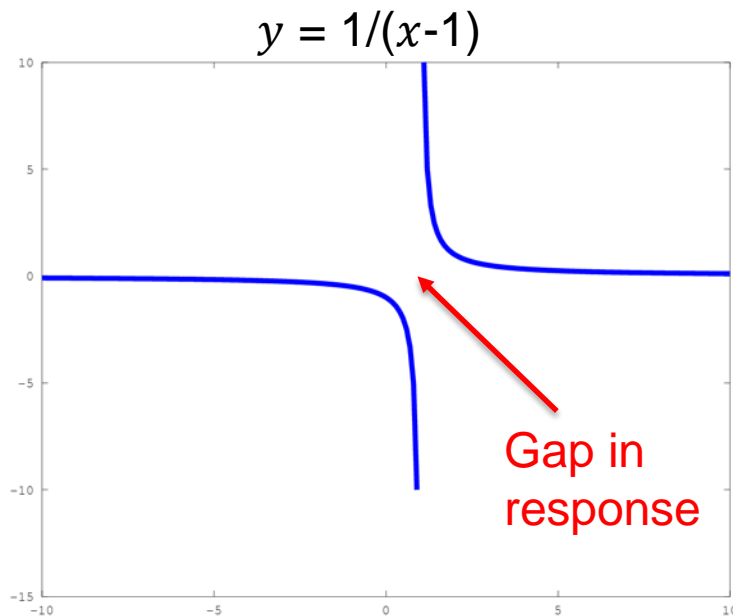


- **Smooth**: derivatives exist and are continuous everywhere



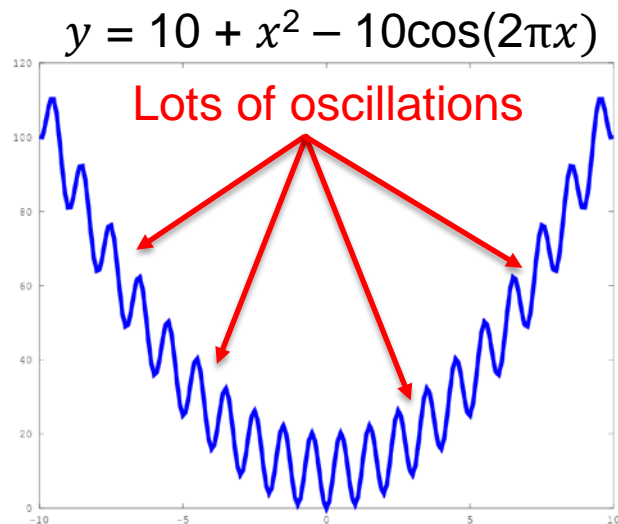
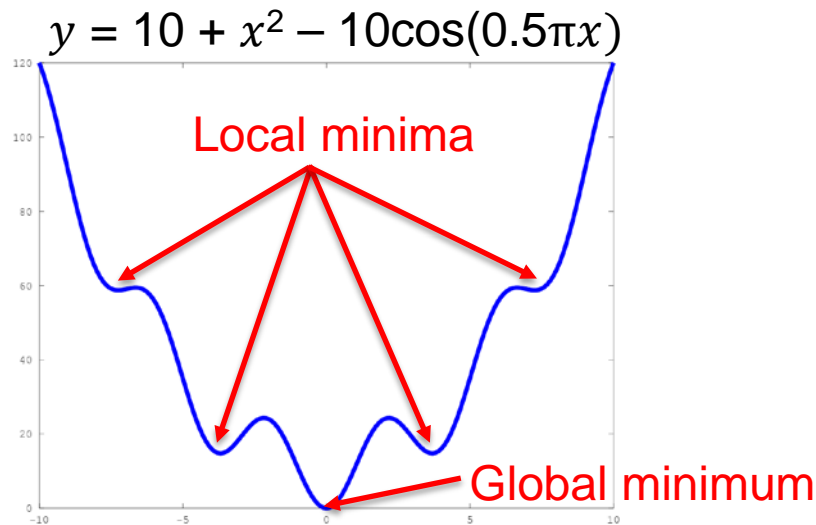
- **Non-smooth**: has “kinks” in it

Model characteristics relevant for Dakota use (2)



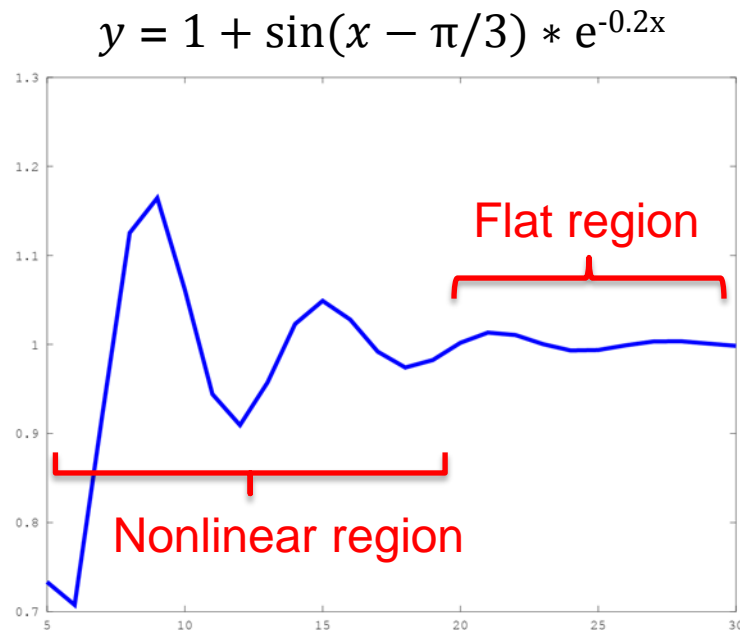
- **Discontinuous**: cannot be drawn without lifting your pencil
 - i.e., has “gaps” in the response
- Note that robustness of simulation can be a factor here
 - i.e., crashes or fails for particular parameter value combinations

Model characteristics relevant for Dakota use (3)



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

Model characteristics relevant for Dakota use (4)



- 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?