SAND2016-XXXXYY

SAND2016-3330PE

Dakota Software Training

Sensitivity Analysis

http://dakota.sandia.gov

Sandia National Laboratories

Exceptional service in the national interest

U.S. DEPARTMENT OF ENERGY

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

- Understand goals and benefits of sensitivity analysis (SA)
- Have a practical process for SA at your disposal
- Be able to formulate your problem, present it to Dakota, and run and understand studies
- Be familiar with key Dakota SA methods
- Know how to use Dakota sensitivity analysis results

Module Outline

- Introduction and motivating application examples
- Sensitivity analysis process, terminology, and Dakota input details

- Centered parameter studies (now for sensitivity analysis)
- Monte Carlo sampling
- Exercise: Determine influential parameters for cantilever

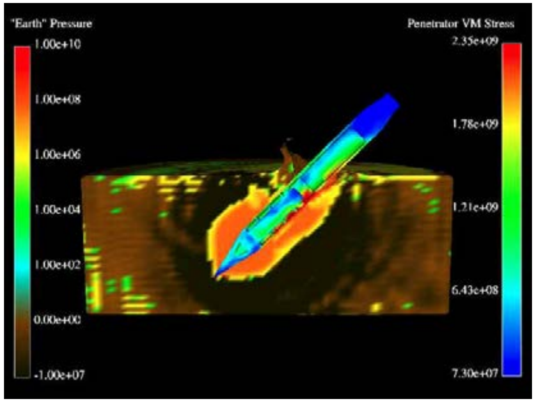
- Other key SA methods: Morris one-at-a-time (MOAT) and variance-based decomposition (VBD)
- Exercise: Explore sensitivity analysis methods

- Beyond Dakota: using SA results, getting more information

Why Sensitivity Analysis?

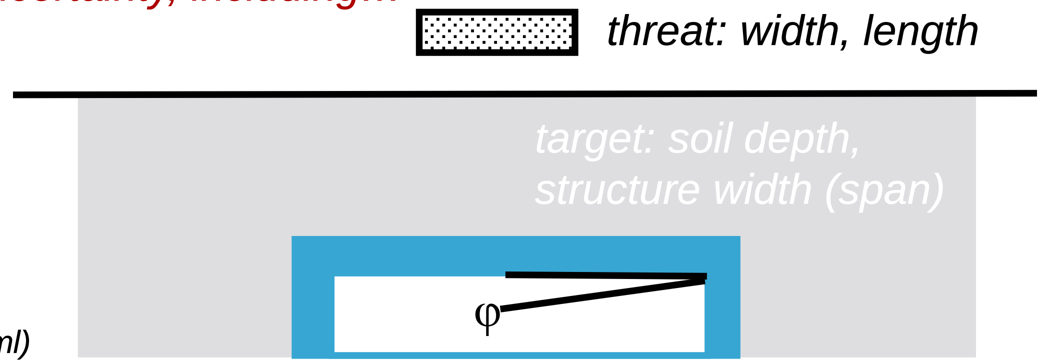
- What? Reveal the extent to which simulation outputs depend on each simulation input
- Why? Identify most important input variables and their interactions
  - Primarily for screening/ranking: Identify the most important variables; down-select for further UQ or optimization analysis
  - Provide a focus for resources
    - Data gathering and model development
    - Code development
    - Uncertainty characterization
  - Identify key model characteristics: smoothness, nonlinear trends, robustness; develop intuition about model
- Related
  - Can have the side effect of identifying code and model issues
  - Generated simulation data can be used to construct surrogate models

Sensitivity Analysis Example: Earth Penetrator

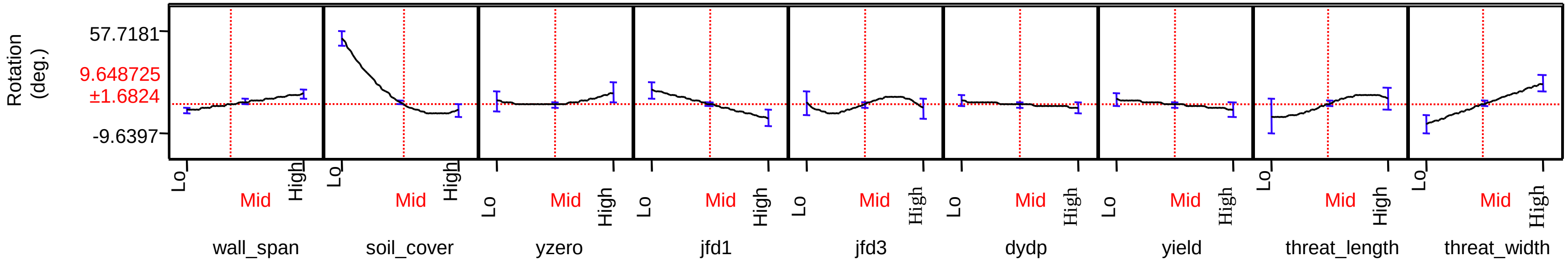


Notional model for illustration purposes only (http://www.sandia.gov/ASC/library/fullsize/penetrator.html)

12 parameters describing target & threat uncertainty, including…



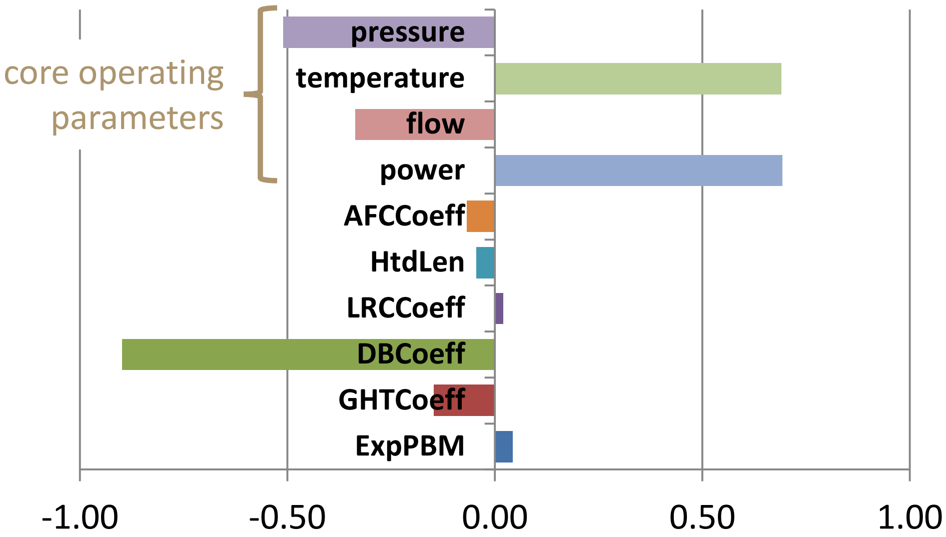
- Underground target with external threat: assess sensitivity in target response to target construction and threat characteristics
- Response: angular rotation (ϕ) of target roof at mid-span
- Analysis: CTH Eulerian shock physics code; JMP stats
- Revealed most sensitive input parameters and nonlinear relationships

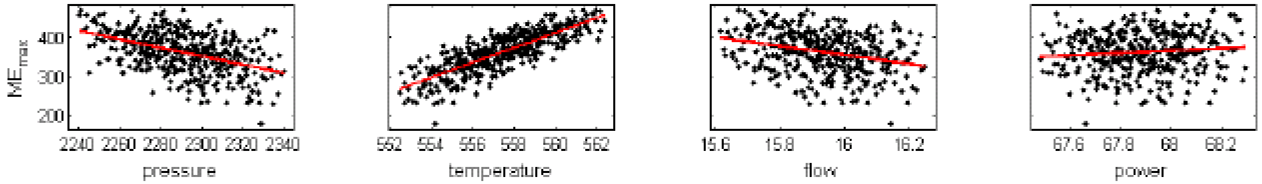


Sensitivity Analysis Example: Nuclear Reactor Thermal-Hydraulics Model

- Assess parameter influence on boiling rate, a key crud predictor
- Dakota correlation coefficients: strong influence of core operating parameters (pressure more important than previously thought)
- Dittus-Bolter correlation model may dominate model form sensitivities (also nonlinear effects of ExpPBM)
- Scatter plots help visualize trend in input/output relationships

parameter influence on number of boiling sites





sensitivity of mass evaporation rate (max) to operating parameters

Discussion:
Your Sensitivity Analysis Practice

- What kinds of parameters are important in your science and engineering computational models?
- What SA questions do (might) you ask with these models?
- How do (might) you answer them?
- What measures of sensitivity, ranking, or importance are you familiar with?
- What challenges do you face?

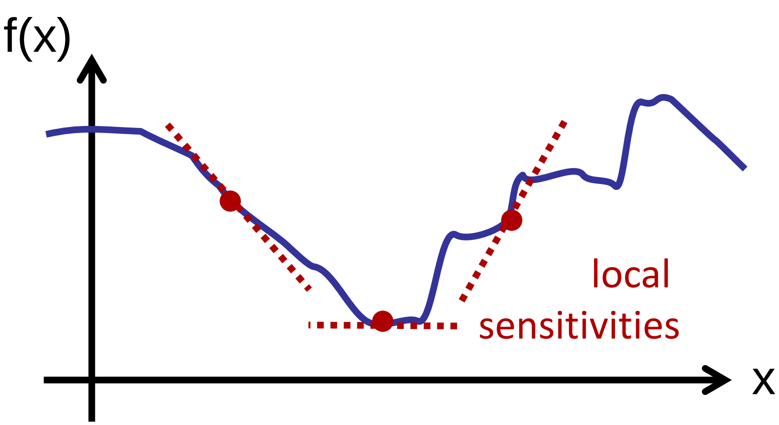
A Practical Process for SA

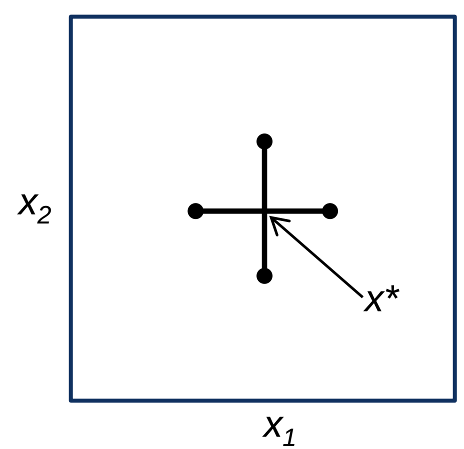
1. What are the key model responses (quantities of interest)?
   What are your follow-on (post-SA) analysis goals?
2. Identify potentially important input parameters
   - Often expert opinion-based with phenomena identification and ranking table (PIRT)
   - Include parameters that likely influence response or might be involved in other studies
3. Pose plausible parameter bounds or steps
4. Set up Dakota input file with variables and interface to simulation
5. Perform an initial centered parameter study
6. Perform additional SA studies based on simulation cost and any known model character
7. Post-process Dakota-generated data with third-party tools

Up next: Some sensitivity analysis terminology

Key Sensitivity Analysis Concepts: Local Sensitivity

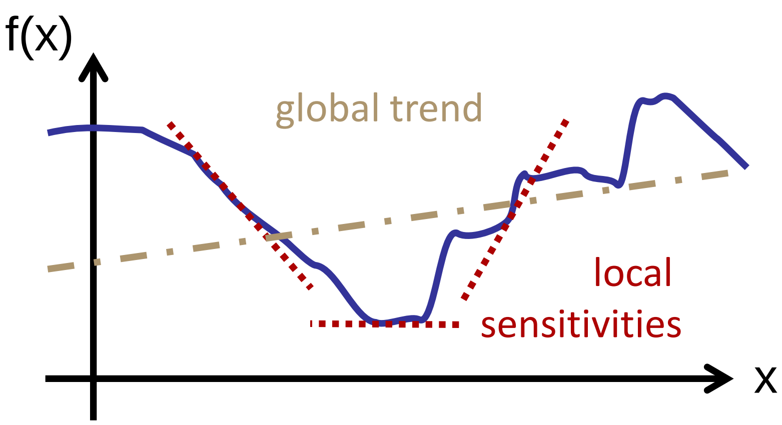
- Local sensitivity measures the relative influence of parameters at a particular point in the input space
- Partial derivatives (slopes) w.r.t. each variable: $\frac{\partial f}{\partial x_1}(x^*),\ \frac{\partial f}{\partial x_2}(x^*)$
- Can be estimated with finite differences (small perturbations); with Dakota: centered parameter study or numerical gradients
- Some simulation codes can compute these directly, e.g., via adjoints

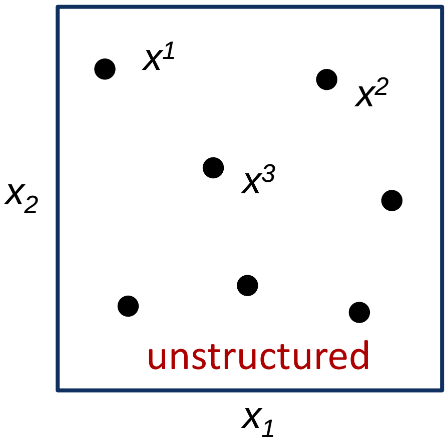


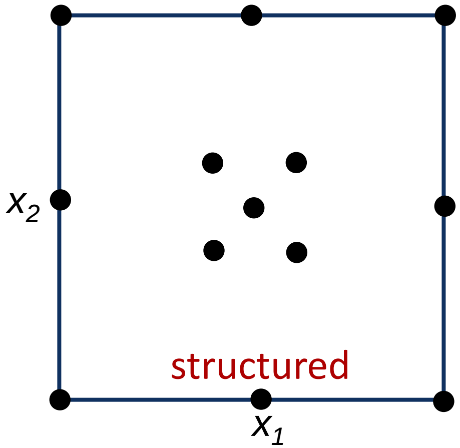


Key Sensitivity Analysis Concepts: Global Sensitivity

- Global sensitivity assesses the relative influence of parameters over the entire input space (typically a hyper-rectangle)
- What is the general trend of the response over all values of x? Does the response depend more nonlinearly on one factor than another?
- How? Evaluate the response at well-distributed points x^j in the input space (a design of computer experiments) and analyze the resulting input/output pairs $\{x^j, f(x^j)\}$
- Dakota (and this training) primarily focus on global SA







Key Sensitivity Analysis Concepts: Measures of Sensitivity

- Correlation coefficient (Pearson) ρ: strength and direction of the linear relationship between two variables (input to output); $\rho \in [-1,1]$
  - Also partial correlation (controls for other variables)
  - Spearman rank correlation: helpful for variables or responses varying over orders
- Main effect: effect of a single variable, averaging over the effects of the other variables
- Sobol indices: measure of output variance attributable to each input variable: first-order/main effect and total effect
- Morris metrics: statistics on elementary effects measure variability of response at various points in input space: main and nonlinear/interaction measures
- Scatter plots: helpful visual diagnostic for trend analysis

A Practical Process for SA

1. What are the key model responses (quantities of interest)?
   What are your follow-on (post-SA) analysis goals?
2. Identify potentially important input parameters
   - Often expert opinion-based with phenomena identification and ranking table (PIRT)
   - Include parameters that likely influence response or might be involved in other studies
3. Pose plausible parameter bounds or steps
4. Set up Dakota input file with variables and interface to simulation
5. Perform an initial centered parameter study
6. Perform additional SA studies based on simulation cost and any known model character
7. Post-process Dakota-generated data with third-party tools

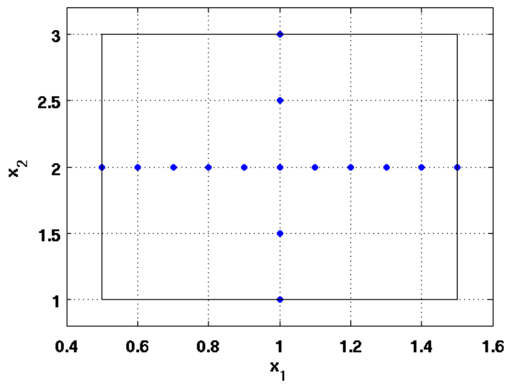
Up next: Discuss 3, 4, and 5

First, how might we pose bounds or increments for non-physical parameters?

Specifying Dakota Variable Ranges for a Sensitivity Study

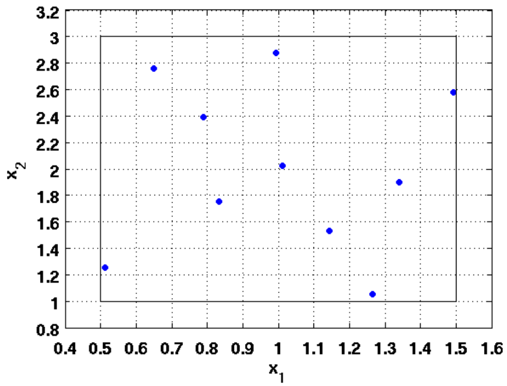
Local or univariate global sensitivity: initial point and steps to take

```
variables
  continuous_design  2
    descriptors      'power'  'expPBM'
    initial_point    1.0      2.0

method centered_parameter_study
  steps_per_variable 5     2
  step_vector        0.1   0.5
```



Global sensitivity: hyper-rectangle bounds

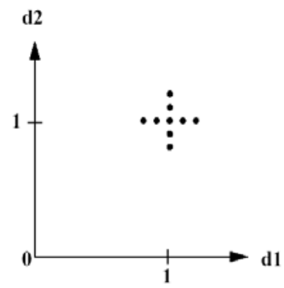
```
variables
  continuous_design  2
    descriptors      'flow'  'power'
    upper_bounds     1.5     3.0
    lower_bounds     0.5     1.0

method sampling
  ...
```



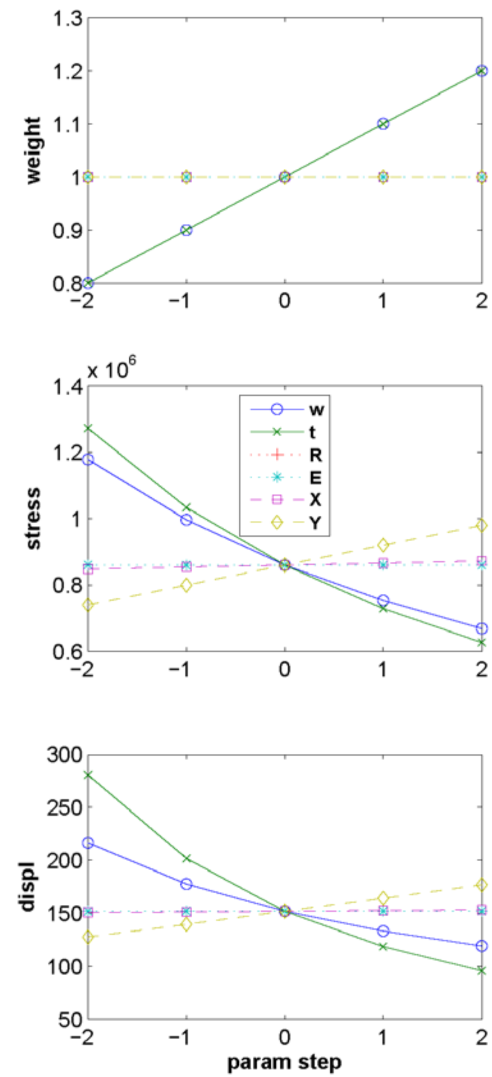
Dakota variable type is not critical. Typically use continuous or discrete design, or uniform or discrete (interval, set) uncertain.

Centered Parameter Study for Univariate Sensitivity

- Exercise 1: Run a centered parameter study similar to that in the Model Characterization module (see **`exercises/sens_analysis/1`**)
- Requires $2 \times d \times steps + 1$ runs
- Similar to perturbation studies you probably already do when learning about a model: *change parameters ±5%, ±10%, etc.*



- How do we interpret this study for SA purposes?
  - Overall range of variability
  - Nonlinear effects
  - Relative influence
  - (Helps to plot the tabular data overlaid to compare)
- What would you conclude from the plots at right?



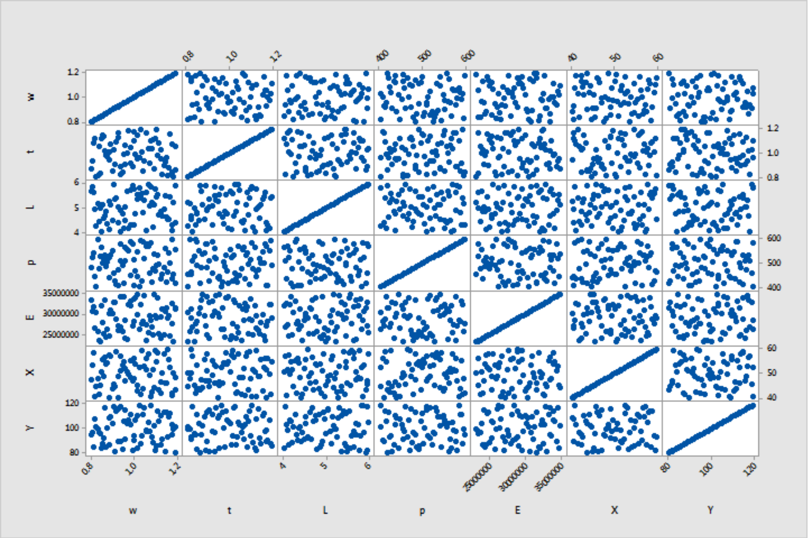
A Practical Process for SA

1. What are the key model responses (quantities of interest)?
   What are your follow-on (post-SA) analysis goals?
2. Identify potentially important input parameters
   - Often expert opinion-based with phenomena identification and ranking table (PIRT)
   - Include parameters that likely influence response or might be involved in other studies
3. Pose plausible parameter bounds or steps
4. Set up Dakota input file with variables and interface to simulation
5. Perform an initial centered parameter study
6. Perform additional SA studies based on simulation cost and any known model character
7. Post-process Dakota-generated data with third-party tools

Up next: 6

Workhorse SA Method: Random Sampling

- Dakota generates a space filling design (most commonly Latin hypercube design) and runs model at each point
- Recommend $10 \times d$ model runs (samples), minimum $2 \times d$
- Analyzes input/output relationships with correlation coefficients
  - Simple correlation: strength and direction of a linear relationship between variables
  - Partial correlation: like simple correlation but adjusts for the effects of the other variables
  - Rank correlations: simple and partial correlations performed on “rank” of data
- Can use for follow-on analysis, such as PCE + VBD with Dakota, or with third-party tools



Two-dimensional projections of a LHD for Cantilever *(plotted with Minitab)*

$$\rho(w,z) = \frac{\sum_i (w^i - \bar{w})(z^i - \bar{z})}{\sqrt{\sum_i (w^i - \bar{w})^2 (z^i - \bar{z})^2}}$$

Simple correlation between factors (input or output) *w* and *z*, taken over samples *i*

Exercise 2: Random Sampling for SA

- Use the Reference Manual to change the Dakota input file in **`exercises/sens_analysis/2`** from a centered study to sampling
  - Configure the sampling method to perform a Latin hypercube sample with an appropriate number of samples. Why might a **seed** specification be important?
  - Use **`uniform_uncertain`** variables to define the hyper-rectangle given by

    $0.8 \le w \le 1.2$ $\quad 0.8 \le t \le 1.2$ $\quad 4.0 \le L \le 6.0$ $\quad 400.0 \le \rho \le 600.0$

    $23.0e{+}6 \le E \le 35.0e{+}6$ $\quad 40.0 \le X \le 60.0$ $\quad 80.0 \le Y \le 120.0$
- Run the study and examine the correlations between inputs and outputs
  - Which parameters most influence mass? Stress? Displacement?
  - How does changing the number of samples affect your conclusions?
  - Do these match your intuition of the cantilever beam analysis? *Recall that Cantilever Physics simulates following simple model…*

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

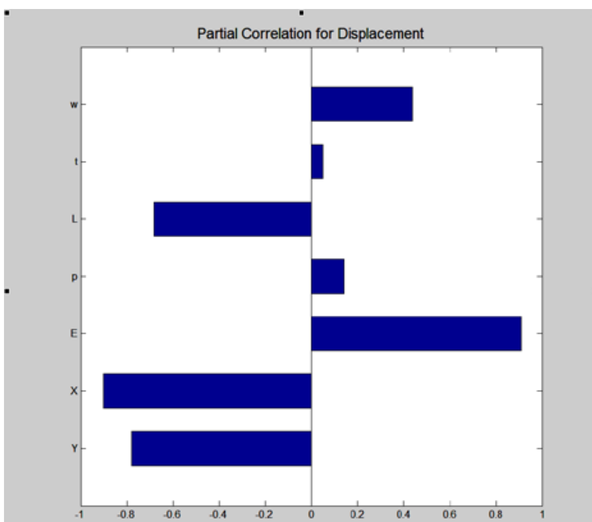
$$S = \frac{600}{wt^2} Y + \frac{600}{w^2 t} X$$

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

Global Sampling Results for Cantilever

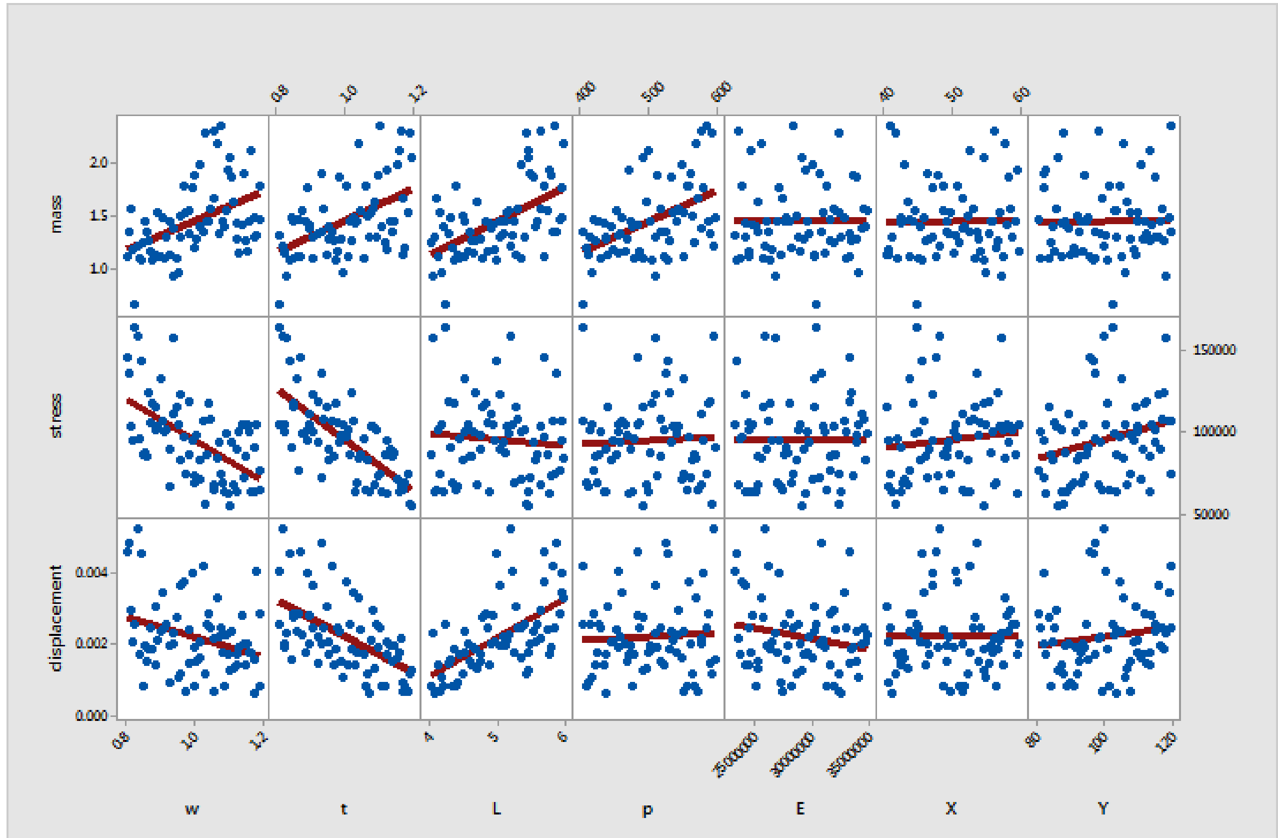
Partial Correlation Matrix for Cantilever			
	mass	stress	displacement
w	0.95	-0.96	-0.78
t	0.95	-0.97	-0.90
L	0.96	-0.17	0.91
p	0.95	0.11	0.14
E	-0.08	-0.13	-0.68
X	-0.03	0.54	0.05
Y	0.12	0.82	0.44

partial correlations from console output (colored w/ Excel)



(plotted with Matlab)

Scatter plots: Dakota tabular data plotted in Minitab (can use Matlab, JMP, Excel, etc.)

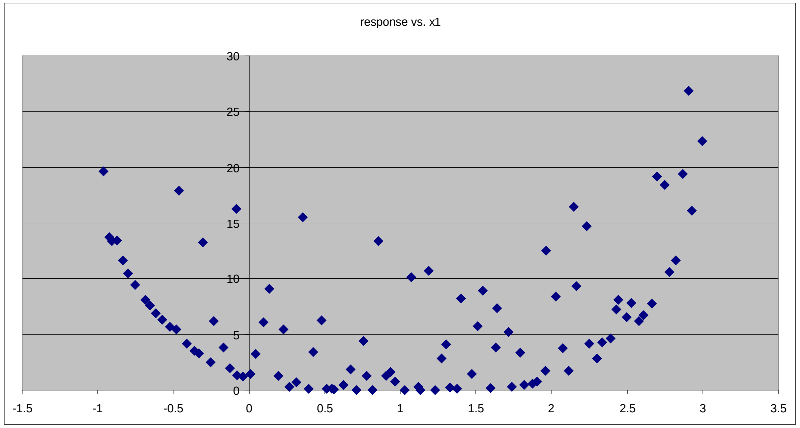


Observation: Correlations

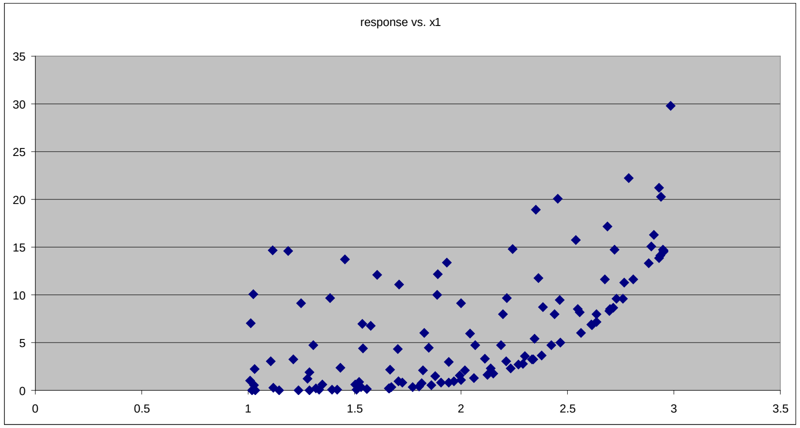
- Large correlation coefficients indicate important factors, however factors with small correlation may still be significant
- Assumptions about input domain (bounds) matter
- Diagnostics like scatter plots can help avoid pitfalls

Example: function with a quartic-like trend over two different domains

Bounds = [-1, 3]



Bounds = [1, 3]



Additional SA Methods: Variance-based Decomposition (VBD)

- VBD assumes an orthogonal decomposition of the response

$$f(x) = f_0 + \sum_i f_i(x_i) + \sum_{i<j} f_{ij}(x_i, x_j) + \cdots$$

- Sensitivity indices summarize how response variability can be apportioned to individual input factors.

$$S_i = \frac{Var_{x_i}[E(f|x_i)]}{Var(f)} \qquad T_i = \frac{E_{x_{-i}}[Var(f|x_{-i})]}{Var(f)} = \frac{Var(f) - Var_{x_{-i}}[E(f|x_{-i})]}{Var(f)}$$

  Main effect S_i measures effect of varying x_i alone (averaging over other factors). Total effect T_i includes its interactions with other variables.

- Directly enabling this for a sampling or DOE method is often prohibitively expensive, requiring *(d+2) x N* runs, where each replicate has *N* samples
- Instead, configure Dakota to automatically build a polynomial chaos expansion (PCE) from the earlier Latin hypercube sampling dataset and compute main and total effects analytically

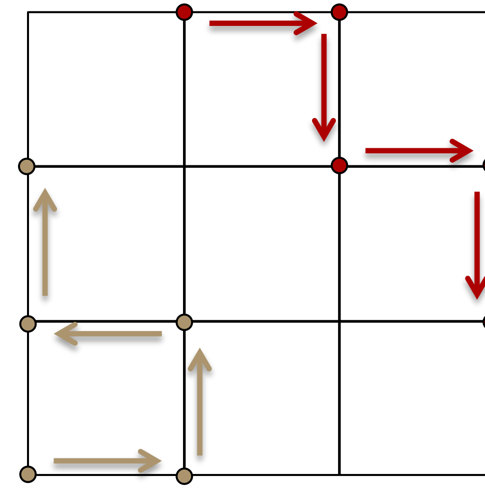
Additional SA Methods: Morris One-at-a-Time (MOAT)

- Conduct "tours" (sampling on coordinate direction paths) around the global space x.

- For each step j in coordinate direction i, compute an elementary effect: $\delta_i(x^j) = \frac{f(x^j+\Delta e_i)-f(x^j)}{\Delta}$
(like a forward difference local sensitivity, but with large step)

- Compute statistics on the elementary effects to assess relative influence of each variable *i* over whole space
  - Mean μ_i: measure of linear/main/first-order effect
  - Modified mean μ_i^*: same, controlling for cancellation
  - Standard deviation σ_i: measure of variability across input space; indicative of interaction and/or nonlinear effects

- Number samples must be a multiple of *(d+1)*; recommend *2 x (d+1) to 10 x (d+1)*



partitions=3 (levels = 4)

$$\mu_i = \frac{1}{N_j}\sum_j \delta_i(x^j)$$

$$\mu_i^* = \frac{1}{N_j}\sum_j |\delta_i(x^j)|$$

$$\sigma_i = \sqrt{\frac{1}{N_j - 1}\sum_j \left(\delta_i(x^j) - \mu_i\right)^2}$$

Other SA Approaches Typically Only Require Changing the Method Block

- Dakota Reference Manual guides in specifying keywords

```
method,
sampling
    sample_type lhs
    seed =52983
    samples = 100
```

LHS Sampling

```
method,
    dace oas
    main_effects
    seed =52983
    samples = 500
```

Main Effects Analysis using Orthogonal Arrays

```
method,
sampling
    sample_type lhs
    seed =52983
    samples = 500
    variance_based_decomp
```

Variance-based Decomposition using LHS Sampling

```
method,
    psuade_moat
    partitions = 3
    seed =52983
    samples = 100
```

Morris One-At-a-Time

Dakota SA Methods Summary

Category	Dakota method names	univariate trends	correlations	modified mean, s.d.	main effects Sobol inds.	importance factors / local sensis
Parameter studies	centered, vector, list	P				
	grid		D		P	
Sampling	sampling, dace lhs, dace random, fsu_quasi_mc, fsu_cvt	P	D			
	with variance_based_decomp...				D	
DACE (DOE-like)	dace {oas, oa_lhs, box_behnken, central_composite}		D		D	
MOAT	psuade_moat			D		
PCE, SC	polynomial_chaos, stoch_collocation				D	D
Mean value	local_reliability					D

also multi-purpose!

D: Dakota-generated
P: Post-processing required (3rd party tools)

Exercise 3: VBD and MOAT

See **exercises/sens_analysis/3**

- Morris One-at-a-Time
  - Copy **dakota_cantilever_lhs.in** from **2/** to **3/**
  - Modify the method to perform a Morris sampling study; note that **samples** must be a multiple of *d+1*
  - Run the study and examine the modified mean and standard deviation of the elementary effects
- Variance-based decomposition with PCE, reusing data from LHS study
  - Copy your tabular data file from **2/** to **3/**
  - Insert the variables specification into **dakota_cantilver_pce_vbd.in**
  - Run the study and examine the Sobol indices (main and total effects)

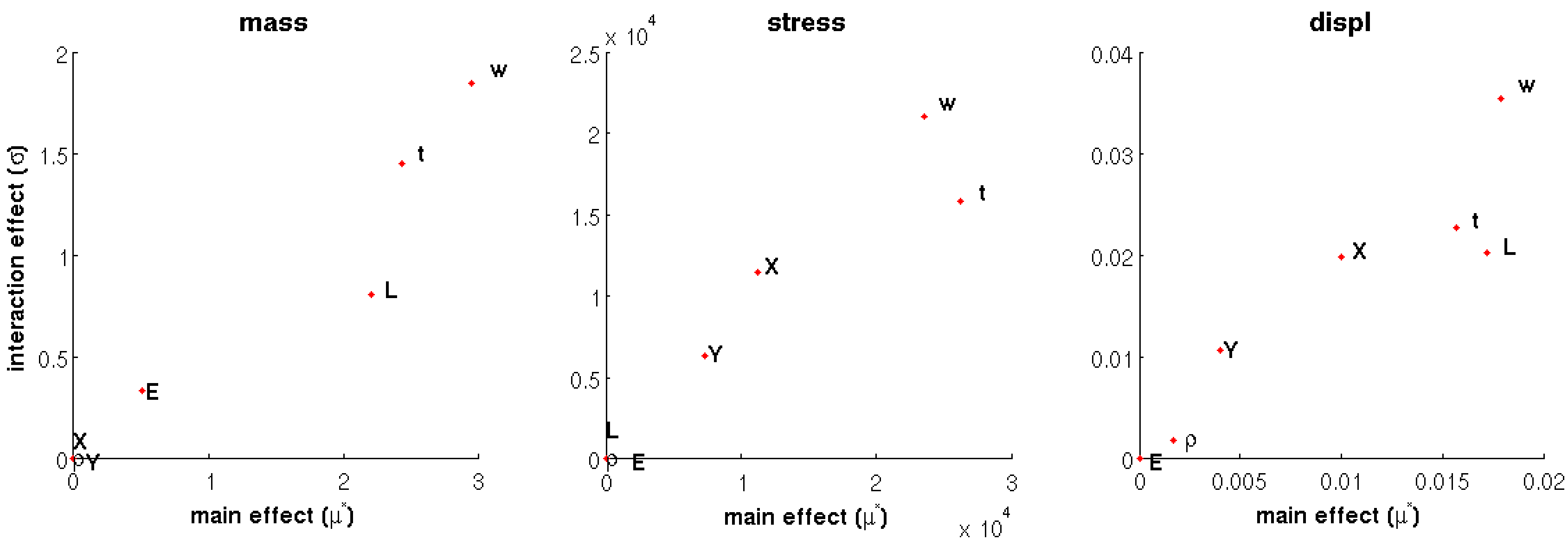
- For each, what do you conclude?
- How might you plot or otherwise analyze/present the results?

Results from Additional SA Methods

- Sobol indices from VBD (for stress):

Main	Total	
3.3760829131e-01	4.2345004119e-01	w
4.6020857475e-01	5.4707791944e-01	t
0.0000000000e+00	2.1120750926e-03	L
0.0000000000e+00	4.1405847238e-03	p
0.0000000000e+00	6.8909143306e-04	E
3.7319366458e-02	6.0826370499e-02	X
5.0936411844e-02	7.5631273252e-02	Y

- Morris metrics



A Practical Process for SA

1. What are the key model responses (quantities of interest)?
   What are your follow-on (post-SA) analysis goals?
2. Identify potentially important input parameters
   - Often expert opinion-based with phenomena identification and ranking table (PIRT)
   - Include parameters that likely influence response or might be involved in other studies
3. Pose plausible parameter bounds or steps
4. Set up Dakota input file with variables and interface to simulation
5. Perform an initial centered parameter study
6. Perform additional SA studies based on simulation cost and any known model character
7. Post-process Dakota-generated data with third-party tools

Up next: Discuss 7

Using Dakota-generated Data

- Users commonly work with the Dakota tabular data file (dakota_tabular.dat by default)
- Import tabular data into Excel, Minitab, Matlab, R, SPlus, JMP, Python to
  - Generate scatter or residual plots to assess trends missed by correlations
  - Perform stepwise or best subsets regression
  - Perform other significance analysis
- Use Dakota results to prune variables and repeat study with more samples

- Decision making considerations
  - Can you gather more data on most influential parameters?
  - Can you afford optimization or UQ using all the influential parameters?

Common Question: UQ versus SA

What distinguishes sensitivity analysis from uncertainty analysis?

- With SA you primarily gain information about variables
  - Rank importance of parameters and characterize in what way they influence responses
  - Sometimes called inverse UQ
  - Secondarily, characterize model properties
- With UQ you primarily gain information about responses
  - Statistical properties of output responses
  - Intervals indicating bounds on response
  - Likelihood (probability of failure)

- Some methods can be used for both, e.g.,
  - LHS is often used for SA (correlations) and UQ (moments, PDFs, CDFs)
  - Polynomial chaos expansions (PCE) thought of as a UQ method, but also efficiently produce Sobol indices for ranking parameter influence

Sensitivity Analysis References

- Saltelli A., Ratto M., Andres T., Campolongo, F., et al., Global Sensitivity Analysis: The Primer, Wiley, 2008.
- J. C. Helton and F. J. Davis. Sampling-based methods for uncertainty and sensitivity analysis. Technical Report SAND99-2240, Sandia National Laboratories, Albuquerque, NM, 2000.
- Oakley, J. and O’Hagan, A. Probabilistic sensitivity analysis of complex models: a Bayesian approach. J Royal Stat Soc B 2004; 66:751–769.

- Dakota User’s Manual
  - Parameter Study Capabilities
  - Design of Experiments Capabilities/Sensitivity Analysis
  - Uncertainty Quantification Capabilities (for MC/LHS sampling)
- Corresponding Reference Manual sections

Sensitivity Analysis: Recommended Practice Summary

- Conduct an initial centered parameter study, requiring $2 \times d \times steps + 1$ runs, ideally with small, then large perturbations
  - Only univariate effects: can't get interactions, however results aren't confounded
- Conduct a global sampling design with from $2 \times d$ to $10 \times d$ samples
  - Input/output pairs with large (> 0.7) simple or partial correlations are significant
  - Smaller ones may still be relevant; to find out, generate scatter plots, analyze same data set using PCE with VBD
- Alternately, or in addition for comparison, conduct a MOAT study to get results similar to VBD
  - From $2 \times d$ to $10 \times d$ samples
- Use third-party tools as needed to generate additional views or conduct analyses

Module Learning Goals
Did We Meet Them?

- Understand goals and benefits of sensitivity analysis (SA)
- Have a practical process for SA at your disposal
- Be able to formulate your problem, present it to Dakota, and run and understand studies
- Be familiar with key Dakota SA methods
- Know how to use Dakota sensitivity analysis results