SAND2016-XXXX

SAND2016-12250C

DAKOTA

CCR
Center for Computing Research

Sandia National Laboratories

Exceptional service in the national interest

A Survey of Probabilistic Uncertainty Propagation and Sensitivity Analysis Methods for Computational Applications

Laura Swiler and Vicente Romero
Sandia National Laboratories
Albuquerque, NM

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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.

Sources of uncertainty in computational models

1. Solution error uncertainty (associated with spatial and temporal discretizations and incomplete convergence of the discretized equations being solved)
2. Uncertainties in boundary or initial conditions
3. Uncertainties in model input parameters
4. Model form uncertainties (e.g. are we using the right model? Does the model incorporate the physics we need?)

This chapter addresses uncertainties in model input parameters where the uncertainties are continuous random variables described by probability distributions or probability density functions (PDFs).

Epistemic vs. Aleatory Uncertainty

- Aleatory uncertainty characterizes the inherent randomness or variability of a quantity.
  - Aleatory uncertainty is irreducible
  - Aleatory uncertainties are almost always characterized by probability distributions
- Epistemic uncertainty characterizes lack of knowledge
  - Epistemic uncertainties can be reduced through increased understanding (research), increased data, or more relevant data.
  - Epistemic uncertainties may be modeled with probability distributions or with intervals, fuzzy sets, Dempster-Shafer belief intervals, etc.

This chapter addresses propagation of both aleatory and epistemic uncertainties assuming the uncertainty is modeled with probability distributions.

Chapter Topics

1. **Sampling design**

   The design identifies how many computer runs will be conducted and what input parameter values will be associated with those samples.

2. **Sensitivity analysis**

   Identify important parameters that most contribute to the output uncertainty.

3. **Model response approximation**

   Response surface approximations (RSAs) are often used as inexpensive replacements – meta-models or *surrogates* for computationally expensive computer simulations.

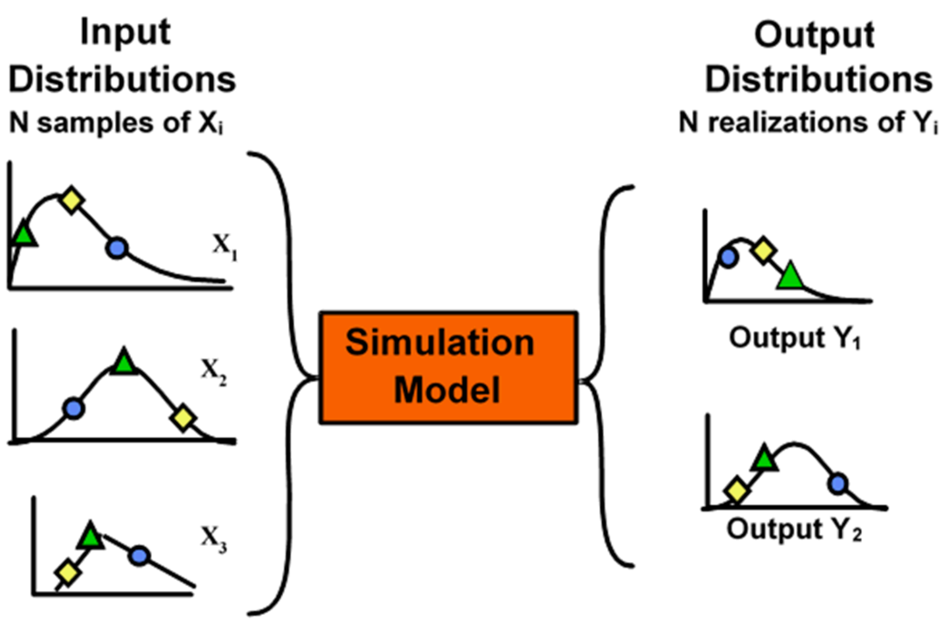
4. **Uncertainty propagation**

   Propagate uncertainty in input parameters to uncertainty in output quantities

   - Sampling
   - Reliability
   - Stochastic expansion

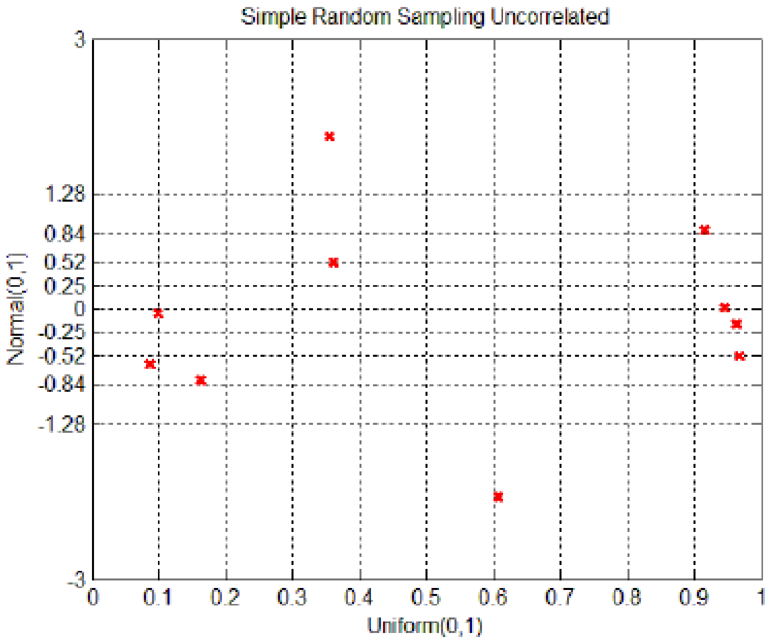
Sample Design

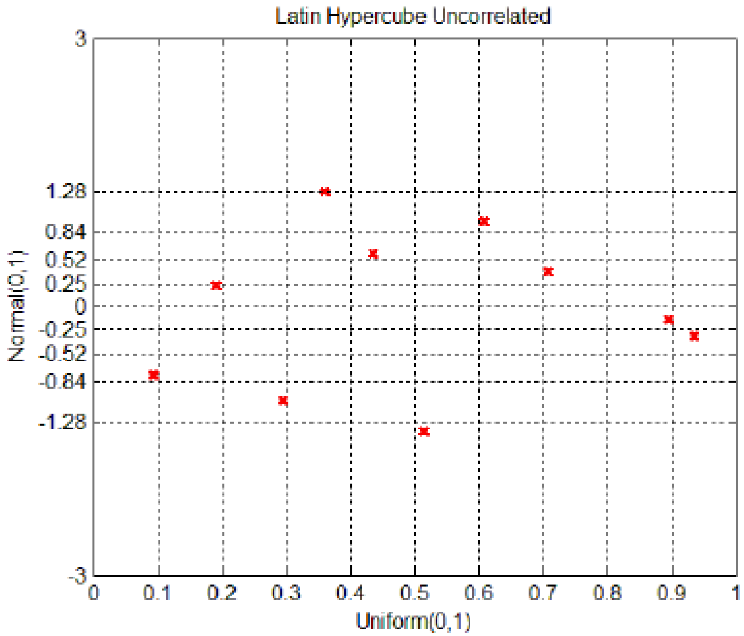
- Monte Carlo Random Sampling is a popular method
  - Generate samples from the input parameter distributions, run the simulation model at those points, generate distributions on the outputs
  - Easy to implement, easy to explain, reproducible
  - Produces unbiased estimates for means, variances and percentiles
  - Preferred when a sufficiently large number of samples are affordable
  - Drawback is the cost: to get accurate estimates of output statistics, a large number of samples is required.



Latin Hypercube Sampling

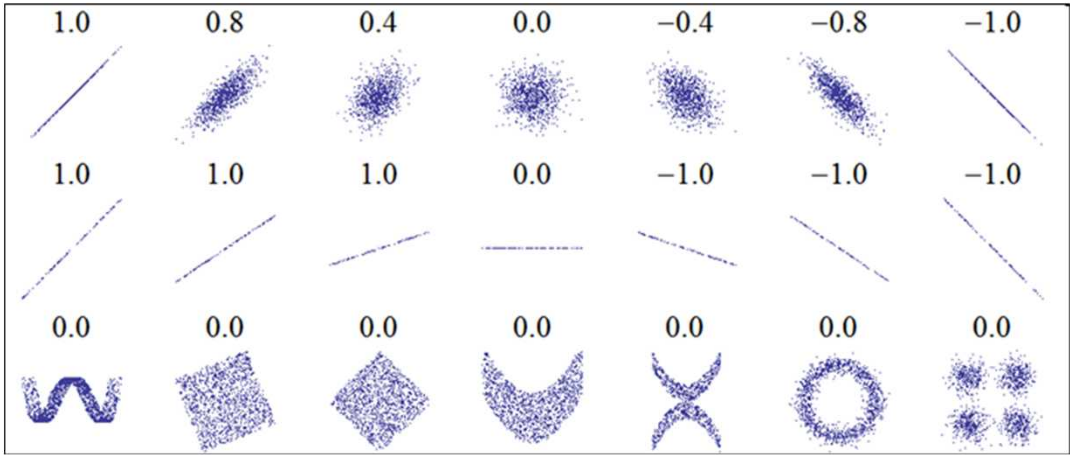
- Stratified Sampling method that decomposes the input into equi-probable strata and assigns one sample to each strata
  - Pairing algorithms for multi-dimensional inputs, to pair the samples for one input with samples from the other inputs to honor a specified correlation structure or (most commonly) ensure independent inputs: ONE SAMPLE IN EACH ROW AND COLUMN
  - Developed by Iman (SNL) and McKay (LANL) in late 1970s, heavily used at DOE labs
  - LHS requires fewer samples than plain Monte Carlo to achieve the same accuracy in statistics (standard error of the computed mean, for example).





Sensitivity Analysis

- Correlation analysis
  - Correlation between inputs and outputs
  - Discussion of simple, partial, rank correlation

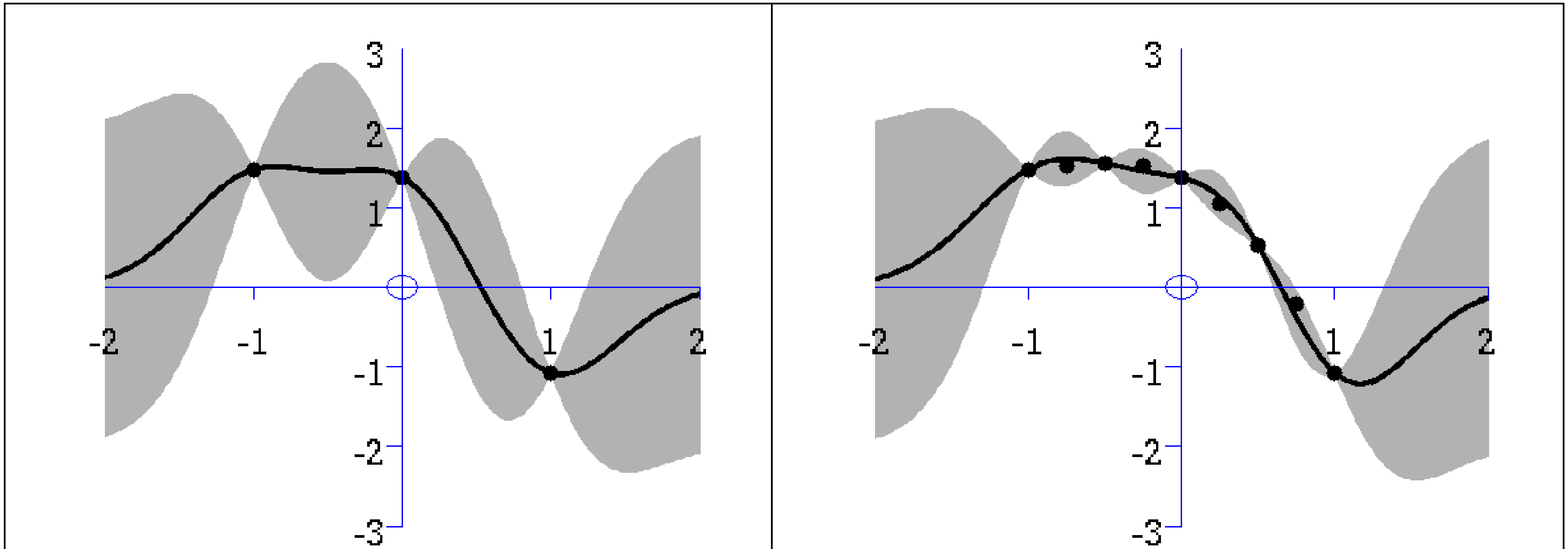


Example correlation relationships
Source:
http://en.wikipedia.org/wiki/Correlation

- Variance-based decomposition
  - Discussion of history of these approaches and computational methods for calculating the indices
  - Main effects indices, $\mathbf{S}_i$, identify the fraction of uncertainty in the output Y attributed to input X_i alone.
  - Total effects indices, $\mathbf{T}_i$, correspond to the fraction of the uncertainty in output Y attributed to X_i and its interactions with other variables.

Response Surface Approximations

- Gaussian Process Models
  - Popular emulators of computer models since 1990s (seminal paper by Sacks et al.)
  - They allow modeling of fairly complicated functional forms
  - They do not just offer a prediction at a new point but an estimate of the uncertainty in that prediction
  - Captures the idea that nearby inputs have highly correlated outputs.
  - The correlation in some dimensions may be more important than others…different “length-scales” in each dimension. This is defined by a correlation function in input space
  - Defined by a mean function and a covariance function: the mean interpolates the data



staffwww.dcs.shef.ac.uk

Response Surface Approximations

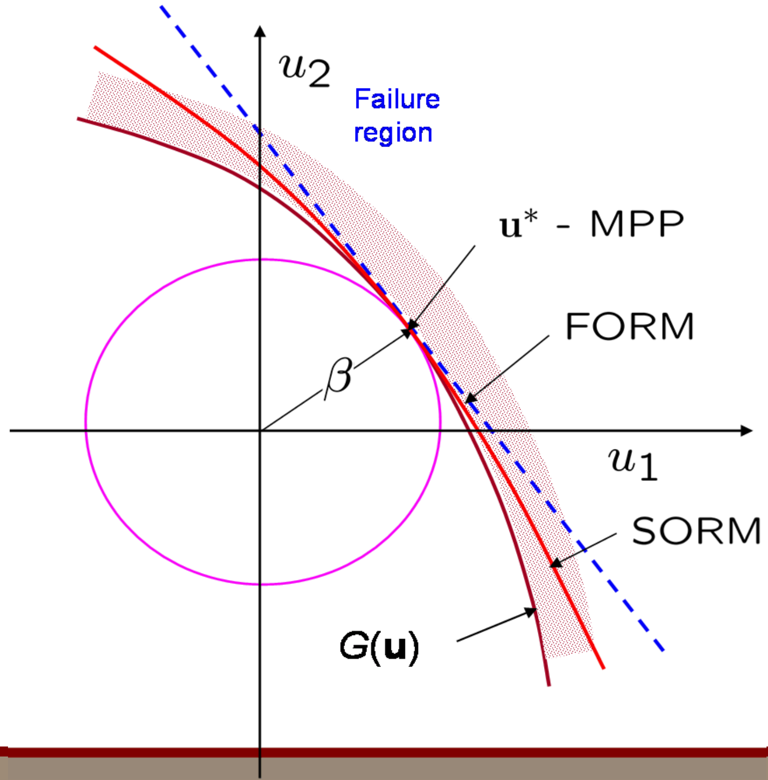
- Stochastic Expansion Methods (Polynomial Chaos Expansion, PCE)
  - PCE models a stochastic response as a function of uncertain input variables using carefully chosen polynomials.
    - Polynomials are chosen according to the Weiner-Askey scheme that provides an orthogonal basis with respect to the probability density function for the input random variables
    - For example, Hermite polynomials are used to model normal random variables

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

  - Structured sampling (typically tensor product grids or sparse grids) are used to estimate the uncertain coefficients α_j.
  - One advantage of stochastic expansions is that the moments of the response can be written analytically
  - Typically, stochastic expansions are more accurate and efficient than sampling if you can sufficiently resolve the order of the polynomials.
  - Have a "curse of dimensionality" issue when tensor grids are used but many approaches (compressive sensing) to address this.

Reliability Methods

- An optimization-based alternative that can be less computationally demanding than sampling techniques for certain types of UQ analysis.
- Often more efficient at computing statistics in the tails of the response distributions (events with low probability).
- Reliability methods address the question: Given a set of uncertain input variables X, and a scalar response function g, what is the probability that the response is below or above a certain level z?”



- Reliability methods involve a lot of assumptions and transformations.
- There use gradient-based optimization (local methods) and derivative-free optimization (global methods)
- We used a global reliability method called EGRA (Efficient Global Reliability Analysis]
- This method involves a GP surrogate

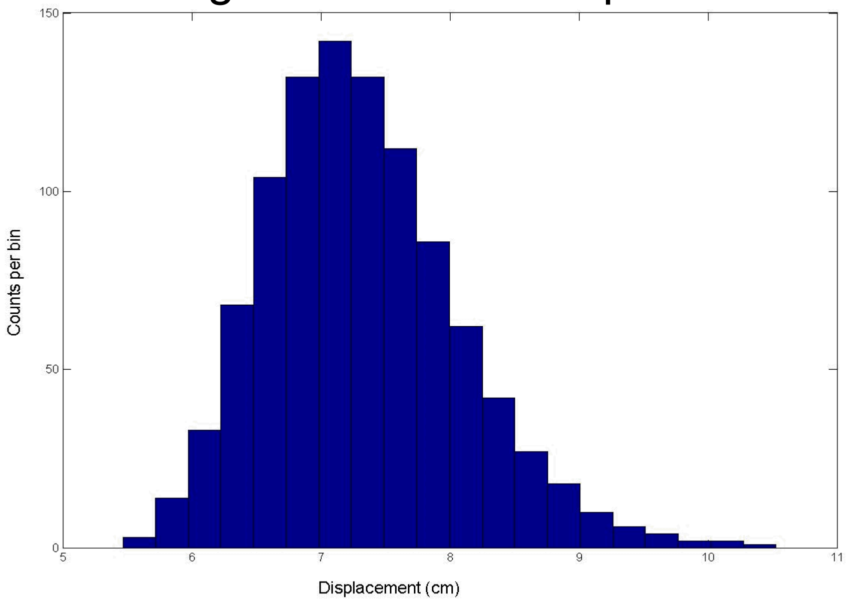
Example Problem: Cantilever Beam

- We provided to readers with the analytic function, values of parameters and their uncertainty
- Beam Deflection $D = PL^3/(3EI)$
- We demonstrated each of the uncertainty propagation methods (sampling, stochastic expansion, reliability, sampling on a surrogate) along with sensitivity analysis for each method
- Comparison CDFs and charts with summary statistics were also provided
- The next slides show a subset of the results

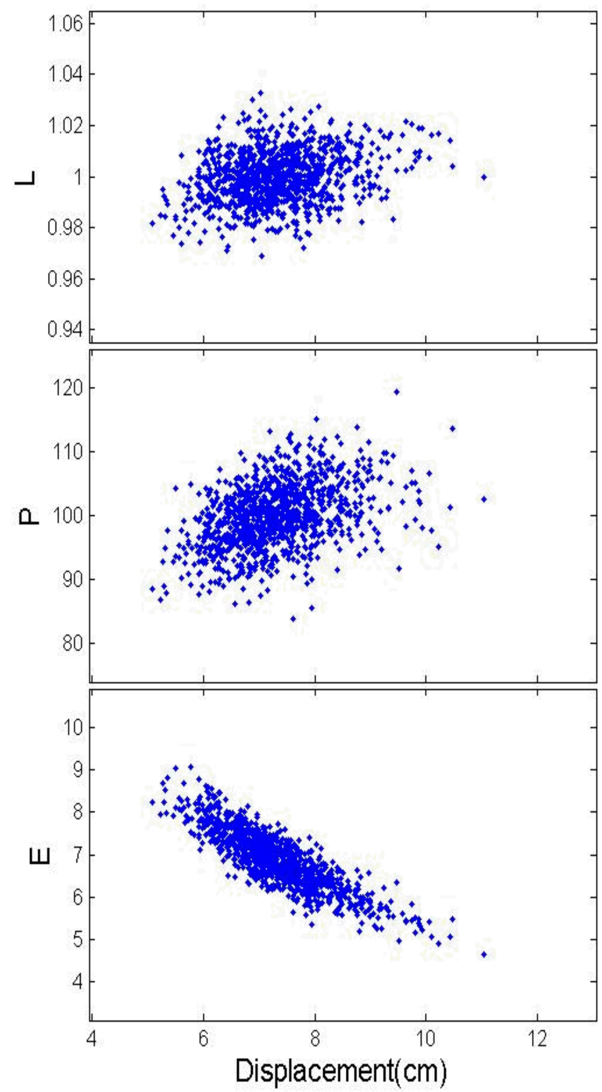
Variable	Distribution	Distribution Parameters
L	Normal	Mean = 1m Std. Dev. = 0.01 m
W	Fixed	1 cm
H	Fixed	2 cm
P	Normal	Mean = 100 N Std. Dev. = 5 N
E	Normal	Mean = 69 GPa Std. Dev. = 6.9 GPa

Cantilever Beam: Sampling Results

Histogram of 1000 Samples

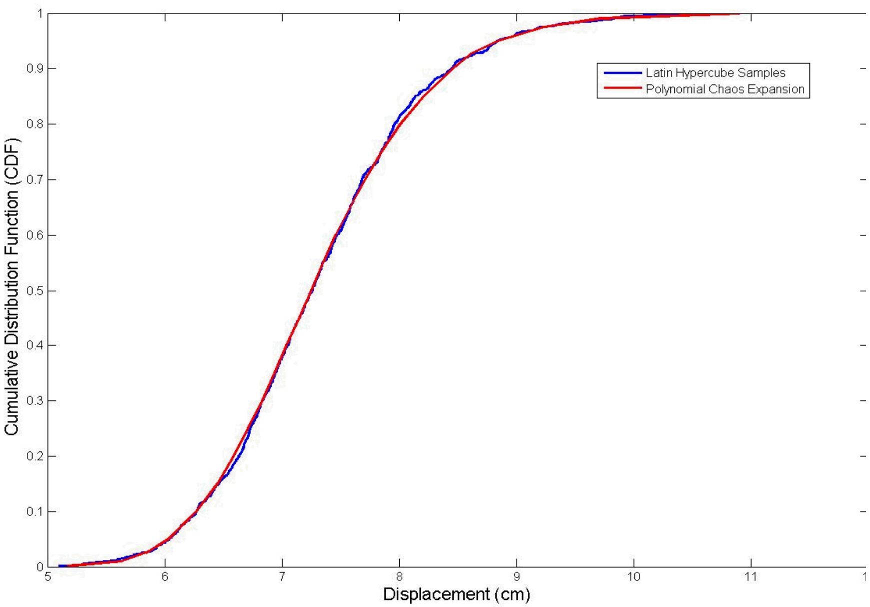


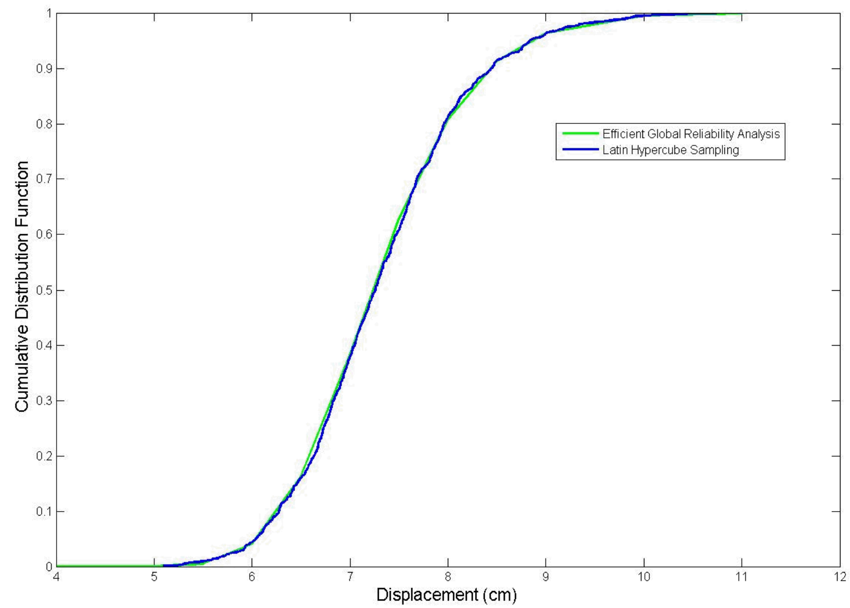
Scatterplots of inputs vs. D



INPUT	Simple Correlation wrt Displacement	Partial Correlation wrt Displacement
L	0.26	0.88
P	0.42	0.95
E	-0.86	-0.99

Cantilever Beam: CDF Comparisons





Cumulative Distribution Comparison of Sampling (Blue line, 1000 samples) vs. PCE (on left in red, 125 samples) vs. EGRA (on right in green, 29 samples)

Moment Comparisons across methods

	First Four Moments of Displacement (cm) Mean estimates from 100 iterations of methods			
Method	Mean	Std. Deviation	Skewness	Kurtosis
Gold Standard 10M Samples	7.323318	0.869388	57.163783	70.471190
LH Sampling	7.323235	0.869277	56.312778	68.359362
PCE	7.323328	0.869415	57.122174	69.576398
GP Surrogate	7.323313	0.869173	56.764502	67.385377

	Mean |% error| First Four Moments of Displacement (cm)			
Method	Mean	Std. Deviation	Skewness	Kurtosis
LH Sampling	0.0061%	0.430%	11.62%	38.93%
PCE	0.0001%	0.003%	0.07%	1.27%
GP Surrogate	0.0012%	0.107%	3.32%	12.46%

	Max |% error| First Four Moments of Displacement (cm)			
Method	Mean	Std. Deviation	Skewness	Kurtosis
LH Sampling	0.0251%	1.688%	44.88%	183.49%
PCE	0.0001%	0.003%	0.07%	1.27%
GP Surrogate	0.0044%	0.392%	11.79%	54.81%

Percentile Comparisons across methods

CDF Percentile	Gold Standard Mean Estimate 10M Samples	LH Sampling Mean Estimate	LH Sampling Max |% error|	PCE Mean Estimate	PCE Max |% error|	GP Surrogate Mean Estimate	GP Surrogate Max |% error|
0.001	5.196	5.152	11.50%	5.1915	2.66%	5.189	2.44%
0.01	5.621	5.612	2.81%	5.6176	0.81%	5.618	0.73%
0.025	5.841	5.848	1.44%	5.8392	0.56%	5.839	0.47%
0.05	6.039	6.042	1.37%	6.0365	0.51%	6.038	0.40%
0.1	6.279	6.279	1.05%	6.2790	0.26%	6.279	0.43%
0.15	6.449	6.447	0.78%	6.4493	0.32%	6.449	0.23%
0.2	6.589	6.586	0.78%	6.5889	0.26%	6.589	0.26%
0.25	6.713	6.709	0.83%	6.7128	0.21%	6.714	0.22%
0.3	6.826	6.822	0.65%	6.8268	0.20%	6.827	0.19%
0.35	6.934	6.931	0.76%	6.9352	0.25%	6.935	0.24%
0.4	7.039	7.036	0.60%	7.0400	0.27%	7.040	0.23%
0.45	7.143	7.139	0.81%	7.1441	0.23%	7.143	0.21%
0.5	7.247	7.244	0.76%	7.2481	0.21%	7.247	0.26%
0.55	7.354	7.350	0.76%	7.3546	0.20%	7.353	0.22%
0.6	7.465	7.463	0.67%	7.4651	0.18%	7.464	0.25%
0.65	7.582	7.579	0.71%	7.5818	0.21%	7.582	0.26%
0.7	7.709	7.711	0.75%	7.7082	0.21%	7.708	0.23%
0.75	7.849	7.848	0.68%	7.8493	0.22%	7.849	0.23%
0.8	8.011	8.008	0.66%	8.0099	0.26%	8.011	0.22%
0.85	8.205	8.198	1.00%	8.2051	0.29%	8.205	0.22%
0.9	8.461	8.462	1.37%	8.4620	0.28%	8.459	0.37%
0.95	8.866	8.871	1.57%	8.8650	0.46%	8.863	0.57%
0.975	9.243	9.238	2.18%	9.2400	0.63%	9.241	0.56%
0.99	9.718	9.696	2.93%	9.7173	1.03%	9.715	0.95%
0.999	10.853	10.685	6.91%	10.8100	3.51%	10.821	2.99%

Approaches for Propagation of Input PDF Uncertainties

Sandia National Laboratories

Structured Sampling based

Statistical Design of Experiments (DOEx)

- ○ sampling stencils of different fidelity levels through which estimates can be upgraded
- ○ final 1-step adaptive samples for upgrading *percentile* estimates

\+

Response Surface Approximations (RSAs) fitted to the samples:

- **Polynomial** RSAs with or w/out regression, e.g.
  - Linear, quadratic
  - MARS (Multivariate Adaptive Regression Splines)
- **Non-Parametric** RSAs with or w/out regression, e.g.
  - Kriging, Gaussian Processes (GPs)
  - Moving Least Squares (MLS)

Quadrature Methods (response statistics from summations of weighted response values at sample points)

- **Point Estimate Methods** (PEMS) with fixed low-order sampling plans for response PDF mean, std. dev., skew, kurtosis
- **Stochastic Expansion Methods** with upgradable-order and dimension-adaptive sampling stencils for response mean, std. dev., higher-order moments, CDF/percentiles
  - Stochastic Collocation (SC)
  - Polynomial Chaos Expansions (PCE)

Random Sampling based

Statistical Sampling

- Hammersley
- LHS
- Halton
- Simple-Random

'Uniform' Sampling over UQ Hypercube

Sampling methods for different circumstances:

- CVT
- LHS
- Halton

\+

Response Surfaces fit to the samples

Non-adaptive

Fit sample values on response axis:

- **PDFs** (full distributions)
  - **Sparse data or economical conservative approx. PDF**: Normal PDF fit to tolerance intervals
  - **Medium to high data**: Beta, Johnson, Lambda families or non-parametric kernel density methods
- **PDF Tail Modeling** for percentiles>10^{-5}. High data (>200 samples) fit w/ optimized Pareto distribution

Compute response statistics directly from samples

or

Fit sample points with a response surface and sample the response surface

Adaptive

- Importance Sampling
- Samples to maximize a criterion, such as D-optimality

Optimization-based Reliability Methods

specialized for nominal estimation of very low-probability response percentiles like $P_l < 10^{-4}$

- Iterative AMV$^+$ (Advanced Mean Value +)
- FORM (First-Order Reliability Method)
- SORM (Second-Order Reliability Method)
- EGRA (Efficient Global Reliability Analysis)
- Etc.

Chapter Summary

- Presented topics relating to how to propagate probabilistic distributions on input parameters through a simulation model
  - **Sampling design**
  - **Sensitivity analysis**
  - **Response Surface Approximations**
  - **Uncertainty Propagation Methods**
- Presented results on a cantilever beam example
  - **Comparison of deflection statistics (mean, variance, percentiles)**
  - **Comparison of sensitivity analysis results**
  - **Accuracy with respect to a gold standard**
- Flowchart summarizing options one can take
- Key references on all topics