SAND2016-3330PE

Dakota Software Training

Sensitivity Analysis

http://dakota.sandia.gov

Sandia National Laboratories

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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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 sensitivity analysis methods
- Know how to use Dakota SA 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

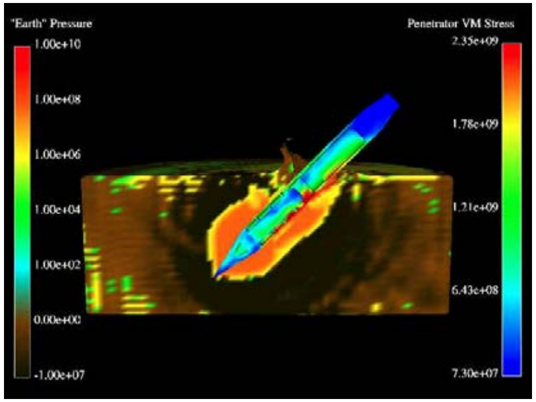
- Other key SA methods: Morris one-at-a-time (MOAT) and variance-based decomposition (VBD)
- Exercise: Explore sensitivity analysis methods

- Beyond Dakota: using SA results, getting more information

Why Sensitivity Analysis?

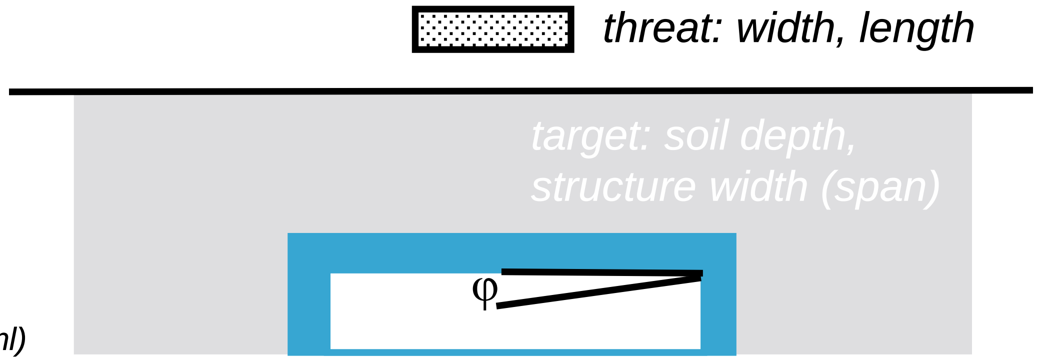
- What? Reveal the extent to which simulation outputs depend on each simulation input
- Why? Identify most important input variables and their interactions
  - Primarily for screening/ranking: Identify the most important variables; down-select for further uncertainty or optimization analysis
  - Provide a focus for resources
    - Data gathering and model development
    - Code development
    - Uncertainty characterization
  - Identify key model characteristics: smoothness, nonlinear trends, robustness; develop intuition about the 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

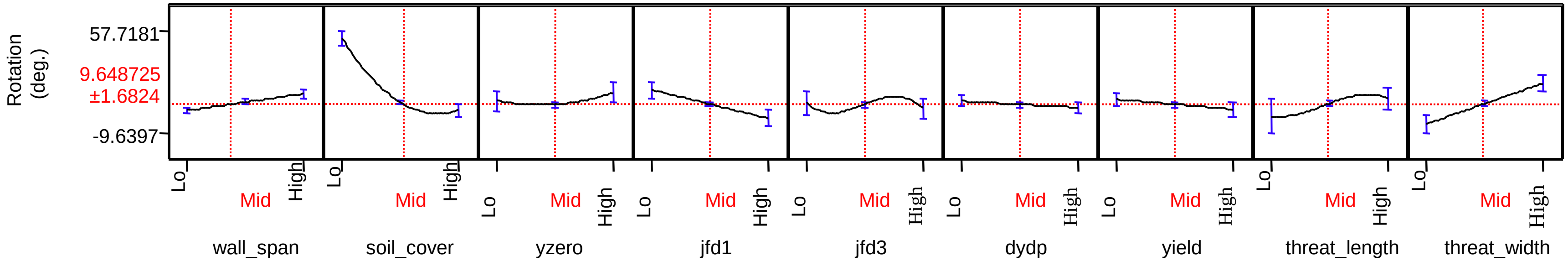


Notional model for illustration purposes only (http://www.sandia.gov/ASC/library/fullsize/penetrator.html)

12 parameters describing target & threat



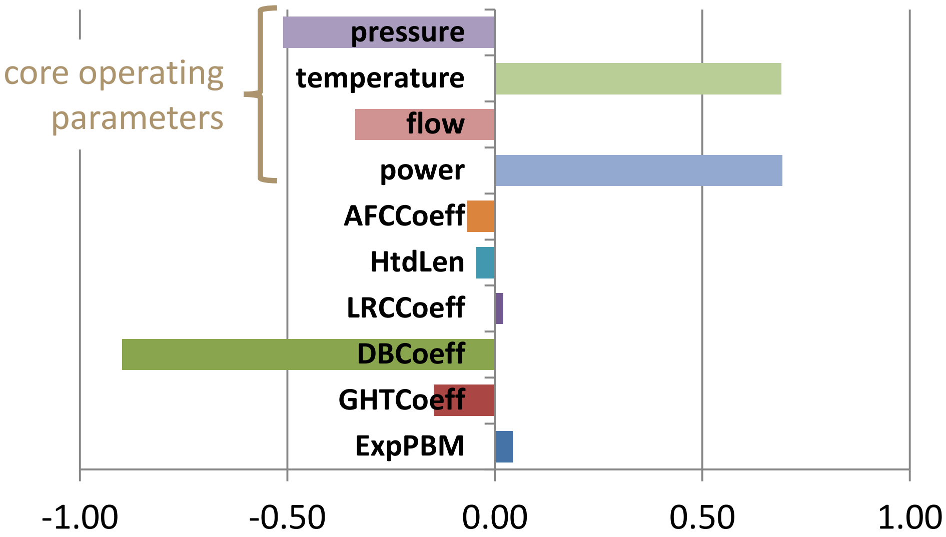
- Underground target with external threat: assess sensitivity in target response to target construction and threat characteristics
- Response: angular rotation (ϕ) of target roof at mid-span
- Analysis: CTH Eulerian shock physics code; JMP for stats
- Revealed most sensitive input parameters and nonlinear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

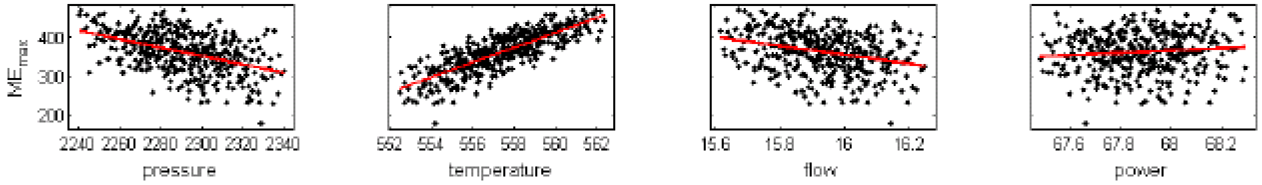


Sensitivity Analysis Example: Nuclear Reactor Thermal-Hydraulics Model

- Assess parameter influence on boiling rate, a key crud predictor
- Dakota correlation coefficients: strong influence of core operating parameters (pressure is 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 (max) mass evaporation rate to operating parameters

Discussion:
Your Sensitivity Analysis Practice

- What kinds of parameters (broadly) 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)
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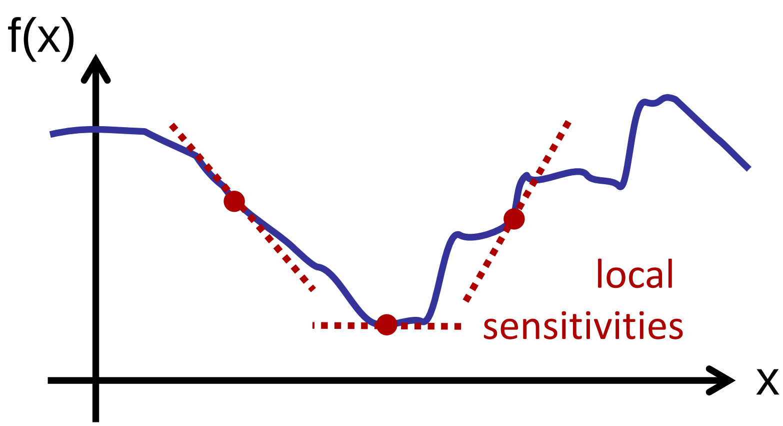
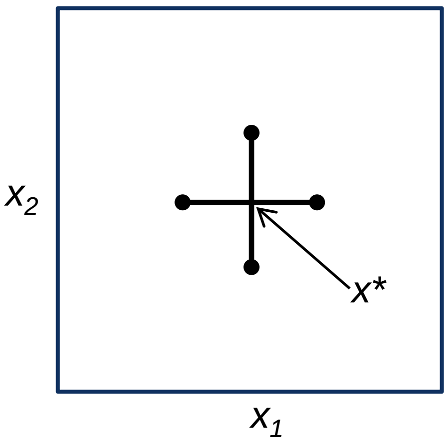
Up next: Some sensitivity analysis terminology

Key Sensitivity Analysis Concepts: Local Sensitivity

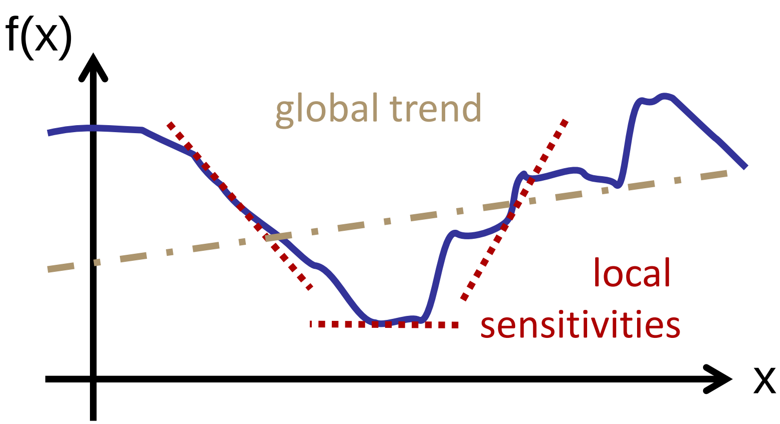
- Local sensitivity measures the relative influence of parameters at a particular point in the input space
- Partial derivatives (slopes) w.r.t. each variable: $\frac{\partial f}{\partial x_1}(x^*), \ \frac{\partial f}{\partial x_2}(x^*)$
- Can be estimated with finite differences (small perturbations);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

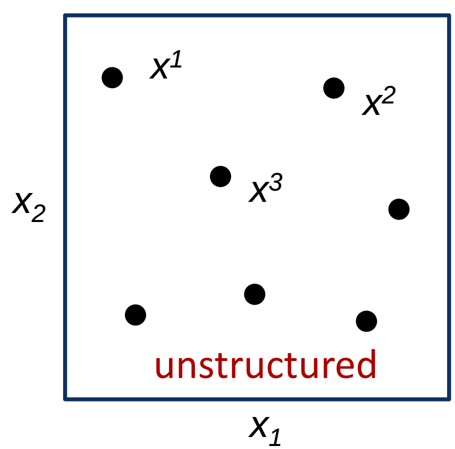


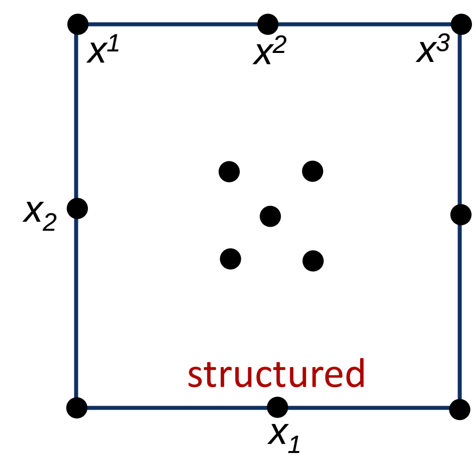


Key Sensitivity Analysis Concepts: Global Sensitivity

- 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 which measure variability of response at various points in input space: main and nonlinear/interaction measures
- Scatter plots: helpful visual diagnostic for trend analysis

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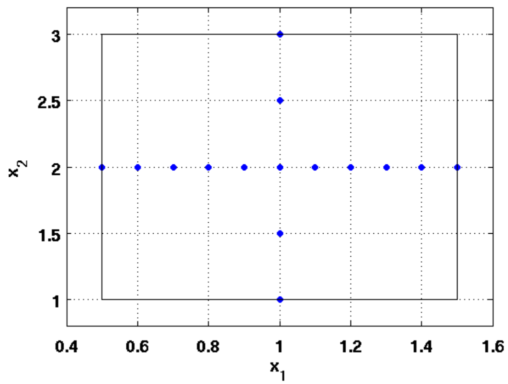
Up next: Discuss 3, 4, and 5

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

Specifying Dakota Variable Ranges for a Sensitivity Study

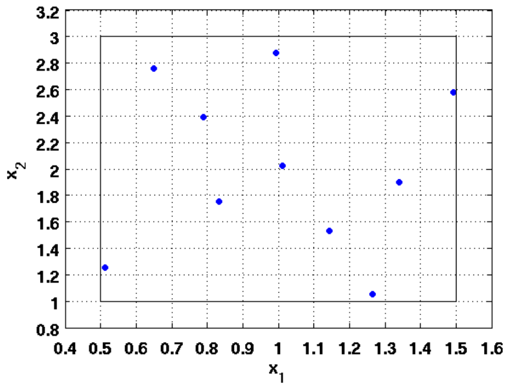
Local or univariate global sensitivity: initial point and steps to take

```
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

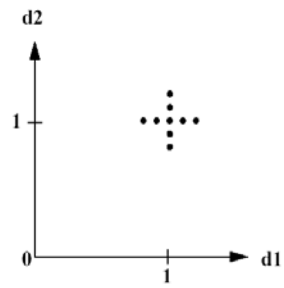
```
variables
  continuous_design  2
    descriptors        'flow'  'power'
    upper_bounds       1.5     3.0
    lower_bounds       0.5     1.0

method sampling
  ...
```



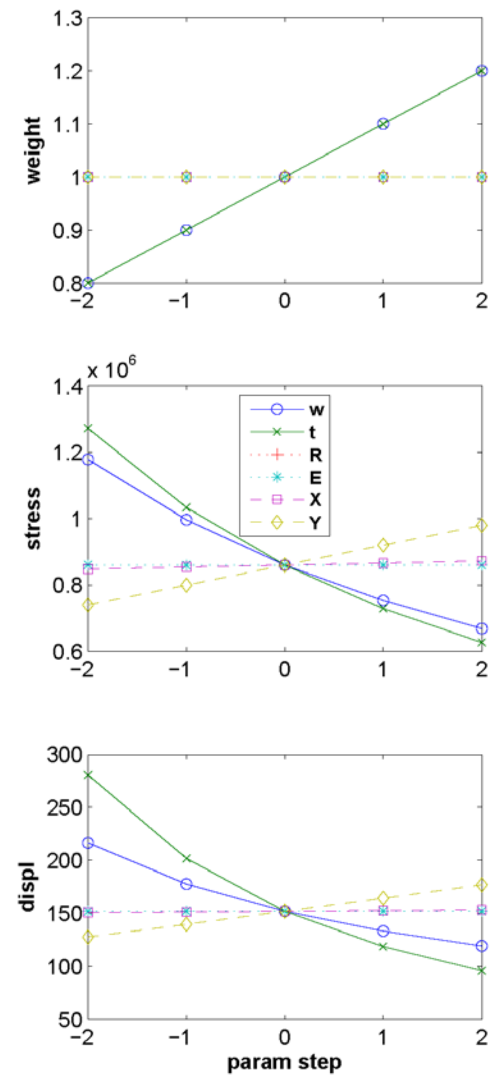
Dakota variable type is not critical. Typically use continuous or discrete design, or uniform or discrete (interval, set) uncertain.

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 $\pm 5\%$, $\pm 10\%$, 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?



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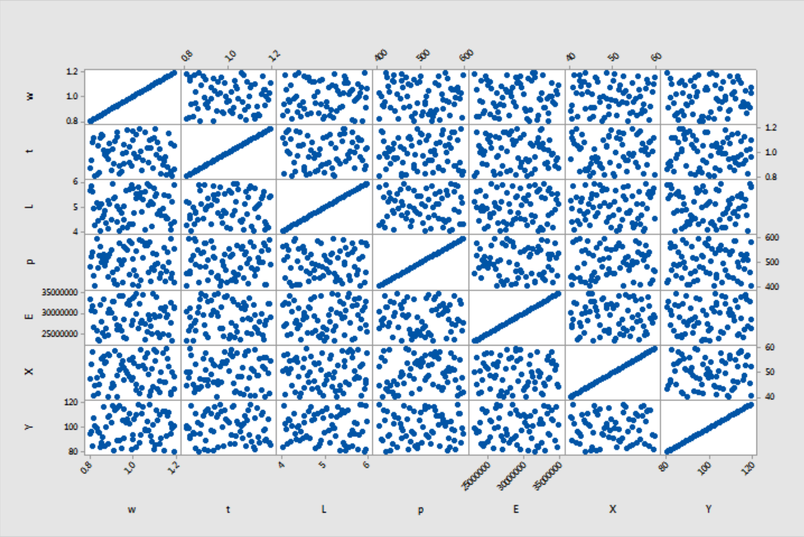
Up next: 6

Workhorse SA Method: Random Sampling

- Dakota generates a space filling design (most commonly a 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
    $0.5 \leq w \leq 1.5$ $\quad 0.5 \leq t \leq 1.5$ $\quad 5.0 \leq L \leq 15.0$ $\quad 450.0 \leq \rho \leq 550.0$
    $2.4e{+}7 \leq E \leq 3.4e{+}7$ $\quad 1.0 \leq X \leq 10.0$ $\quad 5.0 \leq Y \leq 15.0$

- 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…*

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

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

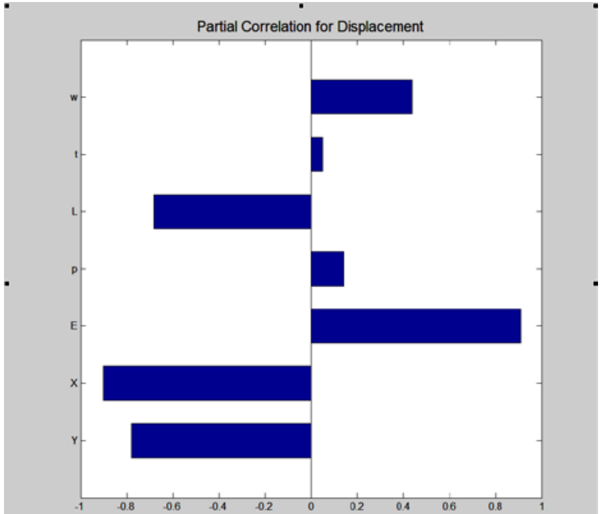
$$S = \frac{600}{wt^2}Y + \frac{600}{w^2 t}X$$

Global Sampling Results for Cantilever

Partial Correlation Matrix for Cantilever

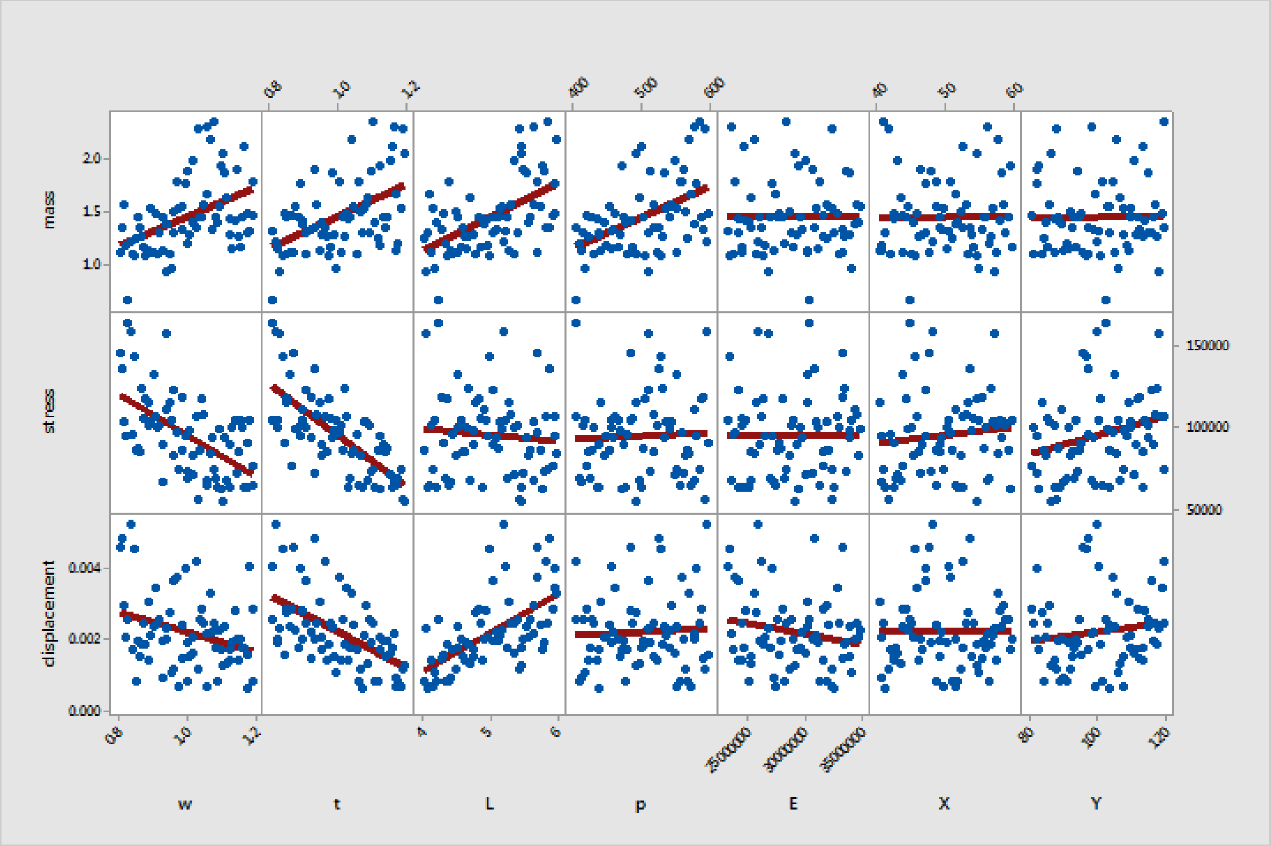
	mass	stress	displacement
w	0.95	-0.96	-0.78
t	0.95	-0.97	-0.90
L	0.96	-0.17	0.91
p	0.95	0.11	0.14
E	-0.08	-0.13	-0.68
X	-0.03	0.54	0.05
Y	0.12	0.82	0.44

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.)

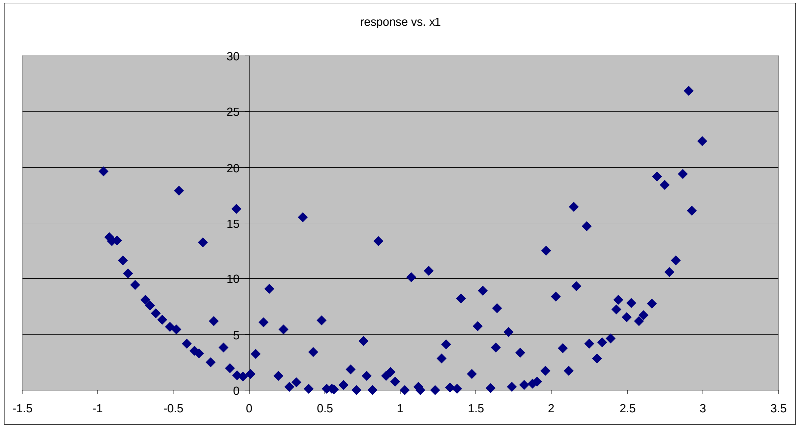


Observation: Correlations

- 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]



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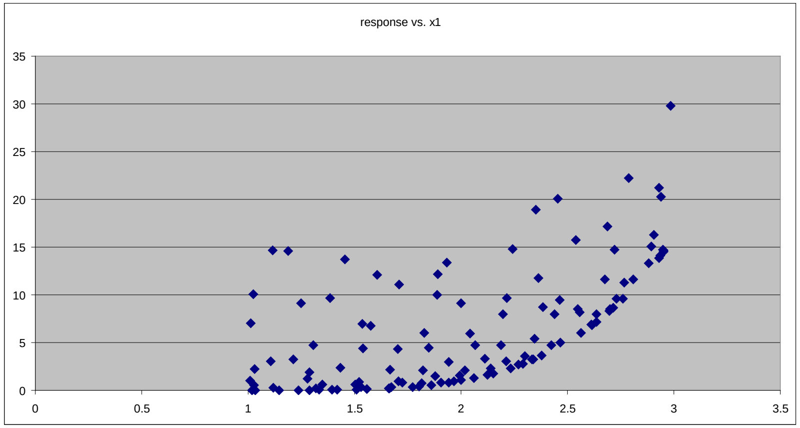


Additional SA Methods: Variance-based Decomposition (VBD)

- 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 $(d+2) \times N$ 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

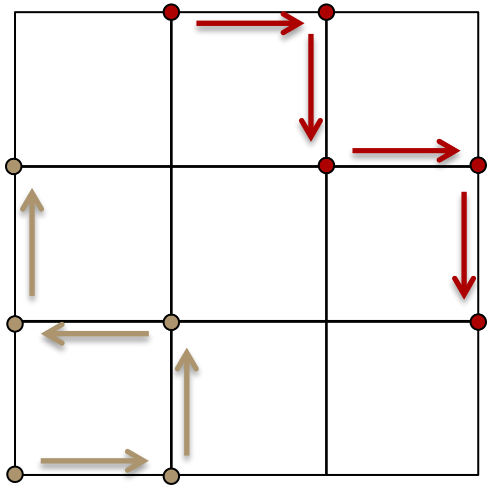
Additional SA Methods: Morris One-at-a-Time (MOAT)

- 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)

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

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

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

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 with variance_based_decomp...	P	D		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)

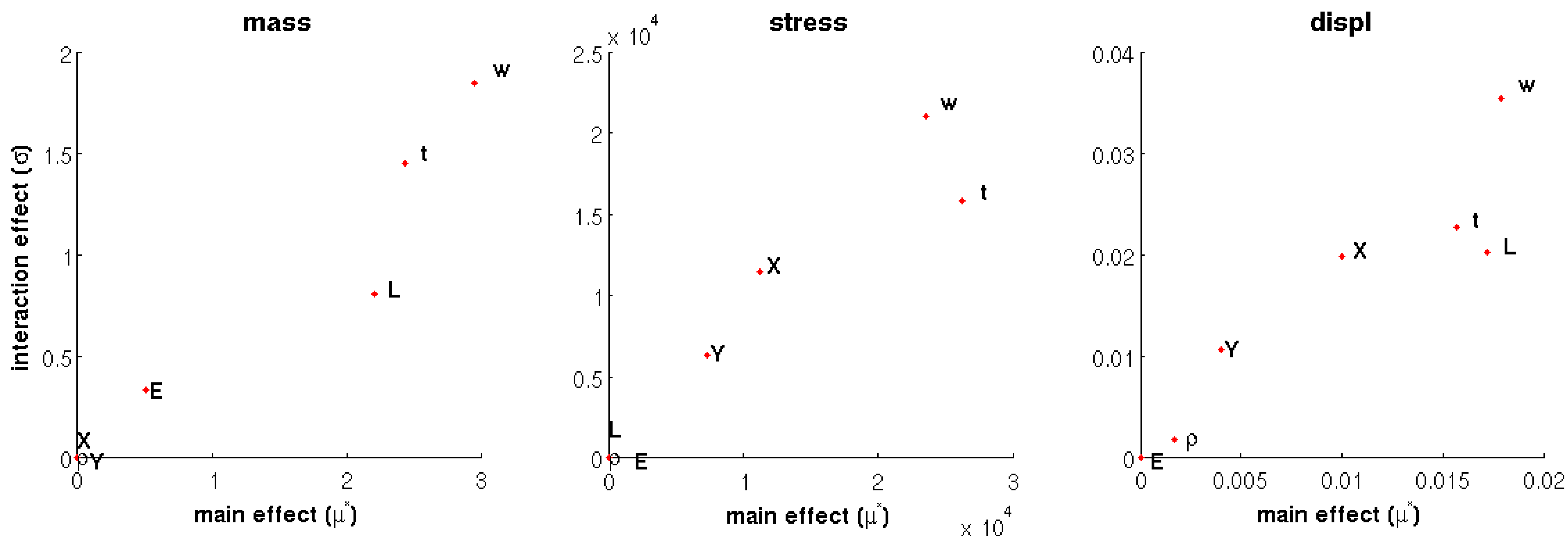
- For each, what do you conclude?
- How might you plot or otherwise analyze/present the results?

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



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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: Uncertainty Quantification 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

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Did We Meet Them?

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