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Global Sensitivity Analysis

Verification and Validation for Nuclear Systems Analysis: Workshop II

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with

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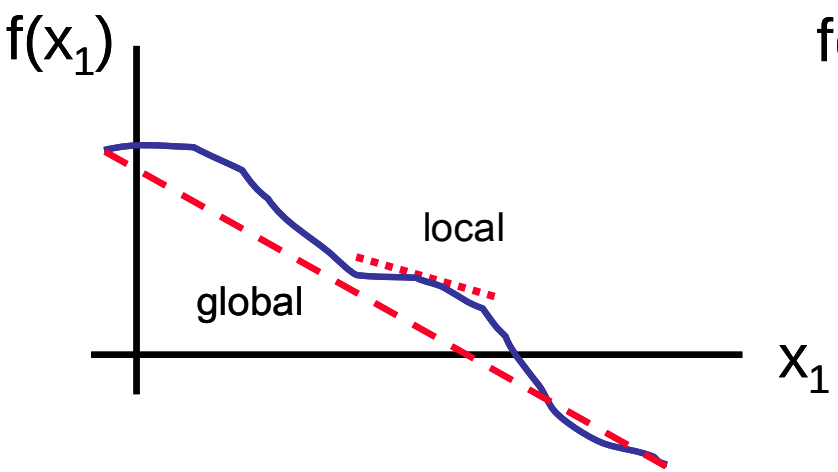
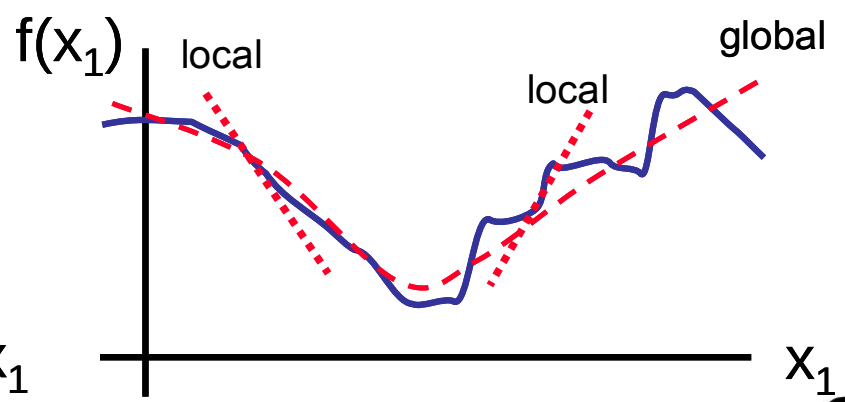
Why Sensitivity Analysis?

Sensitivity Analysis: Rank variables according to importance relative to uncertainty in model output

- **Determine variables important for optimization or UQ, which to gather more data on or control in an experiment, or for guiding anisotropic methods**
- **Local, linear, or under-resolved can mislead**
- **Global: typically computationally expensive**
- **Useful for V&V to check system performance and robustness**





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Key Talk Concepts
(not in outline order)

- Motivation for global sensitivity methods on simulations; non-intrusive/black-box approaches

Example global designs

- Latin Hypercube sampling; replicates for variance-based decomposition
- One-at-a-Time sampling
- Quadrature/cubature

Example analysis techniques

- Regression (linear/ nonlinear), scatter plots
- Elementary effects
- VBD/Sobol indices (directly or with surrogates)

- Current work extending global and nonlinear approaches to leverage adjoint information when available

Local Sensitivity Analysis

- **Calculate sensitivity at one (or a few) locations in input parameter space; typically at nominal values**
- **Deterministic: based on local derivative(s) (possibly via AD or adjoints); or data fit Taylor series with number of points commensurate with # d.o.f. in truncated series**
- **Probabilistic: for example mean-value analysis with importance factors; assume distributions on input parameters (uniform, normal, etc.) and use derivatives:**

$$\mu_f = f(\mu_x) \qquad IF_i = \left(\frac{\sigma_{x_i}}{\sigma_f} \frac{df}{dx_i}(\mu_x) \right)^2$$

$$\left(S^T C S\right) \qquad \sigma_f^2 = \sum_i \sum_j Cov(i,j) \frac{df}{dx_i}(\mu_x) \frac{df}{dx_j}(\mu_x)$$

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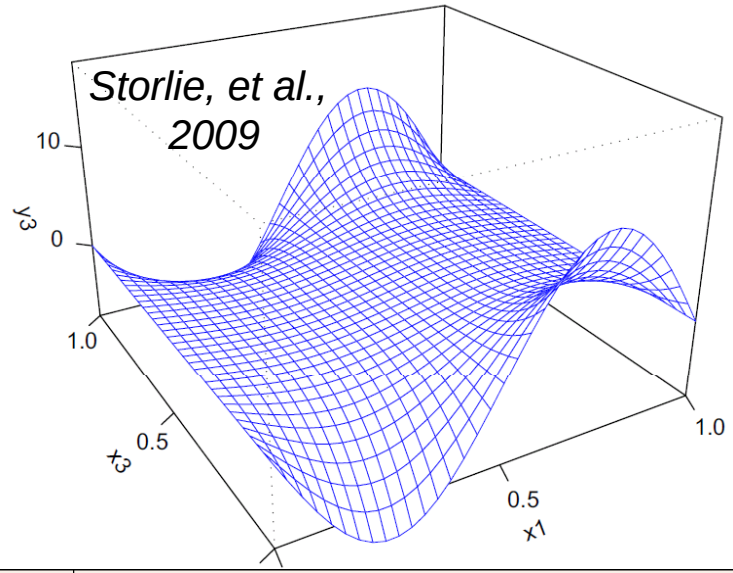
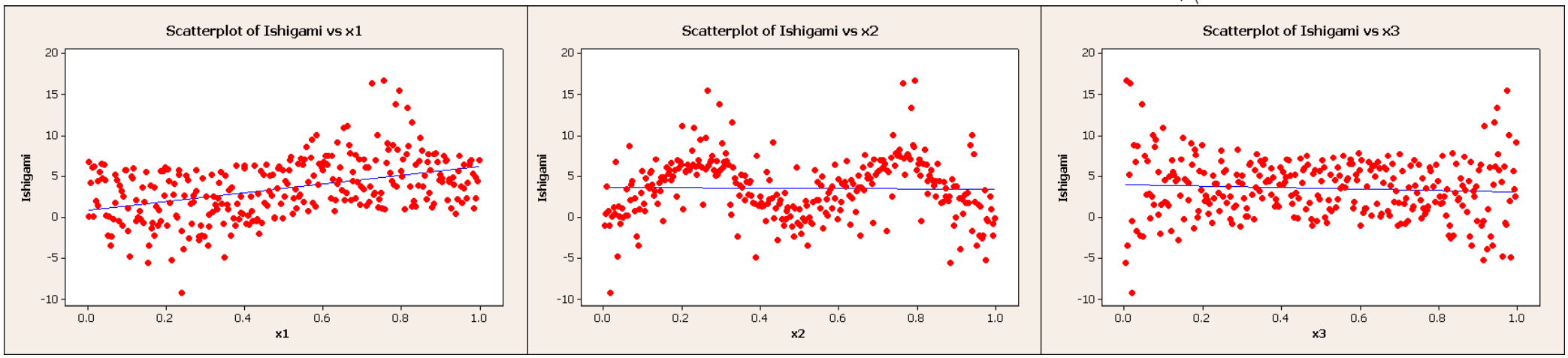
Mildly Nonlinear: "Ishigami" Algebraic Test Function

$$f(x) = \sin(2\pi x_1 - \pi) + 7\sin^2(2\pi x_2 - \pi) + 0.1(2\pi x_3 - \pi)^4 \sin(2\pi x_1 - \pi)$$

- **Even for simple function, local analysis insufficient for sensitivity analysis**
- **Scatterplots of 300 Monte Carlo samples show trend w.r.t each variable**





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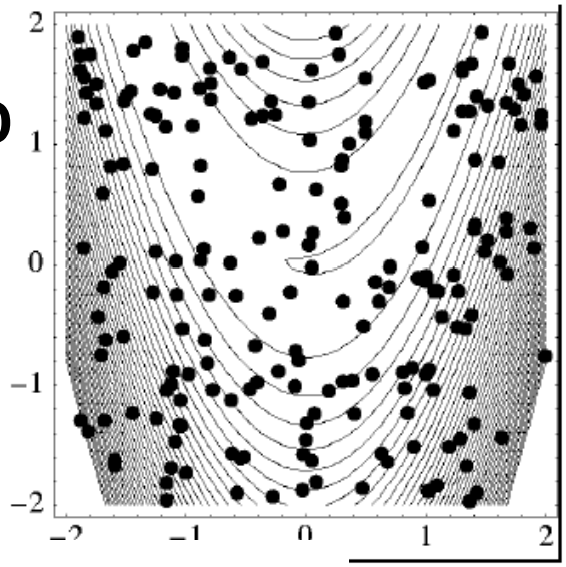
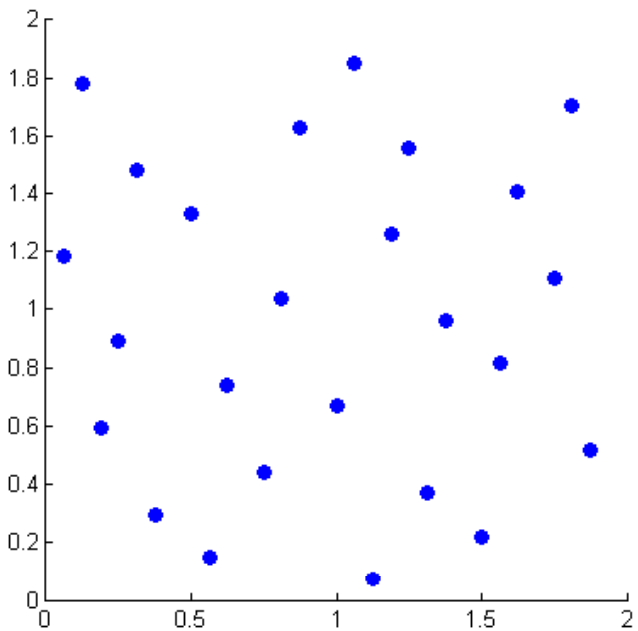
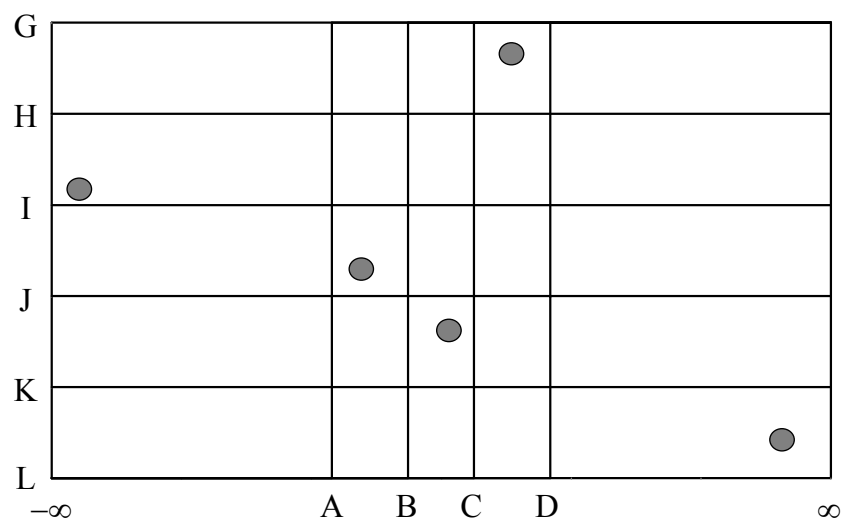
Global Exploration Techniques

- GOAL: assess inputs over hypercube of interest
- Orthogonal arrays (incl. grid), Box-Behnken, CCD
- Monte Carlo, Latin hypercube sampling, low discrepancy: Quasi-MC, CVT
- One-at-a-Time Designs





25 QMC (Halton) points



2-D LHS of size 5 for x1 (normal) and x2 (uniform)

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Ishigami: Analysis of LHS
(misleading correlations)

- **Partial (Pearson) correlations:** strength/direction of linear trend after linear effects due to other parameters removed from x and y
- **Partial (Spearman) rank correlations:** same, but on ranks of data instead of numerical values; good for monotonic over scales, but not nonlinear relationships

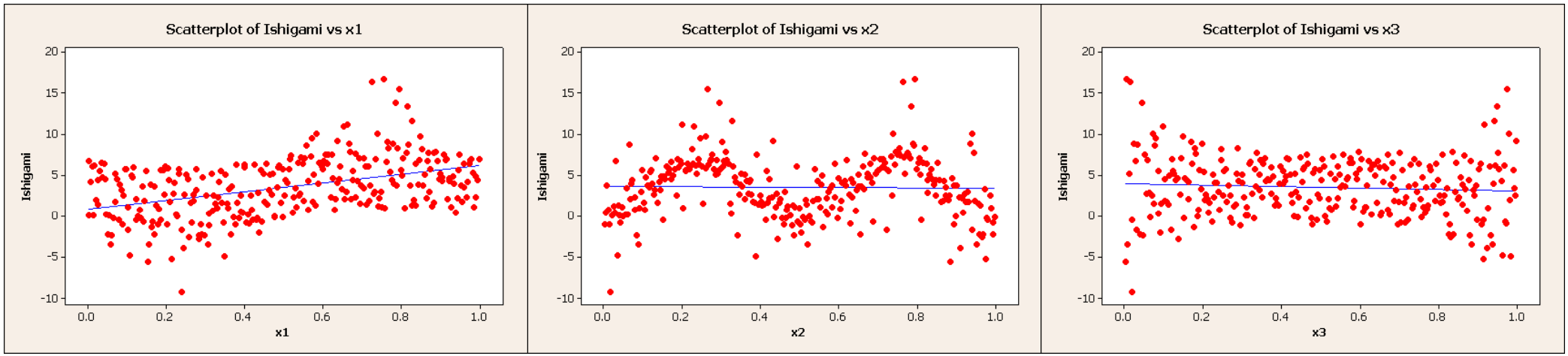
correlation

$$\rho(X_i,Y) = \frac{\mathrm{cov}(X_i,Y)}{\sqrt{\mathrm{var}(X_i).\mathrm{var}(Y)}}$$

partial correlation

$$PC_{(X_i,Y)} = \frac{\mathrm{cov}(rx_i, ry_{i,j})}{\sqrt{\mathrm{var}(rx_i).\mathrm{var}(ry_{i,j})}}$$

	30 samples		300 samples	
	corr	rank corr	corr	rank corr
x1	0.51	0.54	0.42	0.41
x2	-0.06	-0.03	-0.01	-0.01
x3	0.08	0.05	-0.06	-0.05



Versatility of LHS Designs

- Can perform linear, nonlinear (higher-order), or non-parametric statistical analysis of LHS (or other space-filling) samples

- For example, construct regression models or global surrogates, from which statistics can be computed

- Comparison of global and local linear (adjoint-based) methods for SA / UQ of SFR neutronics using DAKOTA and ERANOS:
  C. Rabiti, G. Palmiotti, M. Assawaroongruengchot, and Adams, B.M., *Comparison of uncertainty quantification methods for fast reactor neutronics*, PHYSOR2010, Pittsburgh, PA, May 9—14, 2010

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One-at-a-Time/Elementary Effects (Morris, Saltelli)

- **Make large perturbations; calculate differences (elementary effects d_i)**

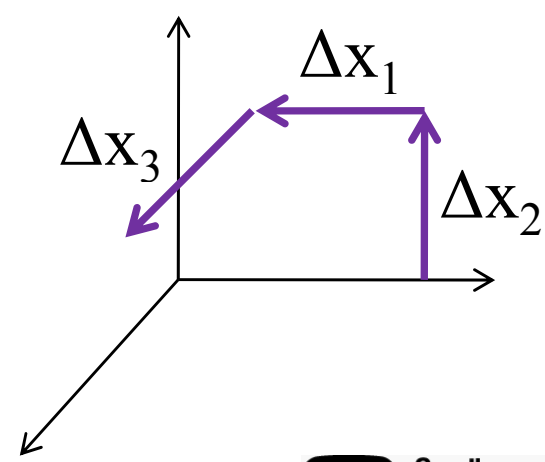
$$d_i(x) = \frac{y(x + \Delta e_i) - y(x)}{\Delta}$$

- **Compute statistics on these differences to summarize how each variables affects y:**

$$\mu_i = \frac{1}{r}\sum_{j=1}^{r} d_i^{(j)} \qquad \mu_i^* = \frac{1}{r}\sum_{j=1}^{r} \left| d_i^{(j)} \right| \qquad \sigma_i = \sqrt{\frac{1}{r}\sum_{j=1}^{r}\left(d_i^{(j)} - \mu_i\right)^2}$$

mean of d_i *modified mean of d_i* *standard deviation of d_i*

- **With k variables and r replicates, need not do 2*k*r samples; reuse to get same results in (k+1)*r evaluations**
- **Can be very effective for screening large numbers of parameters w/nonlinear models**



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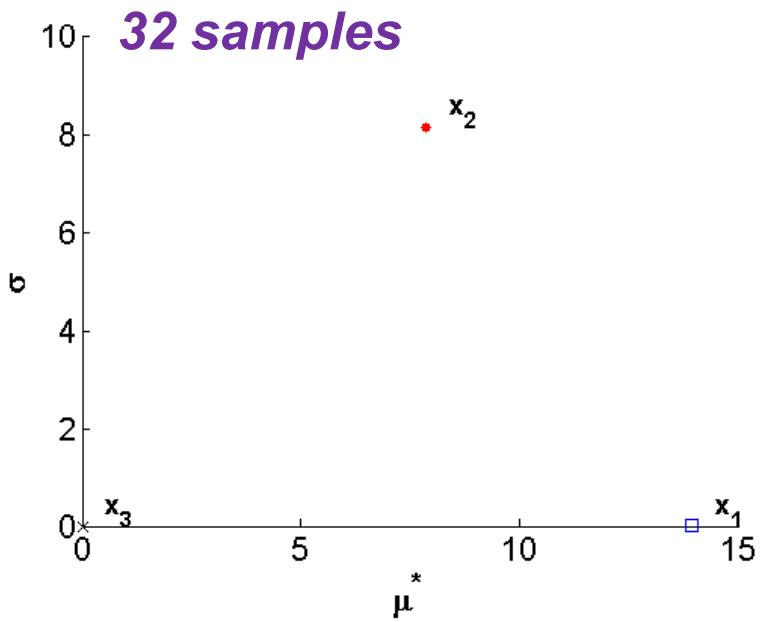
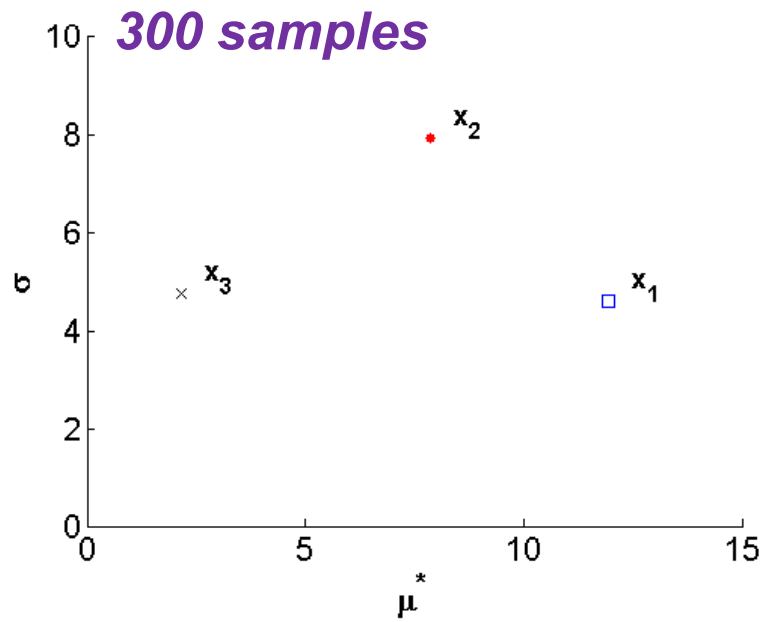
Morris OAT for Ishigami

	32 samples		300 samples	
	mod mean	std dev	mod mean	std dev
x1	13.95	0.00	11.95	4.61
x2	7.88	8.15	7.88	7.93
x3	0.00	0.00	2.17	4.76

- **Identifies parameters contributing to overall variation across parameter space (μ*) and those with different effect in different areas in parameter space (σ, measure of interactions/nonlinearity)**
- ***Can gain some insight even with few samples***





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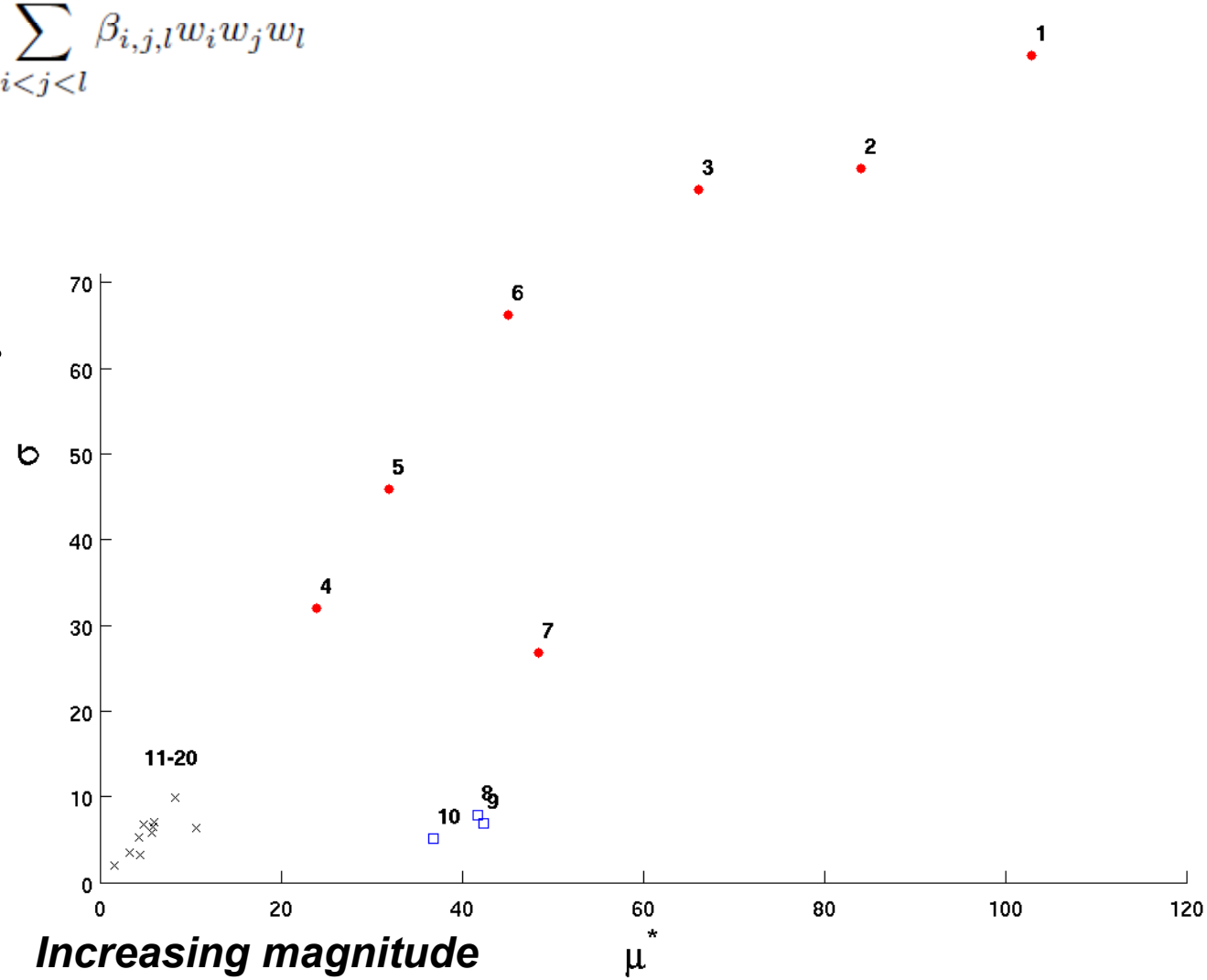
Morris Example

$$y = \beta_0 + \sum_{i=1}^{20} \beta_i w_i + \sum_{i<j}^{20} \beta_{i,j} w_i w_j + \sum_{i<j<l}^{20} \beta_{i,j,l} w_i w_j w_l + \sum_{i<j<l<s}^{20} \beta_{i,j,l,s} w_i w_j w_l w_s,$$

Increasing variability in elementary effects due to factor β_i



Increasing magnitude of elementary effects due to factor β_i

Good screening of 20 parameters with 84 samples

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Variance-Based Decomposition

- Identify fraction of output variance that can be attributed to an individual variable alone, or with interaction effects
- Sensitivity indices (Sobol); popularized by Saltelli, et al.

main effect (x_j alone); [0,1]

$$S_j = \frac{V(E(Y \mid X_j))}{V(Y)}$$

total effect (with interactions)

$$T_j = \frac{E[Var(Y \mid X_{-j})]}{V(Y)}$$

(k-dimensional integrals)

- Benefit: sensitivity indices are model-free (not regression-based), global, and capture interactions
- Costly! Calculation typically sampling-based requiring (*k*+2)**N* points (*k* variables, *N* samples per replicate)
- Can accelerate with surrogates or PCE/SC

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Alternative: Meta-models (Response Surfaces)

- **Create two sample matrices (2*N* samples); build a meta-model, e.g., regression, spline, neural network, Kriging; feasible for moderately high dimension**
- **Calculate the remaining *k* matrices using the meta-model and compute VBD indices**
- **Further use of meta-models: repeat the process to obtain bootstrap estimates of the indices, generate confidence intervals on the indices *(measure of convergence)***
- **Exploration of various nonparametric regression models and Gaussian process models:**
  Implementation and Evaluation of Nonparametric Regression Procedures for Sensitivity Analysis of Computationally Demanding Models. **C.B. Storlie, L.P. Swiler, J.C. Helton, and C.J. Sallaberry.** ***Reliability Engineering and System Safety*** **Vol. 94, pp. 1735–1763, 2009.**

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Alternative: Stochastic Expansions

- Create polynomial approximation to response function
- Polynomial chaos expansions (PCE): known basis, compute coefficients

$$R = \sum_{j=0}^{P} \alpha_j \Psi_j(\boldsymbol{\xi})$$

$$\alpha_j = \frac{\langle R, \Psi_j \rangle}{\langle \Psi_j^2 \rangle} = \frac{1}{\langle \Psi_j^2 \rangle} \int_\Omega R\, \Psi_j\, \varrho(\boldsymbol{\xi})\, d\boldsymbol{\xi}$$

- (Lagrange) Stochastic collocation (SC): known coefficients, form interpolant

$$R = \sum_{j=1}^{N_p} r_j L_j(\boldsymbol{\xi})$$

- Form basis, then sample, calculate moments, probabilities, etc.
- Tailoring → fine-grained algorithmic control:
  - Synchronize PCE form with numerical integration
  - Optimal basis & Gauss pts/wts for arbitrary input PDFs
  - Anisotropic approaches: emphasize key dimensions
- h/p-adaptive collocation (FY10-12)

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Stochastic Expansions: Analytic Sensitivity Indices

- Stochastic expansion methods produce functional representations of stochastic variability (e.g. polynomial chaos expansion or stochastic collocation)

- Sudret 2008: sensitivity indices are analytic functions of the PCE
- Tang, et al., 2009: sensitivity indices as analytic functions of SC; implementation in DAKOTA

- Efficient: calculation of input sensitivities does not require additional function evaluations beyond those needed to construct the stochastic expansion

VBD with Sampling, Surrogate-based Sampling, PCE

Analytic values of T_i: 0.55, 0.45, 0.24

	LHS-based VBD			
	30*5 = 150 samples		300*5 = 1500 samples	
	S_i	T_i	S_i	T_i
x1	0.62	1.06	0.28	0.54
x2	0.25	0.17	0.47	0.51
x3	*-0.04*	0.17	0.03	0.27

	Surrogate with VBD			
	30 samples		300 samples	
	S_i	T_i	S_i	T_i
x1	0.56	0.85	0.31	0.49
x2	0.02	*-0.03*	0.45	0.39
x3	0.06	0.37	0.01	0.17

still under-resolved: need 1000s of samples

	quadrature order 3: 27 evals			quadrature order 7: 343 evals		
	S_i	T_i	local	S_i	T_i	local
x1	0.42	0.56	1.68	0.29	0.52	6.20
x2	0.44	0.44	0.00	0.48	0.48	0.00
x3	0.00	0.14	0.00	0.00	0.23	0.00
x1,x2	0.00			0.00		
x1,x3	0.14			0.23		
x2,x3	0.00			0.00		
x1,x2,x3	0.00			0.00		

(also get local sensitivities analytically)

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Key Points

- Typically care about global sensitivity, though local analysis may give a good approximation to it
- Global importance can be hard to assess
- Modest computational model evaluations can offer considerable insight
- With tailored surrogates, can accelerate calculation

Near-term Plans for NE Problems

- Examples here on algebraic function; summer 2010: Cyrus applying to coupled flux/burnup calculation
  - R-Z neutronics flux solver coupled to
  - Quasi-static point depletion code for coupled neutron/nuclide fields
  - Tracking 45 isotopes for fast reactor simulation
  - Compare global methods to ESM

- Future work (with Proctor, Abdel-Khalik, Eldred)
  - Hybrid approaches: linear SA/UQ for flux with loose ("network") coupling to nonlinear SA/UQ for depletion or T-H
  - Scalability in dimension, convergence detection, use of derivatives
  - Extend ESM to handle nonlinear phenomena; hybridize with global methods that sample in principal directions

Improve Scalability with Derivative Enhancement

PCE: linear regression with derivatives; gradients/Hessians add equations

$$\begin{bmatrix} \vdots & \vdots & & \vdots \\ \pi_{0,j}(\vec{\xi}_i) & \pi_{1,j}(\vec{\xi}_i) & \cdots & \pi_{P,j}(\vec{\xi}_i) \\ \frac{\partial \pi_{0,j}}{\partial \xi_1}(\vec{\xi}_i) & \frac{\partial \pi_{1,j}}{\partial \xi_1}(\vec{\xi}_i) & \cdots & \frac{\partial \pi_{P,j}}{\partial \xi_1}(\vec{\xi}_i) \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial \pi_{0,j}}{\partial \xi_{n_\xi}}(\vec{\xi}_i) & \frac{\partial \pi_{1,j}}{\partial \xi_{n_\xi}}(\vec{\xi}_i) & \cdots & \frac{\partial \pi_{P,j}}{\partial \xi_{n_\xi}}(\vec{\xi}_i) \\ \vdots & \vdots & & \vdots \end{bmatrix} \begin{pmatrix} \vdots \\ \vec{u}^{(m,j)} \\ \vec{u}^{(m+1,j)} \\ \vdots \\ \vec{u}^{(m+n_\xi,j)} \\ \vdots \end{pmatrix} = \begin{pmatrix} \vdots \\ \vec{u}_i \\ \frac{\partial \vec{u}_i}{\partial \xi_1} \\ \vdots \\ \frac{\partial \vec{u}_i}{\partial \xi_{n_\xi}} \\ \vdots \end{pmatrix}$$

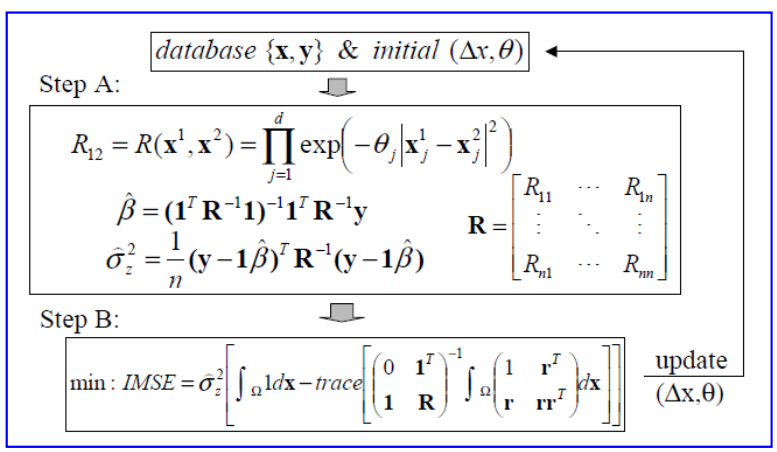
SC: enhanced interpolants

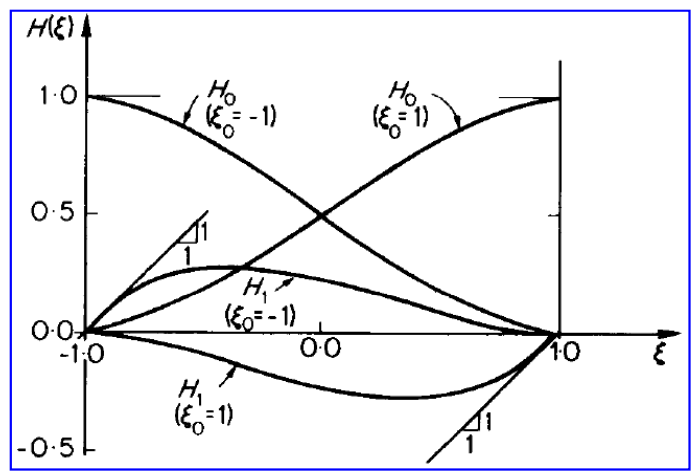
- cubic Lagrange splines (discretization → h-adaptive)
- Hermitian polynomials

$$a_j^i = 1 \text{ for } i = 1$$

$$a_j^i = \begin{cases} \prod_{\substack{l=j-1 \\ l \neq j}}^{j+2} \frac{x - x_l^i}{x_j^i - x_l^i} & \text{if } x \in \left[x_j^i, x_{j+1}^i\right], \quad j = 2, \ldots, m_i - 2 \\ \prod_{l=j+1}^{j+2} \frac{x - x_l^i}{x_j^i - x_l^i} & \text{if } x \in \left[x_j^i, x_{j+1}^i\right], \quad j = 1 \\ \prod_{\substack{l=j-1 \\ l \neq j}}^{j+1} \frac{x - x_l^i}{x_j^i - x_l^i} & \text{if } x \in \left[x_j^i, x_{j+1}^i\right], \quad j = m_i - 1 \\ 0 & \text{otherwise} \end{cases}$$

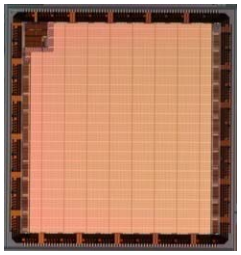
EGRA: gradient-enhanced Kriging interpolates function values and gradients





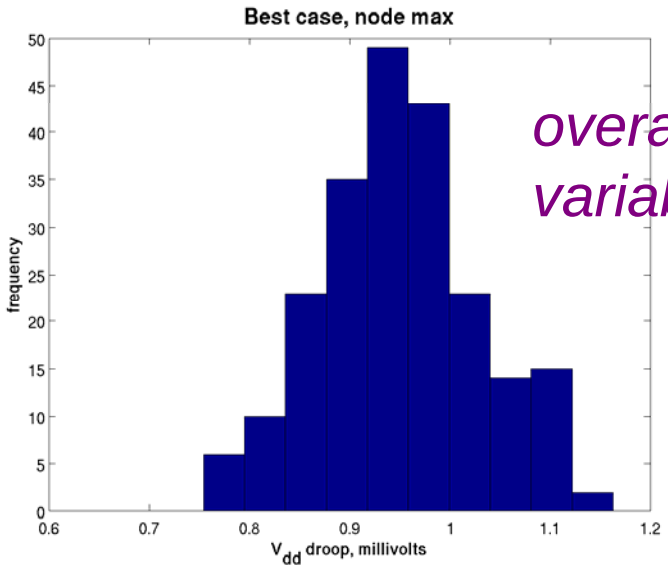
SA for Electrical Circuits

- **CMOS7 ViArray:** generic ASIC implementation platform; ***applications in NW, satellite, command & control***
- **Modeling and simulation used in design phase to assess predicted performance during photocurrent event, including sensitivity/variability of supply voltage**
- **DAKOTA coupled to Xyce circuit simulator to determine which process layers contributed most to device performance (1000s of simulation runs, each 2.0h to 4.5h)**



	Vdd Metrics	
	node max	node avg
METAL1	0.96	0.82
METAL2	0.11	0.04
METAL3	0.10	0.05
METAL4	0.80	0.81
METAL5	0.86	0.91
VIA1	0.71	0.66
VIA2	0.80	0.76
VIA3	0.57	0.60
VIA4	0.91	0.94
CONTACT	0.21	0.13
polyc	0.04	0.05

correlations



overall variability

Thank you for your attention!

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publicly available implementations of these and more algorithms:

http://www.cs.sandia.gov/dakota

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Abstract: Global Sensitivity Analysis

Global sensitivity methods assess the sensitivity of a computational model to inputs considered over their full parametric range. Global approaches are essential when dealing with nonlinear models, where linear/local methods could be misleading. They are typically used for parameter screening to determine factors for which to gather supplementary data, variables most important for optimization, calibration, or uncertainty quantification, or dimensions crucial to refine with adaptive methods. This talk will address both sample design and statistical analysis concerns for global sensitivity analysis, drawing from examples such as Latin hypercube sampling with linear and nonlinear regression, Morris screening designs and analysis, and stochastic expansion methods with Sobol indices.