SAND2016-3330PE

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Dakota Software Training

Sensitivity Analysis

http://dakota.sandia.gov

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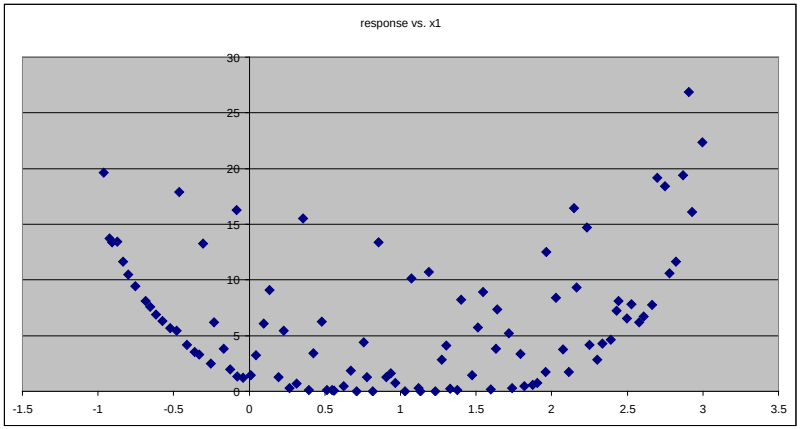
Observation: Correlations

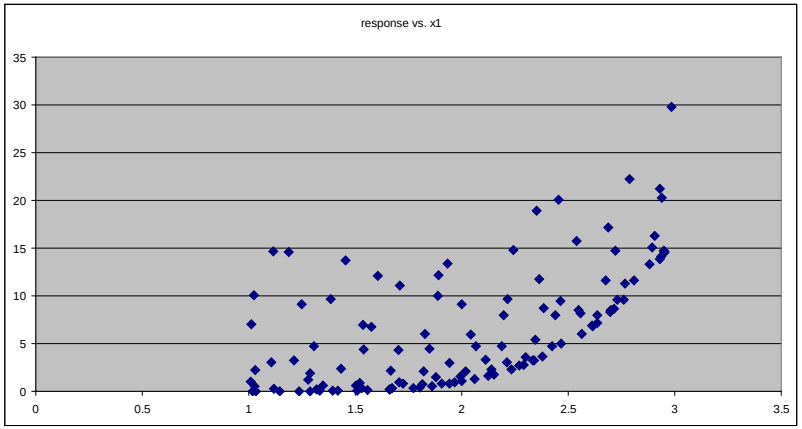
- Large correlation coefficients indicate important factors, however factors with small correlation may still be significant
- Assumptions about input domain (bounds) matter
- Diagnostics like scatter plots can help avoid pitfalls

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.

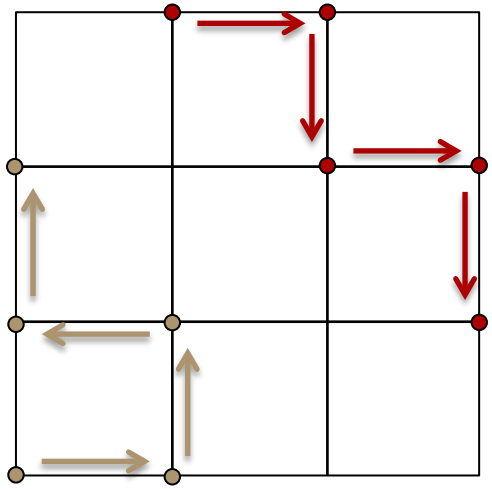
$$S_i = \frac{Var_{x_i}[E(f|x_i)]}{Var(f)} \qquad T_i = \frac{E_{x_{-i}}[Var(f|x_{-i})]}{Var(f)} = \frac{Var(f) - Var_{x_{-i}}[E(f|x_{-i})]}{Var(f)}$$

  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 $(d+2) \times N$ 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)

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

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

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

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)

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