



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? (including exercise)
 - 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

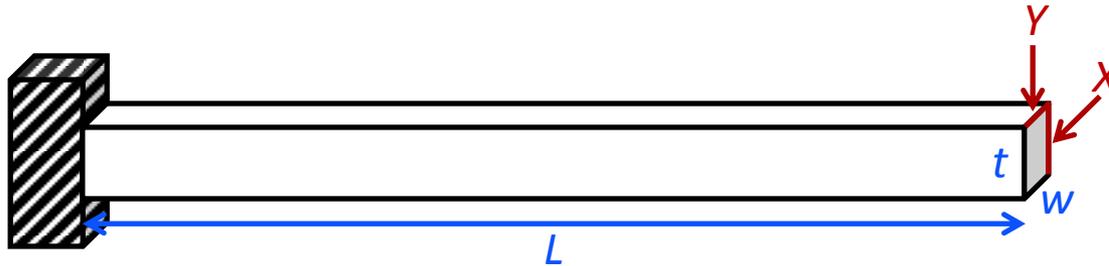
THE CANTILEVER BEAM MODEL

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 Beam Model



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)

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

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

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



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?

Given the cantilever model, how would you go about exploring it?



- 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?

Exercise 1: Explore cantilever model using approaches just identified



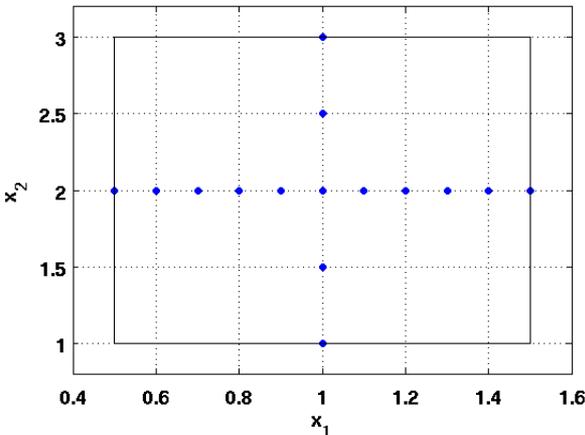
- Exercise materials are in `~/exercises/characterization/1`
- Try running the Cantilever Physics executable, `cantilever`, using the input file named `cantilever.i`:
 - `./cantilever cantilever.i`
- Now change values of L , ρ , and E in `cantilever.i` according to the just articulated approaches and rerun for each
 - Use a spreadsheet to make your favorite plots of the responses (*mass*, *stress*, *displacement*) with respect to those parameters
- Discussion: What do you observe about the behavior of the responses? E.g.,
 - Are the responses linear/nonlinear, monotonic/non-monotonic, increasing/decreasing with respect to parameters?
 - Do the responses change gradually or abruptly across the parameter ranges?

Model exploration using Dakota



Centered Parameter Study

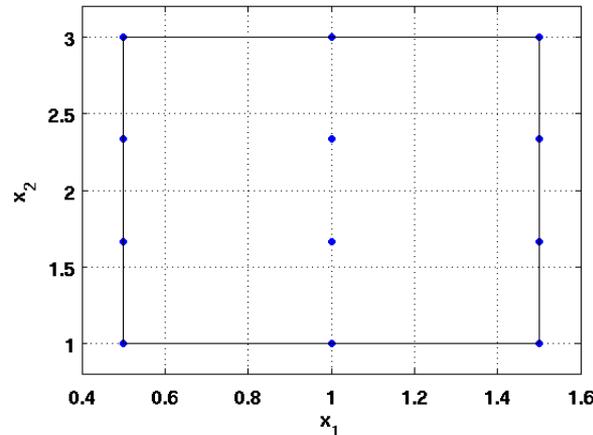
Centered Parameter Study



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

Multi-Dimensional (Grid) Parameter Study

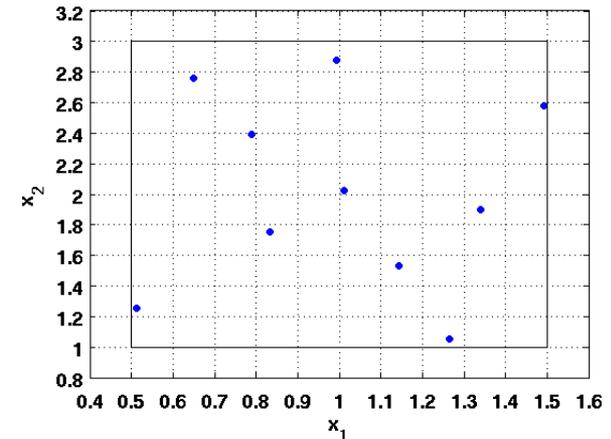
Multidim Parameter Study



- 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



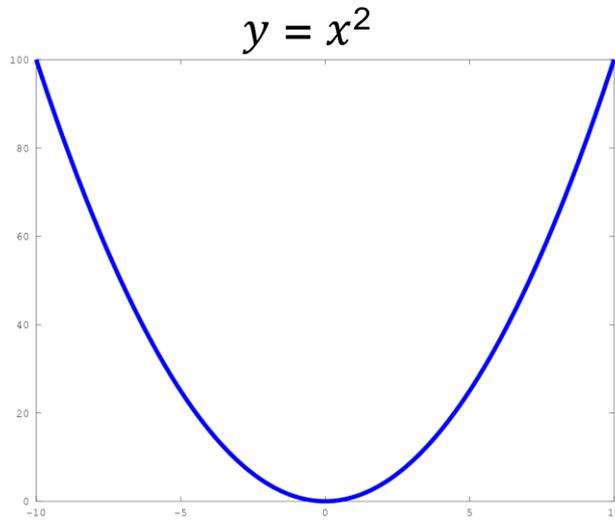
- Exercise materials are in ~/exercises/characterization/2
- Along with the cantilever files, you will find some Dakota input files
 - dakota_cantilever_centered.in, dakota_cantilever_grid.in, dakota_cantilever_lhs.in
- Run the Dakota studies and plot the results
 - dakota -i <dakota_input_file> -o <dakota_output_file>
 - plot_dakota_centered cantilever_centered_tabular.dat L,p,E mass,stress,displacement
 - plot_dakota_scatter cantilever_grid(lhs)_tabular.dat L,p,E mass,stress,displacement
- Discussion
 - Are your observations any different than those you ran by hand?
 - How did the amount of time and effort to generate and look at results compare to when you did it by hand?
- Let's take a quick look at the Dakota output...



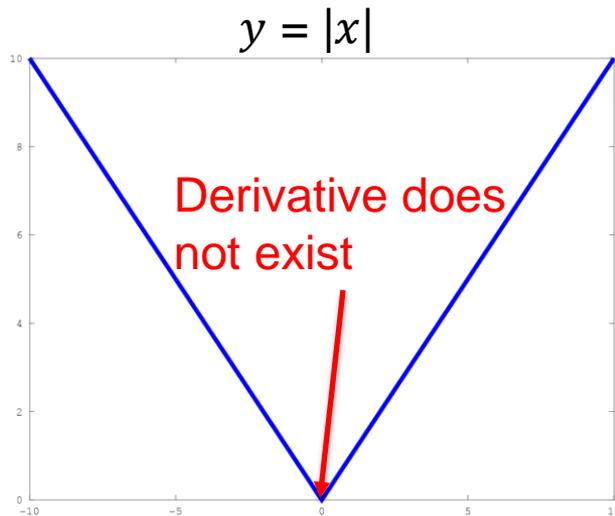
Model Characterization

RELEVANT MODEL CHARACTERISTICS

Model characteristics relevant for Dakota use (1)

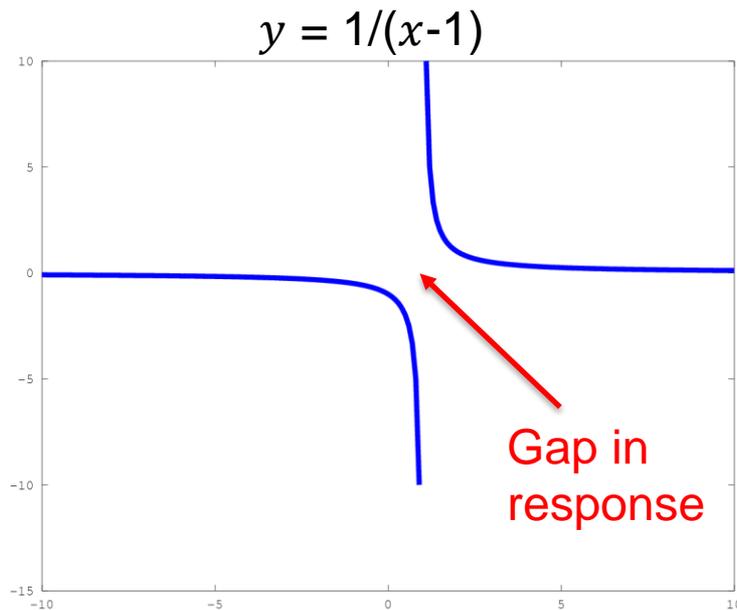


- **Smooth**: derivatives exist and are continuous everywhere



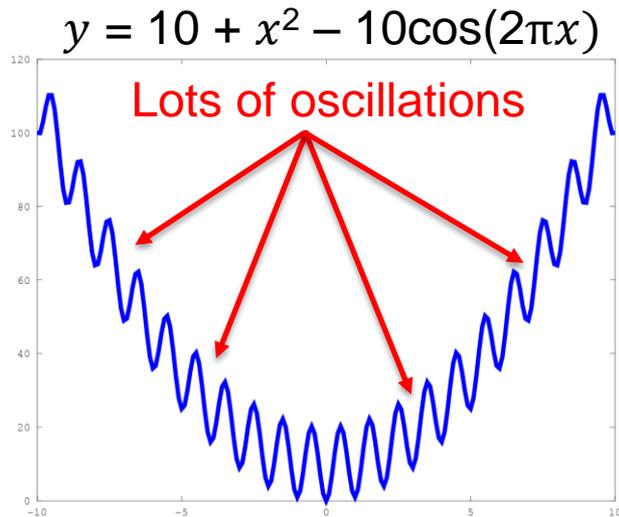
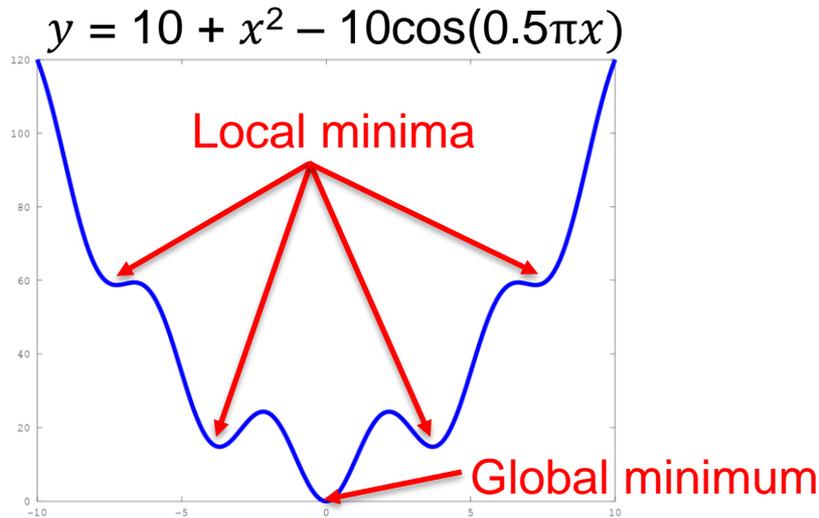
- **Non-smooth**: has “kinks” in it

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)

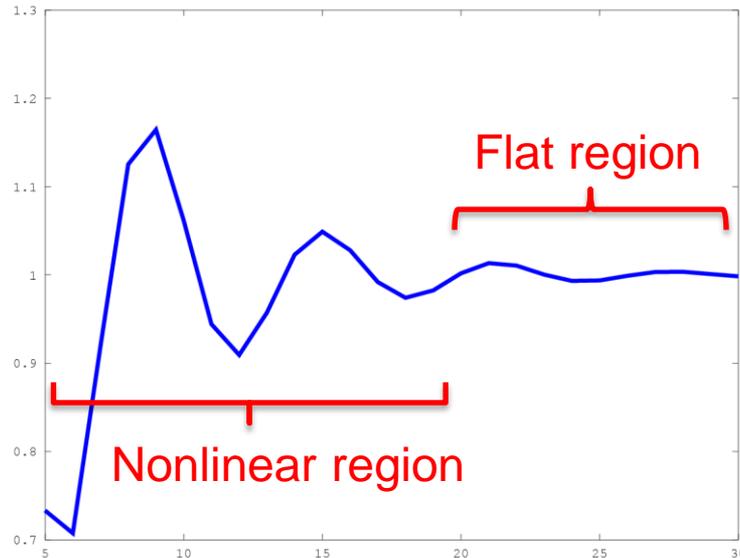


- **Multi-modal:** having multiple local minima
- **Noisy:** multi-modal “on steroids”
 - Often has some underlying trend

Model characteristics relevant for Dakota use (4)



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



- 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: `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?