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Uncertainty Quantification: Part 3

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Last time (January 2011)
Uncertainty Quantification: Parts 1 and 2

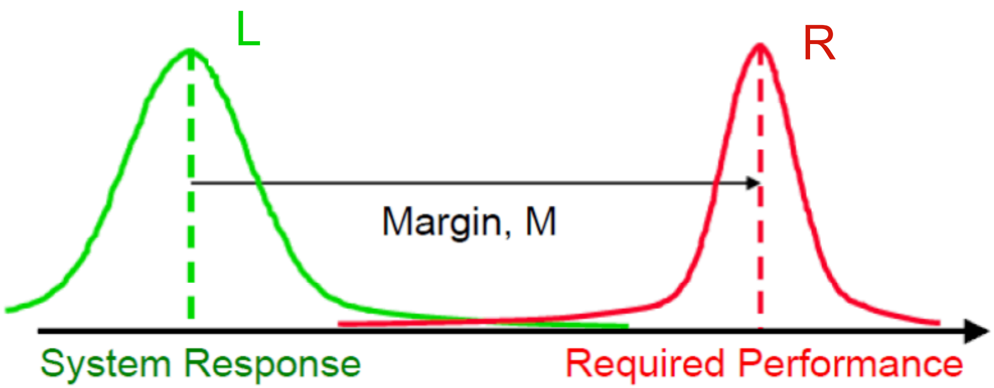
- Part 1:
  - Sampling methods:
    - Monte Carlo, Latin Hypercube
    - Adaptive Methods: Importance Sampling
  - Sensitivity analysis:
    - Scatterplots, correlation analysis (simple, partial, rank)
    - Variance-based methods
    - Surrogate methods
- Part 2:
  - Surrogate Methods
    - Stochastic Expansion: Polynomial Chaos/Stochastic Collocation
    - Gaussian Process Models
  - Epistemic/Aleatory Distinction
    - History
    - Approaches

This time (November 2011) Uncertainty Quantification: Part 3

- Part 3:
  - Reliability Methods
    - Limit state surface
    - Optimization approaches (local/global)
  - Kelly/Swiler analysis of surrogates
  - Next steps
    - Reliability methods
    - Importance sampling

Safety Factors

- Much of the early work on engineering reliability comes from the civil engineering field, concerned with reliability of structures
- In this lecture, the notation of L = load, R = resistance, we want L < R
- Nominal safety factor: $SF = R_{nom}/L_{nom}$, where $R_{nominal}$ is usually a conservative value (e.g. 2-3 standard deviations below the mean) and $L_{nominal}$ is also a conservative value (2-3 standard deviations above the mean)
- Problem: the nominal safety factor may not convey the true margin of safety in a design



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Probability of Failure

$$p_f = P(failure) = P(R < L)$$

$$p_f = \int_0^{\infty} \left[\int_0^{l} f_R(r)dr \right] f_L(l)dl$$

$$p_f = \int_0^{\infty} F_R(l) f_L(l)dl$$

In practice, this integration is hard to perform and doesn't always have an explicit form, except in some special cases

Probability of Failure

- Special Case: $R \sim N(\mu_R, \sigma_R)$, $L \sim N(\mu_L, \sigma_L)$
- Define $Z = R - L$

$$p_f = P(failure) = P(Z < 0)$$

$$p_f = \Phi\left[\frac{0 - (\mu_R - \mu_L)}{\sqrt{\sigma_R^2 + \sigma_L^2}}\right]$$

$$p_f = 1 - \Phi\left[\frac{(\mu_R - \mu_L)}{\sqrt{\sigma_R^2 + \sigma_L^2}}\right]$$

- There are also modifications which treat multiple loads, or lognormal distributions (Haldar and Mahadevan)

Reliability Analysis

- Assume that the probability of failure is based on a specific performance criterion which is a function of random variables, denoted X_i.
- The performance function is described by Z:

  $Z = g(X_1, X_2, X_3, \ldots, X_n)$
- The failure surface or limit state is defined as Z = 0. It is a boundary between safe and unsafe regions in a parameter space.
- Now we have a more general form of $P_{failure}$

$$p_f = P(failure) = P(Z < 0)$$

$$p_f = \int \ldots \int_{g() < 0} f_X(x_1, x_2, \ldots, x_n) dx_1 dx_2 \ldots dx_n$$

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Reliability Analysis

- Note that the failure integral has the joint probability density function, f, for the random variables, and the integration is performed over the failure region

$$p_f = \int \cdots \int_{g() < 0} f_X(x_1, x_2, \ldots, x_n) dx_1 dx_2 \ldots dx_n$$

- If the variables are independent, we can replace this with the product of the individual density functions
- In general, this is a multi-dimensional integral and is difficult to evaluate.
- People use approximations. If the limit state is a linear function of the inputs (or is approximated by one), first-order reliability methods (FORM) are used.
- If the nonlinear limit state is approximated by a second-order representation, second-order reliability methods (SORM) are used.

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Mean Value Method (FOSM)

- Often called the First-Order Second-Moment (FOSM) method or the Mean Value FOSM method
- The FOSM method is based on a first-order Taylor series expansion of the performance function
- It is evaluated at the mean values of the random variables, and only uses means and covariances of the random variables
- The mean value method only requires one evaluation of the response function at the mean values of the inputs, plus *n* derivative values if one assumes the variables are independent → n+1 evaluations in the simplest approach (CHEAP!)

$$\mu_g = g(\mu_{\mathbf{x}})$$

$$\sigma_g^2 = \sum_{i=1}^{n} \sum_{i=1}^{n} Cov(i,j) \frac{dg}{dx_i}(\mu_{\mathbf{x}}) \frac{dg}{dx_j}(\mu_{\mathbf{x}})$$

$$\sigma_g^2 = \sum_{i=1}^{n} \left(\frac{dg}{dx_i}(\mu_{\mathbf{x}}) \right)^2 Var(x_i)$$

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Mean Value Method (FOSM)

- Introduce the idea of a safety index β (think of this as how far in "normal space" that your design is away from failure)

$$\beta = \frac{\mu_g}{\sigma_g}$$

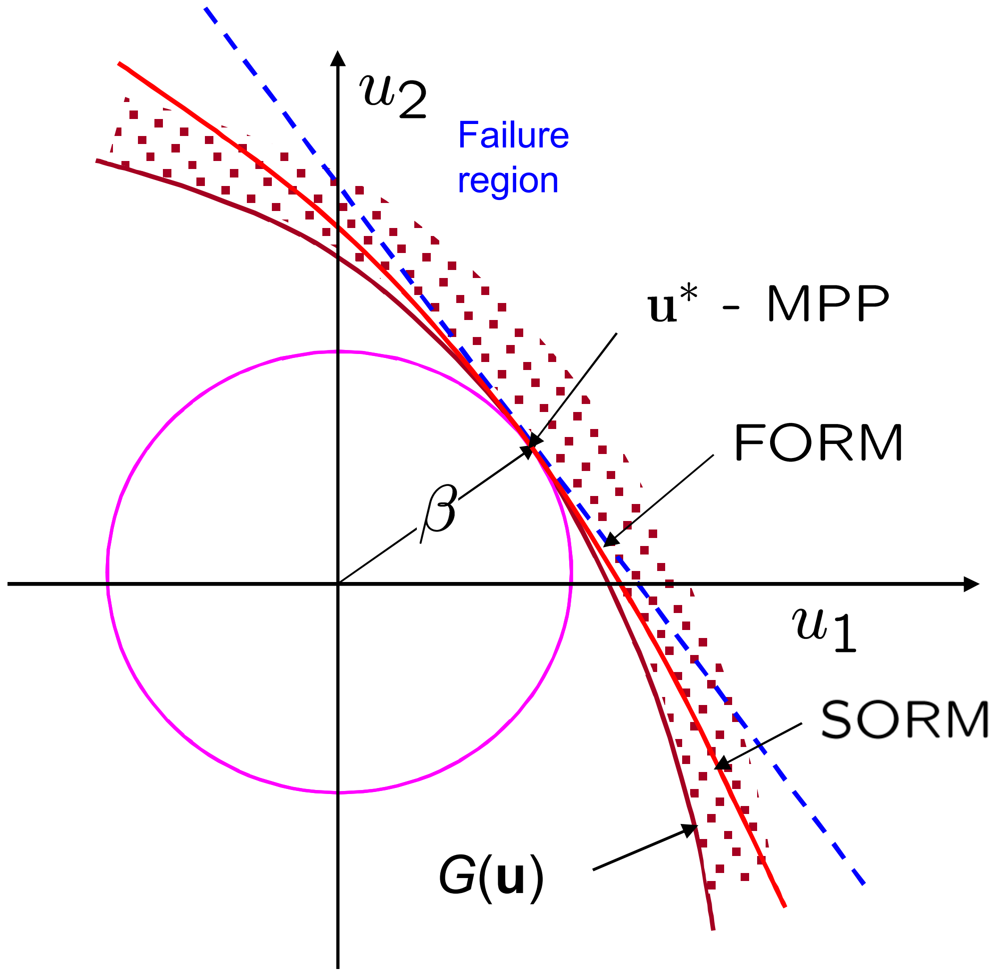
$$p_f = \Phi[-\beta] = 1 - \Phi[\beta]$$

- FOSM does not use distribution information when it is available
- When g(x) is nonlinear, significant error may be introduced by neglecting higher order terms in the expansion
- The safety index fails to be constant under different problem formulations
- It can be very efficient. When g(x) is linear and the input variables are normal, the mean value method gives exact results!

Most Probable Point Methods

- Transform the uncertainty propagation problem into an optimization one: first transform all of the non-normal random variables into independent, unit normal variables. Then, find the point on the limit state surface with minimum distance to the origin.
- The point is called the Most Probable Point (MPP). The minimum distance, β, is called the safety index or reliability index.
- X is often called the original space, U is the transformed space.

MPP Search Methods



Uncertainty Transformations

- Want to go from correlated non-normals to uncorrelated standard normals (*u*)
- Several methods
  - Rosenblatt
  - Rackwitz-Fiesler
  - Chen-Lind
  - Wu-Wirshing
  - Nataf
- Rosenblatt: First transform a set of arbitrarily, correlated random variables $X_1 \ldots X_n$ to uniform distributions, then transform to independent normals.
- Nataf: First transform to correlated normals (*z*), then to independent normals *u*. L is the Cholesky factor of the correlation matrix

$$
\begin{aligned}
U_1 &= F_{X_1}(X_1) \\
U_2 &= F_{X_2|X_1}(X_2 \mid x_1) \\
&\ldots \\
U_n &= F_{X_n|X_1,X_2,\ldots}(X_n \mid x_1, x_2, \ldots x_{n-1})
\end{aligned}
$$

$$
\begin{aligned}
u_1 &= \Phi^{-1}(U_1) \\
u_2 &= \Phi^{-1}(U_2) \\
&\ldots \\
u_n &= \Phi^{-1}(U_n)
\end{aligned}
$$

$$\Phi(z_i) = F(x_i)$$

$$\mathbf{z} = \mathbf{L}\mathbf{u}$$

MPP Search Methods

<u>Reliability Index Approach (RIA)</u>

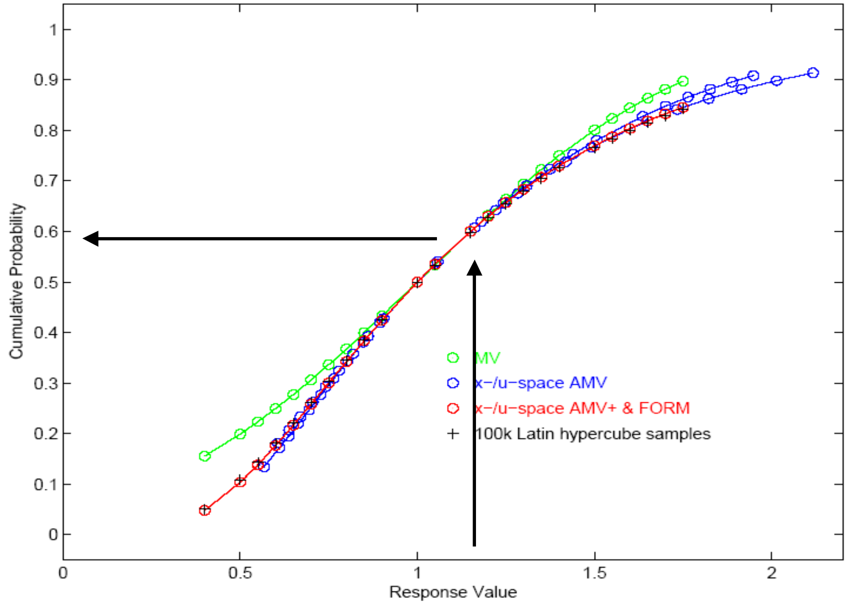
$$\text{minimize} \quad \mathbf{u}^T\mathbf{u}$$
$$\text{subject to} \quad G(\mathbf{u}) = \bar{z}$$

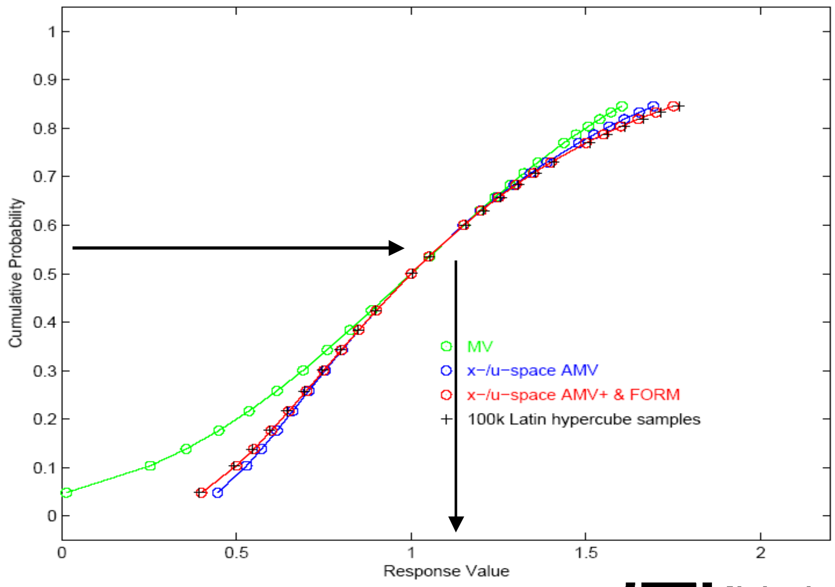
Find min dist to *G* level curve
Used for fwd map *z* → *p*/*β*

<u>Performance Measure Approach (PMA)</u>

$$\text{minimize} \quad \pm G(\mathbf{u})$$
$$\text{subject to} \quad \mathbf{u}^T\mathbf{u} = \bar{\beta}^2$$

Find min *G* at *β* radius
Used for inv map *p*/*β* → *z*





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Reliability Algorithm Variations: First-Order Methods

Limit state linearizations

AMV: $g(\mathbf{x}) = g(\mu_{\mathbf{x}}) + \nabla_x g(\mu_{\mathbf{x}})^T (\mathbf{x} - \mu_{\mathbf{x}})$

u-space AMV: $G(\mathbf{u}) = G(\mu_{\mathbf{u}}) + \nabla_u G(\mu_{\mathbf{u}})^T (\mathbf{u} - \mu_{\mathbf{u}})$

AMV+: $g(\mathbf{x}) = g(\mathbf{x}^*) + \nabla_x g(\mathbf{x}^*)^T (\mathbf{x} - \mathbf{x}^*)$

u-space AMV+: $G(\mathbf{u}) = G(\mathbf{u}^*) + \nabla_u G(\mathbf{u}^*)^T (\mathbf{u} - \mathbf{u}^*)$

FORM: no linearization

Integrations

1st-order: $\begin{cases} p(g \le z) = \Phi(-\beta_{cdf}) \\ p(g > z) = \Phi(-\beta_{ccdf}) \end{cases}$

MPP search algorithm

[HL-RF], Sequential Quadratic Prog. (SQP), Nonlinear Interior Point (NIP)

Warm starting

***When:* AMV+ iteration increment, *z*/*p*/β level increment, or design variable change**

***What:* linearization point & assoc. responses (AMV+) and MPP search initial guess**

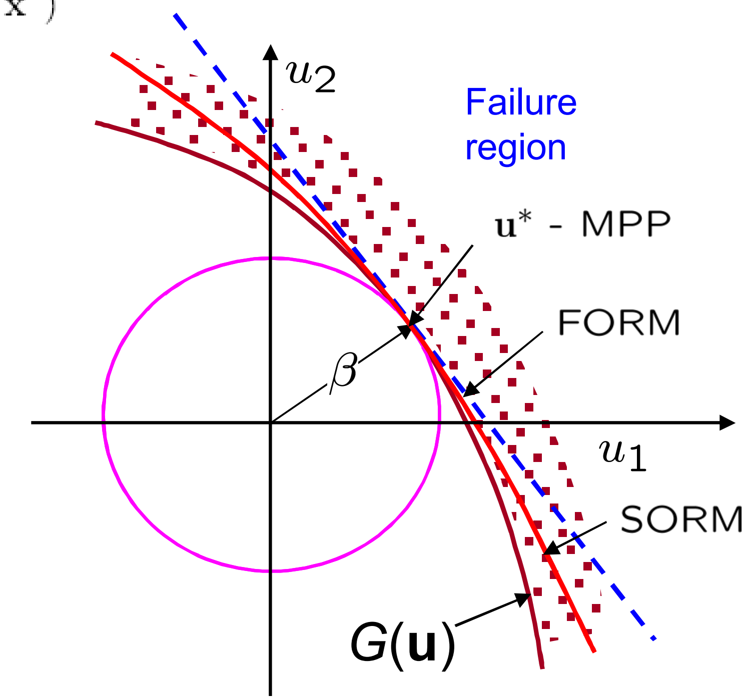
Reliability Algorithm Variations: Second-Order Methods

2nd-order local limit state approximations

- **e.g., x-space AMV²+:**

$$g(\mathrm{x}) \cong g(\mathrm{x}^*) + \nabla_x g(\mathrm{x}^*)^T(\mathrm{x}-\mathrm{x}^*) + \frac{1}{2}(\mathrm{x}-\mathrm{x}^*)^T \nabla_x^2 g(\mathrm{x}^*)(\mathrm{x}-\mathrm{x}^*)$$

- **Hessians may be full/FD/Quasi**
- **Quasi-Newton Hessians may be BFGS**



2nd-order integrations

$$p = \Phi(-\beta) \prod_{i=1}^{n-1} \frac{1}{\sqrt{1+\beta\kappa_i}}$$

curvature correction

Synergistic features:

Hessian data needed for SORM integration can enable more rapid MPP convergence

[QN] Hessian data accumulated during MPP search can enable more accurate probability estimates

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Reliability Algorithm Variations: Second-Order Methods

Multipoint limit state approximations

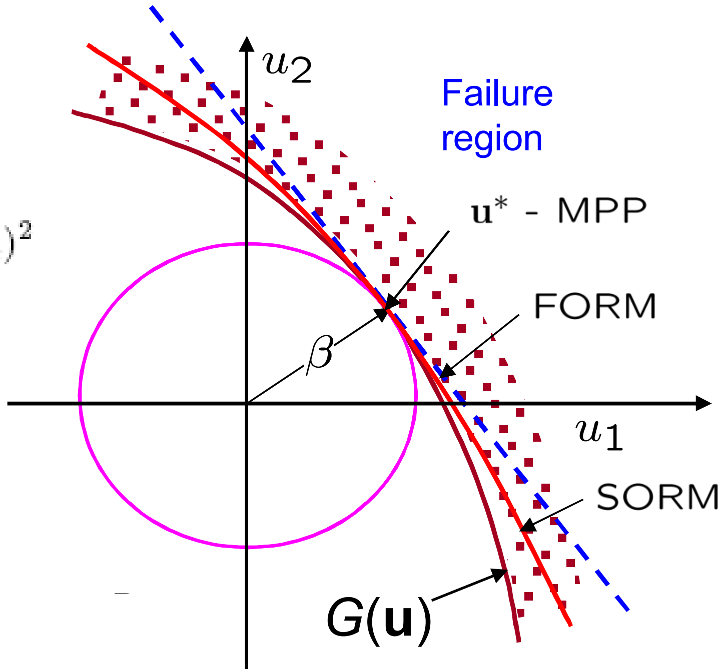
- **e.g., TPEA, TANA:**

$$g(\mathrm{x}) \cong g(\mathrm{x}_2) + \sum_{i=1}^{n} \frac{\partial g}{\partial x_i}(\mathrm{x}_2)\frac{x_{i,2}^{1-p_i}}{p_i}(x_i^{p_i} - x_{i,2}^{p_i}) + \frac{1}{2}\epsilon(\mathrm{x})\sum_{i=1}^{n}(x_i^{p_i} - x_{i,2}^{p_i})^2$$

$$p_i = 1 + \ln\left[\frac{\frac{\partial g}{\partial x_i}(\mathrm{x}_1)}{\frac{\partial g}{\partial x_i}(\mathrm{x}_2)}\right] \Big/ \ln\left[\frac{x_{i,1}}{x_{i,2}}\right]$$

$$\epsilon(\mathrm{x}) = \frac{H}{\sum_{i=1}^{n}(x_i^{p_i} - x_{i,1}^{p_i})^2 + \sum_{i=1}^{n}(x_i^{p_i} - x_{i,2}^{p_i})^2}$$

$$H = 2\left[g(\mathrm{x}_1) - g(\mathrm{x}_2) - \sum_{i=1}^{n}\frac{\partial g}{\partial x_i}(\mathrm{x}_2)\frac{x_{i,2}^{1-p_i}}{p_i}(x_{i,1}^{p_i} - x_{i,2}^{p_i})\right]$$



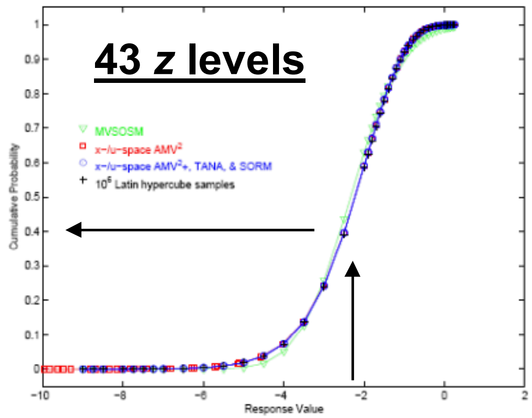
Importance Sampling

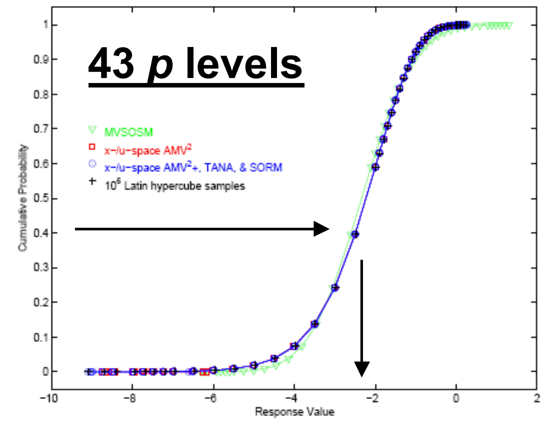
Use of importance sampling to calculate prob of failure:

- After MPP is identified, sample around MPP to estimate P_f more accurately

Reliability Algorithm Variations: Sample Results

Analytic benchmark test problems: lognormal ratio, short column, cantilever



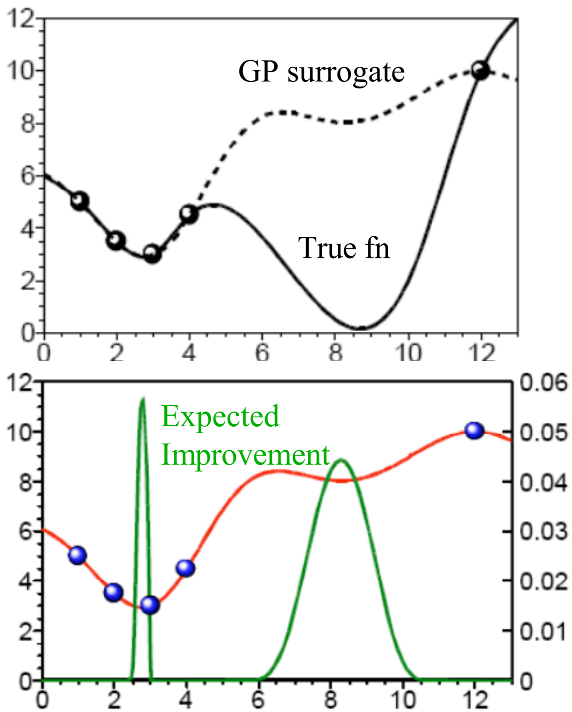


RIA Approach	SQP Function Evaluations	NIP Function Evaluations	CDF p Error Norm	Target z Offset Norm
MVFOSM	1	1	0.1548	0.0
MVSOSM	1	1	0.1127	0.0
x-space AMV	45	45	0.009275	18.28
u-space AMV	45	45	0.006408	18.81
x-space AMV^2	45	45	0.002063	2.482
u-space AMV^2	45	45	0.001410	2.031
x-space AMV+	192	192	0.0	0.0
u-space AMV+	207	207	0.0	0.0
x-space AMV^2+	125	131	0.0	0.0
u-space AMV^2+	122	130	0.0	0.0
x-space TANA	245	246	0.0	0.0
u-space TANA	296*	278*	6.982e-5	0.08014
FORM	626	176	0.0	0.0
SORM	669	219	0.0	0.0

PMA Approach	SQP Function Evaluations	NIP Function Evaluations	CDF z Error Norm	Target p Offset Norm
MVFOSM	1	1	7.454	0.0
MVSOSM	1	1	6.823	0.0
x-space AMV	45	45	0.9420	0.0
u-space AMV	45	45	0.5828	0.0
x-space AMV^2	45	45	2.730	0.0
u-space AMV^2	45	45	2.828	0.0
x-space AMV+	171	179	0.0	0.0
u-space AMV+	205	205	0.0	0.0
x-space AMV^2+	135	142	0.0	0.0
u-space AMV^2+	132	139	0.0	0.0
x-space TANA	293*	272	0.04259	1.598e-4
u-space TANA	325*	311*	2.208	5.600e-4
FORM	720	192	0.0	0.0
SORM	535	191*	2.410	6.522e-4

Efficient Global Reliability Analysis (EGRA)

- Address known failure modes of local reliability methods:
  - Nonsmooth: fail to converge to an MPP
  - Multimodal: only locate one of several MPPs
  - Highly nonlinear: low order limit state approxs. fail to accurately estimate probability at MPP
- Based on EGO (surrogate-based global opt.), which exploits special features of GPs
  - Mean and variance predictions: formulate expected improvement (EGO) or expected feasibility (EGRA)
  - Balance explore and exploit in computing an optimum (EGO) or locating the limit state (EGRA)



From Jones, Schonlau, Welch, 1998

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Efficient Global Reliability Analysis (EGRA)

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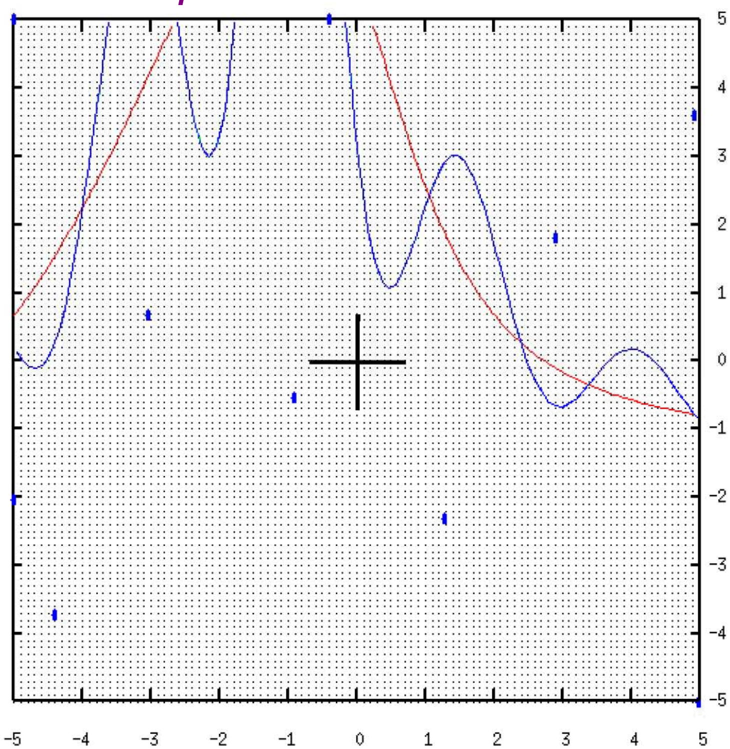
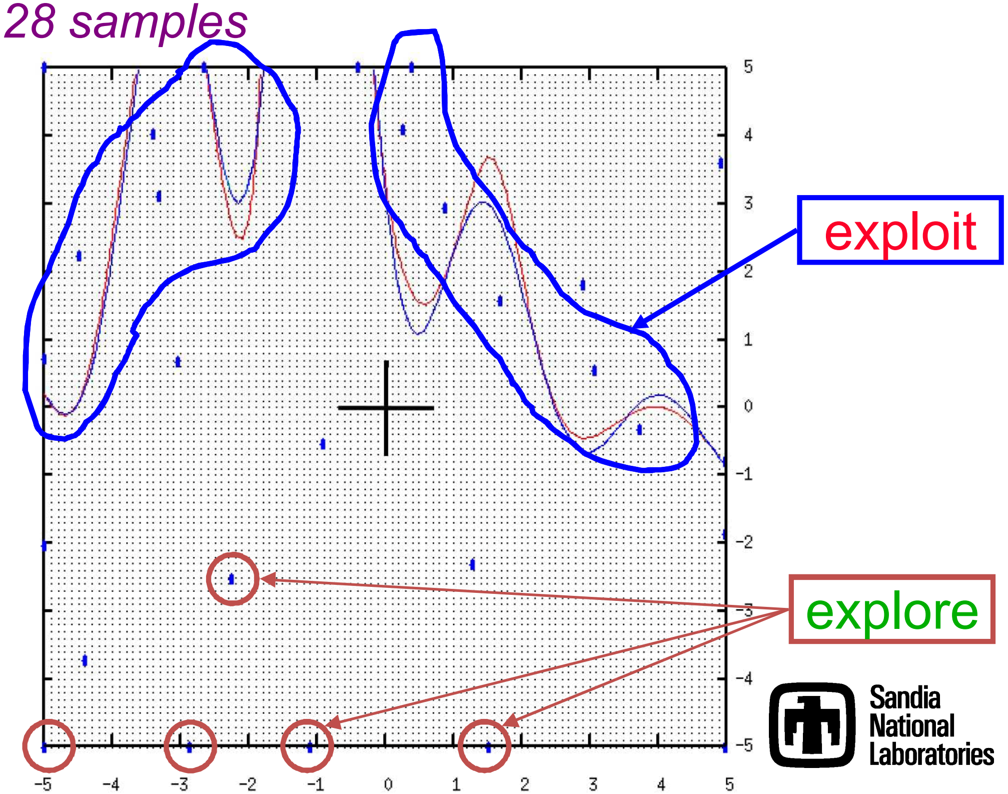
10 samples



28 samples



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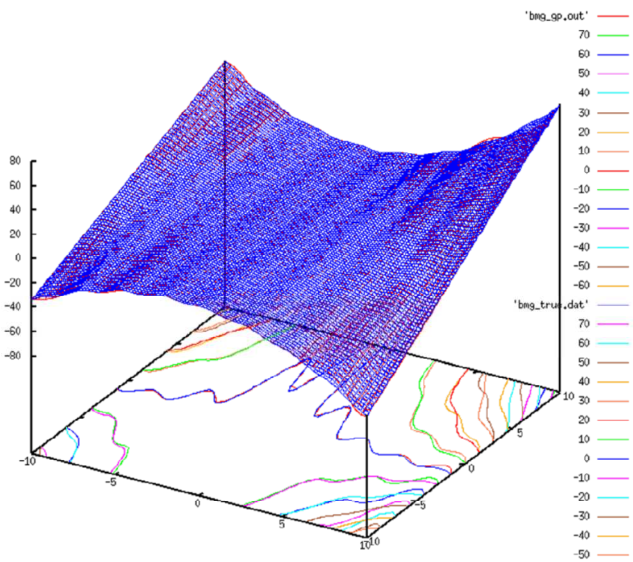
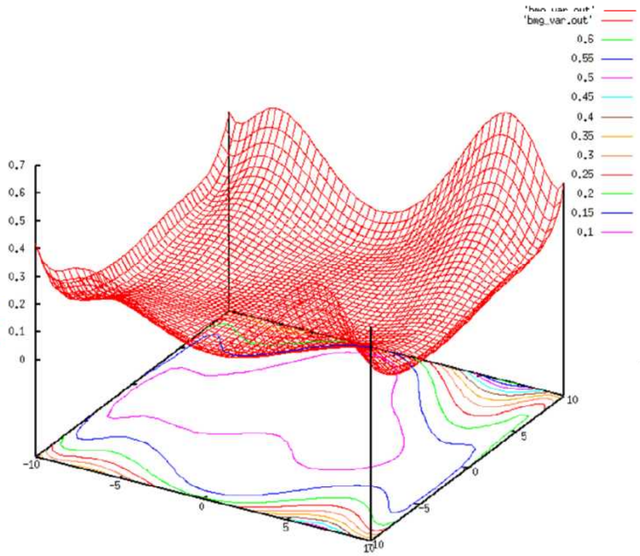
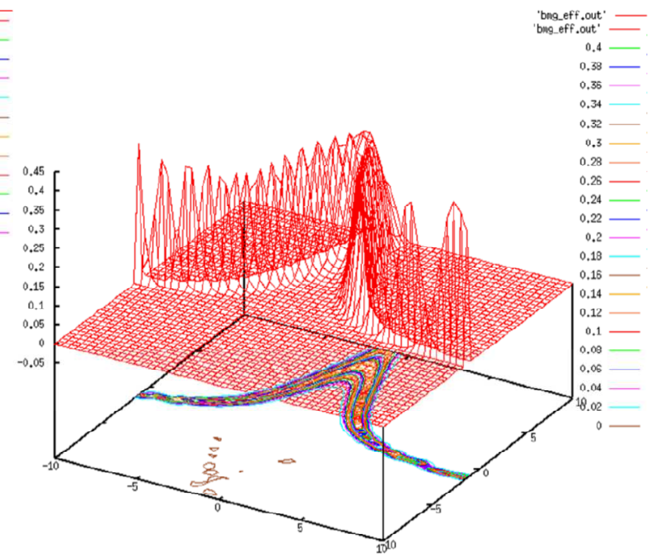
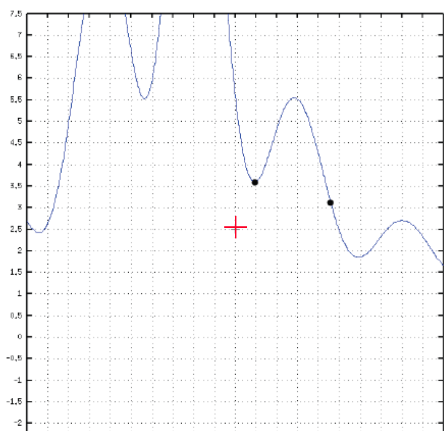
Efficient Global Reliability Analysis (EGRA)

Mean | Variance | Expected Feasibility









Reliability Method	Function Evaluations	First-Order p_f (% Error)	Second-Order p_f (% Error)	Sampling p_f (% Error, Avg. Error)
No Approximation	70	0.11797 (277.0%)	0.02516 (-19.6%)	—
x-space AMV^2+	26	0.11797 (277.0%)	0.02516 (-19.6%)	—
u-space AMV^2+	26	0.11777 (277.0%)	0.02516 (-19.6%)	—
u-space TANA	131	0.11797 (277.0%)	0.02516 (-19.6%)	—
LHS solution	10k	—	—	0.03117 (0.385%, 2.847%)
LHS solution	100k	—	—	0.03126 (0.085%, 1.397%)
LHS solution	1M	—	—	0.03129 (truth , 0.339%)
x-space EGRA	35.1	—	—	0.03134 (0.155%, 0.433%)
u-space EGRA	35.2	—	—	0.03133 (0.136%, 0.296%)

Accuracy similar to exhaustive sampling at cost similar to local reliability assessment

References

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- Li, J., Li, J. and D. Xiu. "An Efficient Surrogate-based Method for Computing Rare Failure Probability" *Journal of Computational Physics*, 2011.
- RIAC (Reliability Information Analysis Center): DoD site with useful information, guides on failure rates, accepted practices, etc.: http://www.theriac.org/

Surrogate Exercise

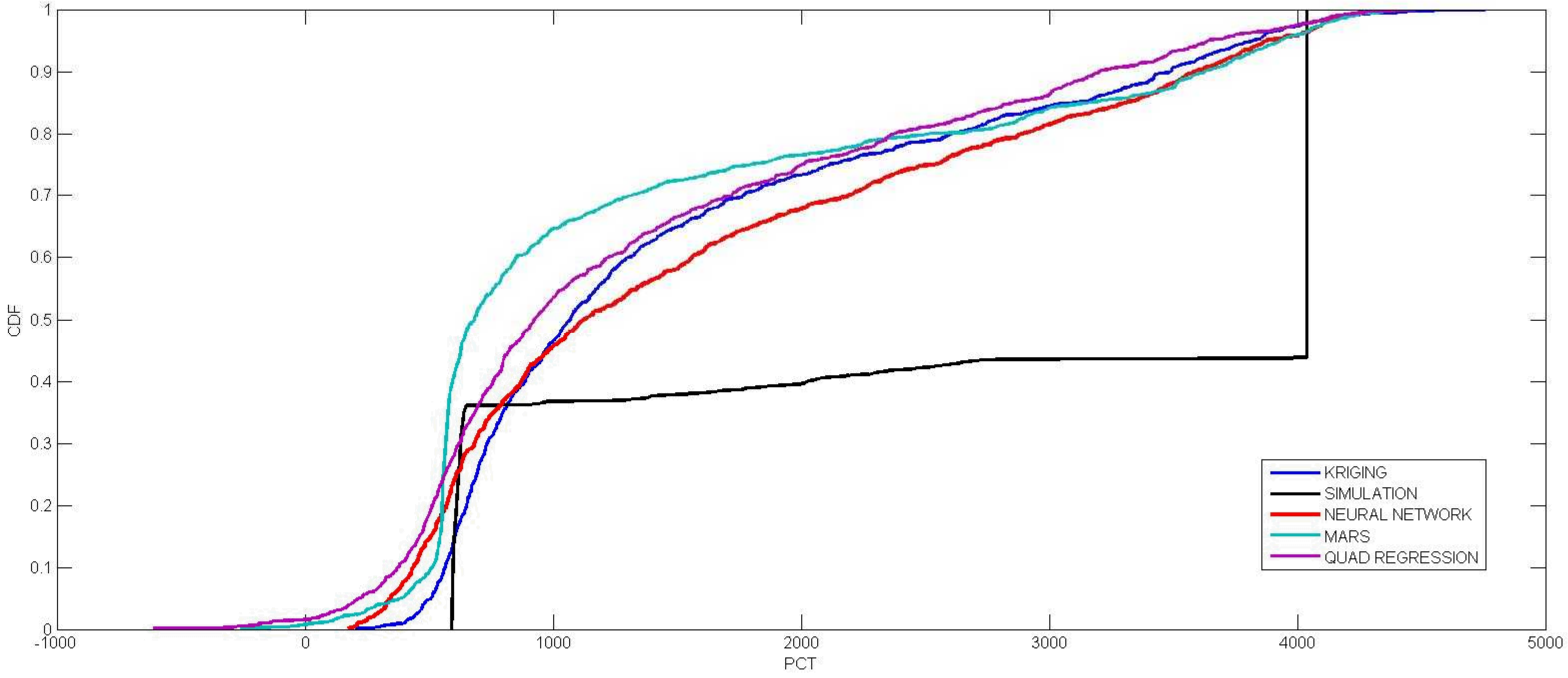
- MAAP data provided by Rick Sherry
- 7 inputs, PCT output
- Example Data Points:

1.743111057	182799.5467	0.955967773	0.988974257	12214102556	1.941626994	0.542751523	4040
5.462543971	210542.5794	0.923124154	0.992020895	7328733829	2.591832158	1.378279799	626.65
2.674710746	237825.6961	1.020738132	0.951296806	12324543052	0.939464609	1.700512893	2058.8
3.329309419	208744.735	0.883249726	1.021922709	12334040643	1.330167851	0.291383003	4040
1.715799521	183364.9316	1.04383727	0.963999398	12175622386	1.771614952	0.266097902	4040
2.304336794	188262.2584	0.984127727	1.048833468	12200355093	3.053181734	0.459711939	4040
6.585511973	209736.5804	1.041076319	1.024155978	12136328119	2.05280482	1.123557699	4040
4.293919875	219027.6166	0.904034142	1.010287086	11075618901	2.415474448	0.687599633	4040
2.106734623	232051.7923	0.992982254	1.000366752	11325441596	4.294646801	1.293444688	2332.05
2.262055459	203886.1326	1.018127502	0.968931448	5366045950	3.392389074	0.926106795	624.85

Bimodal Distribution on PCT

Surrogate Exercise

DAKOTA methods not able to match well



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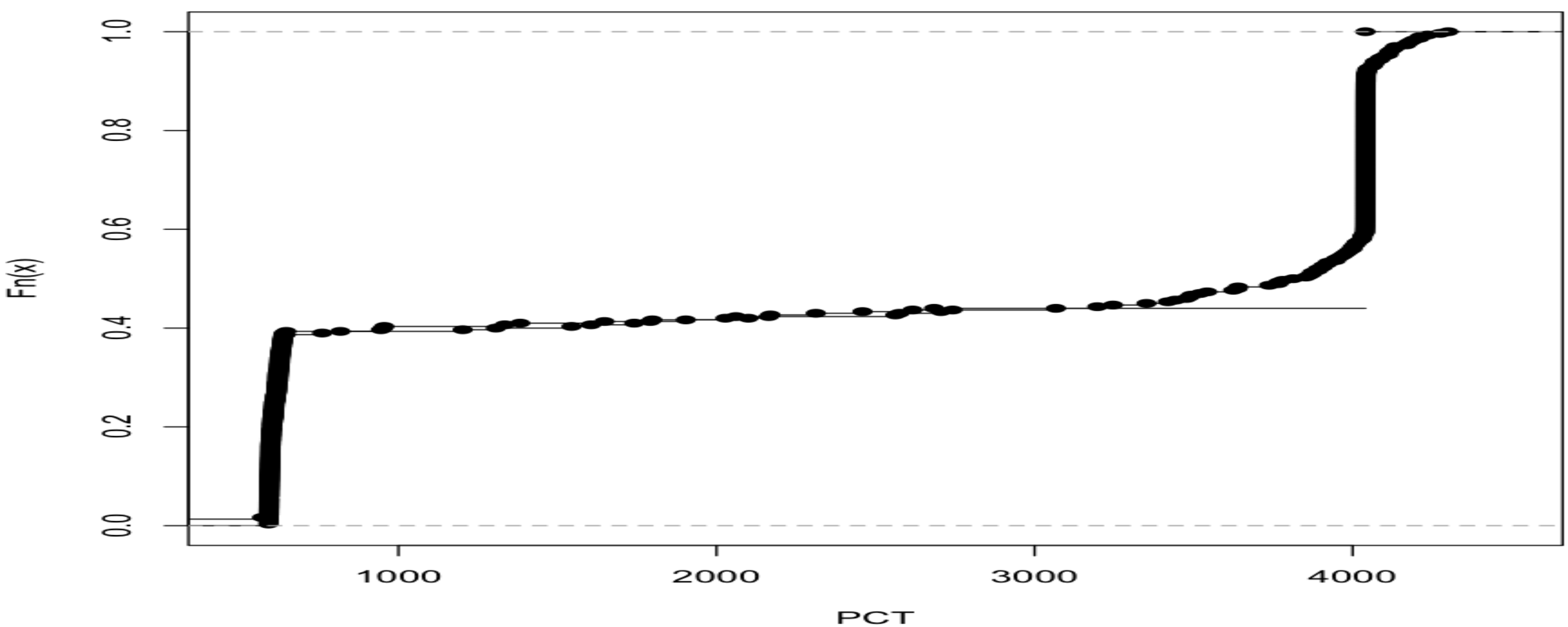
Surrogate Exercise

Treed Gaussian Process (TGP) does better because it generates separate GPs in different regions of space:



Surrogate Exercise

Overall RMSE error metrics when building on 700 points, predicting on 300:

Poly	NN	Kriging	Mars	TGP
398.88	368.86	300.92	374.85	300.00

TGP and kriging very similar…CDFs better with TGP.

Still need to investigate some issues (discuss).

DAKOTA Sensitivity Analysis

- Parameter study, design and analysis of computer experiments, and general sampling methods (heavy global focus):
  - Single and multi-parameter studies (grid, vector, centered)
  - DDACE (grid, sampling, orthogonal arrays, Box-Behnken, CCD)
  - FSUDACE (Quasi-MC, CVT)
  - PSUADE (Morris designs)
  - Monte Carlo, Latin hypercube sampling (with correlation or variance analysis, including variance-based decomposition)
  - Mean-value with importance factors
  - Stochastic expansion (PCE/SC) yielding Sobol indices

- DAKOTA outputs can include correlations, main/total effects, interaction effects; tabular output can be analyzed with any third-party statistics package
- Determine main effects and key parameter *interactions*
- In SA, typically no distribution assumption

DAKOTA UQ

- Techniques for propagating aleatory uncertainty (variables characterized by probability distributions) through models:
  - Latin hypercube (and other) sampling
  - Local reliability methods (mean value, MPP search, FORM, SORM)
  - Global reliability methods (EGRA)
  - Non-intrusive stochastic expansion methods (polynomial chaos and stochastic collocation)
  - *Reliability and importance sampling help with low probability events*
- Methods for epistemic uncertainty (variables characterized by intervals or basic probability assignments):
  - Local/global interval estimation
  - Local/global Dempster-Shafer evidence theory (belief/plausibility)
  - “Second-order” probability via sampling

- DAKOTA can output moments, probability of response thresholds, reliability metrics, response corresponding to a metric, etc.

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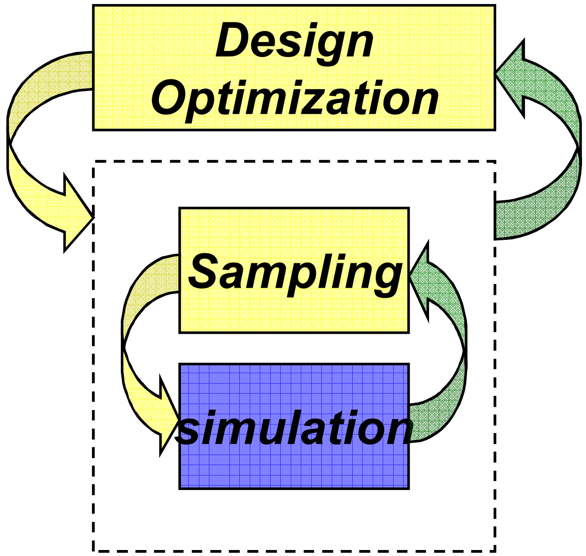
Extra Slides

Optimization under Uncertainty

- Design for reliability is a classic OUU problem, often called RBDO (reliability-based design optimization)
- Nice properties in that the reliability formulation itself generates quantities such as derivatives of performance function with respect to uncertain variables
- Variety of approaches (next page)
- Simplest case: think of a “nested” algorithm, with an optimization outer loop and sampling inner loop



RBDO Algorithms

Bi-level RBDO

- **Constrain RIA z → p/β result**
- **Constrain PMA p/β → z result**

RIA RBDO
$$\begin{cases} \text{minimize} & f \\ \text{subject to} & \beta \geq \bar{\beta} \\ \text{or} & p \leq \bar{p} \end{cases}$$

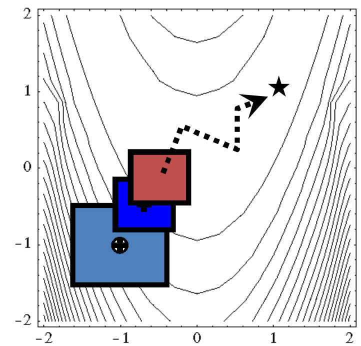
PMA RBDO
$$\begin{cases} \text{minimize} & f \\ \text{subject to} & z \geq \bar{z} \end{cases}$$

Sequential/Surrogate-based RBDO:

- **Break nesting: iterate between opt & UQ until target is met. Trust-region surrogate-based approach is non-heuristic.**

$$\begin{aligned} \text{minimize} \quad & f(\mathbf{d}_0) + \nabla_d f(\mathbf{d}_0)^T (\mathbf{d} - \mathbf{d}_0) \\ \text{subject to} \quad & \beta(\mathbf{d}_0) + \nabla_d \beta(\mathbf{d}_0)^T (\mathbf{d} - \mathbf{d}_0) \geq \bar{\beta} \\ & \| \mathbf{d} - \mathbf{d}_0 \|_\infty \leq \Delta^k \end{aligned}$$

1st-order (also 2nd-order w/ QN)



Unilevel RBDO:

- **All at once: apply KKT conditions of MPP search as equality constraints**
  - Opt. increases in scale (***d***,***u***)
  - Requires 2nd-order info for derivatives of 1st-order KKT

$$\begin{aligned} \min_{\mathbf{d}_{aug}=(\mathbf{d},\mathbf{u}_1,..,\mathbf{u}_{N_{hard}})} \quad & : f(\mathbf{d},\mathbf{p},\mathbf{y}(\mathbf{d},\mathbf{p})) \\ \text{s. t.} \quad & : G_i^R(\mathbf{u}_i,\eta) = 0 \\ & \beta_{allowed} - \beta_i \geq 0 \\ \|\mathbf{u}_i\| \, \|\nabla_{\mathbf{u}} G_i^R(\mathbf{u}_i,\eta)\| + \mathbf{u}_i^T \nabla_{\mathbf{u}} G_i^R(\mathbf{u}_i,\eta) & = 0 \\ \beta_i & = \|\mathbf{u}_i\| \\ \mathbf{d}^l \leq \mathbf{d} & \leq \mathbf{d}^u \end{aligned}$$

KKT of MPP

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Mean Value Method (FOSM)

Some extensions/notation

$$\bar{z} \Rightarrow p, \beta$$

$$\beta_{cdf} = \frac{\mu_g - \bar{z}}{\sigma_g},$$

$$\beta_{ccdf} = \frac{\bar{z} - \mu_g}{\sigma_g}$$

$$\bar{p}, \bar{\beta} \Rightarrow z$$

$$z = \mu_g - \sigma_g \bar{\beta}_{cdf},$$

$$z = \mu_g + \sigma_g \bar{\beta}_{ccdf}$$

$$p_f = \Phi[-\beta] = 1 - \Phi[\beta]$$

p = probability of failure
β= reliability index
z = response level

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