NORTHWESTERN UNIVERSITY

Computer Experiments and Model Uncertainty Quantification in Engineering Design

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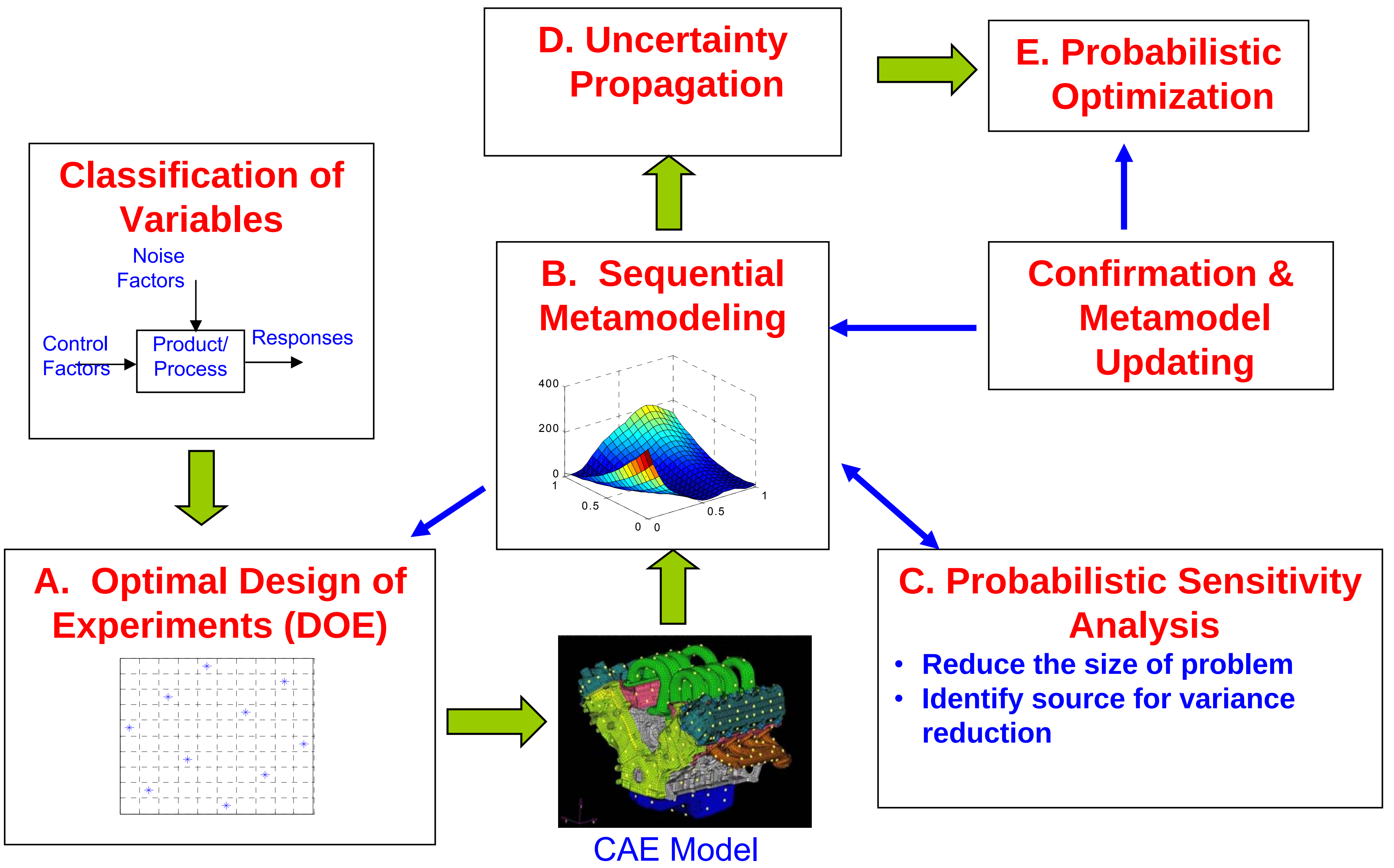
Metamodeling for Simulation Based Design under Uncertainty

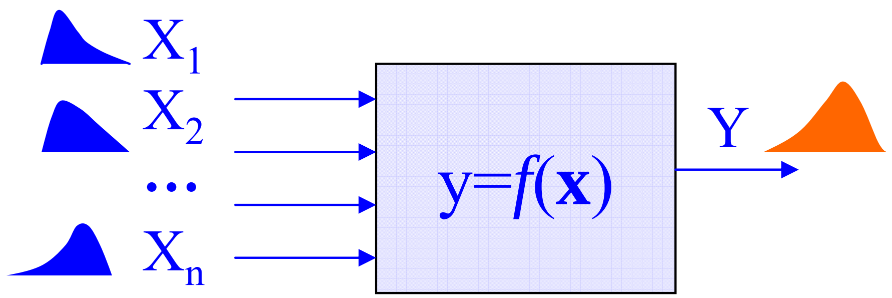


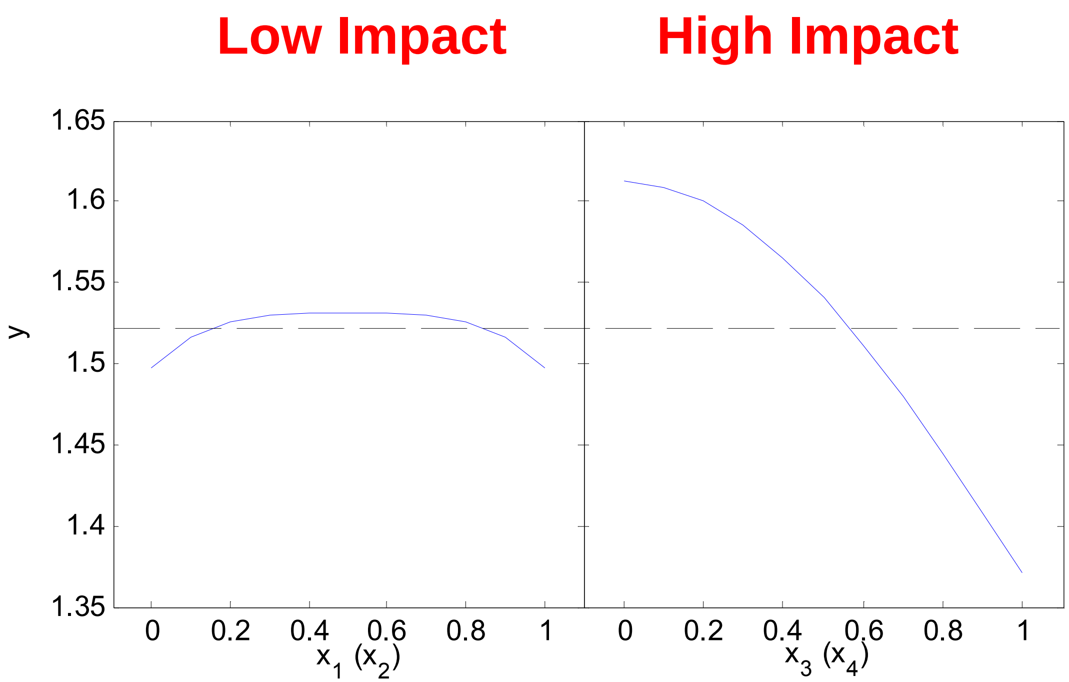
Research Developments

- *Analytical uncertainty propagation (UP) and Statistical Sensitivity Analysis (SSA)*
- *Quantification of model (interpolation) uncertainty*
- *Sampling of computer experiments*

Statistical Sensitivity Analysis (SSA)

SSA study of how the variation in the output of a model can be apportioned, qualitatively or quantitatively, to different sources of variation (Saltelli, et al. 2000)





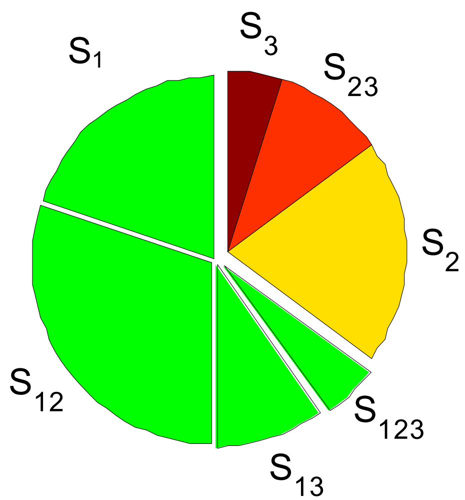
- Reduce the dimension of a design problem
- Investigate resources for uncertainty reduction
- Study the interaction of control & noise variables

Variance-Based SSA Method

Variance-based methods investigate the impact of uncertainty in a random variable on the variance of a random response, derived from the concept of variance decomposition.

$$V = \sum_i V_i + \sum_{i<j} V_{ij} + \ldots + V_{1,2,3,\ldots,n}$$

- V: **Total variance of Y**
- $\sum_i V_i$: **Partial variance form X_i**
- $\sum_{i<j} V_{ij}$: **Partial variance from X_i and X_j interaction**
- $V_{1,2,3,\ldots,n}$: **Partial variance from all variable interaction**



Main Sensitivity Index (MSI)	$S_i = \dfrac{V_i}{V}$	(3)
Interaction Sensitivity Index (ISI)	$S_{1,2,\ldots,m} = \dfrac{V_{1,2,3,\ldots,m}}{V}$	(4)
Total Sensitivity Index (TSI)	$S_{Ti} = 1 - S_{\sim i}$	(5)

For a function with 3 variables, TSI of X_1:

$$\begin{aligned} S_{T1} &= S_1 + S_{12} + S_{13} + S_{123} \\ &= 1 - \left(S_2 + S_3 + S_{23}\right) \\ &= 1 - S_{\sim 1} \end{aligned}$$

Computational Challenge of SSA

ANOVA Decomposition

$$f(\mathbf{x}) = f_0 + \sum_{i=1}^{M} \phi_i(x_i) + \sum_{i_1=1}^{M} \sum_{i_2 \geq i_1}^{M} \phi_{i_1 i_2}(x_{i_1}, x_{i_2}) + \ldots + \phi_{1\ldots M}(x_1, \ldots, x_M)$$

- f_0: **Constant**
- $\phi_i(x_i)$: **Functions of one input only**
- $\phi_{i_1 i_2}(x_{i_1}, x_{i_2})$: **Functions of two input interaction**
- $\phi_{1\ldots M}(x_1, \ldots, x_M)$: **Functions of high-order interaction**

Main Effect

$$\phi_i(x_i) = \int f(\mathbf{x}) \prod_{j \neq i} [p_j(x_j) d\mathbf{x}_j] - f_0 \qquad f_0 = \int f(\mathbf{x}) \prod_{i=1}^{M} [p_i(x_i) dx_i]$$

Two-Variable Interaction Effect

$$\phi_{i_1 i_2}(x_{i_1}, x_{i_2}) = \int f(\mathbf{x}) \prod_{j \neq i_1, i_2} [p_j(x_j) dx_j] - \phi_{i_1}(x_{i_1}) - \phi_{i_2}(x_{i_2}) - f_0$$

Separable Variances

$$V = Var\{f(\mathbf{X})\} = \int f^2(\mathbf{x}) p(\mathbf{x}) d\mathbf{x} - f_0^{\,2}$$

$$V_{i_1 \ldots i_s} = Var\{\phi_{i_1 \ldots i_s}(x_{i_1}, \ldots, x_{i_s})\} = \int \phi^2_{i_1 \ldots i_s}(x_{i_1}, \ldots, x_{i_s}) \prod_{j=i_1}^{i_s} [p_j(x_j) dx_j]$$

Analytical SSA and UA

- Subset Decomposition

$$V = \sum \widehat{V}_{\mathbf{U}_i} + \sum_{i_1 < i_2} \widehat{V}_{\mathbf{U}_{i_1}\mathbf{U}_{i_2}} + \ldots + \widehat{V}_{\mathbf{U}_1 \ldots \mathbf{U}_T}$$

$$\widehat{\phi}_{\mathbf{U}_{i_1} \ldots \mathbf{U}_{i_s}}(\mathbf{x}_{\mathbf{U}_{i_1}}, \ldots, \mathbf{x}_{\mathbf{U}_{i_s}}) = \sum_{l=1}^{s} \sum_{j_1, \ldots, j_l \in (i_1, \ldots, i_s)} (-1)^{s-l} \widehat{\phi}_{\mathbf{U}_{j_1} + \ldots \mathbf{U}_{j_l}}(\mathbf{x}_{\mathbf{U}_{j_1}}, \ldots, \mathbf{x}_{\mathbf{U}_{j_l}})$$

- Transform multivariate to univariate integration for tensor product basis functions

Chen, W., Jin, R., and Sudjianto, A., 2006, “Analytical Global Sensitivity Analysis and Uncertainty Propagation for Robust Design”, *Journal of Quality Technology, in press.*

SSA in Robust Design

- Let D for the set of design variables, R for the set of noise variables

$$V = \widehat{V}_{\mathbf{D}} + \widehat{V}_{\mathbf{R}} + \widehat{V}_{\mathbf{DR}}$$

- Variance reduction of eliminating uncertainty

$$\Delta\sigma_{yi}^{2} = Var[f(\mathbf{X}) \mid \mathbf{x}_{\mathbf{D}})] - Var[f(\mathbf{X}) \mid \mathbf{x}_{\mathbf{D}}, x_i)]$$

- Sensitivity Index for uncertainty reduction

$$S_i^u = \overline{\Delta\sigma_{yi}^{2}} / V = \widehat{S}_{\mathbf{D}+i} - \widehat{S}_{\mathbf{D}} = S_i + \widehat{S}_{i\mathbf{D}}$$

Tensor Product Basis Functions

$$f(\mathbf{x}) = a_0 + \sum_{i=1}^{N_b} a_i B_i(\mathbf{x}) = a_0 + \sum_{i=1}^{N_b} [a_i \prod_{l=1}^{M} h_{il}(x_l)]$$

$$f(\mathbf{x}) = x_1^{\ 2} + x_1 \sin(x_2)$$

Two tensor-product basis functions

$$f(\mathbf{x}) = B_1(\mathbf{x}) + B_2(\mathbf{x})$$

$$B_1(\mathrm{x}) = h_{11}(x_1) h_{12}(x_2) \qquad B_2(\mathrm{x}) = h_{21}(x_1) h_{22}(x_2)$$

Four univariate basis functions

$$h_{11}(x_1) = x_1^{\ 2}, \qquad h_{21}(x_1) = x_1,$$

$$h_{12}(x_2) = 1, \qquad h_{21}(x_2) = \sin(x_2).$$

Generalized Analytical Formulations

Subset Main Variance

$$\widehat{V}_{\mathbf{U}} = \int \left\{ \sum_{i=1}^{N_b} [a_i \prod_{l \notin \mathbf{U}} C_{1,il} \prod_{l \in \mathbf{U}} h_{il}(x_l)] - \sum_{i=1}^{N_b} (a_i \prod_{l=1}^{M} C_{1,il}) \right\}^2 \prod_{l \in \mathbf{U}} [p_l(x_l) dx_l]$$

$$= \int \left\{ \sum_{i=1}^{N_b} [a_i \prod_{l \notin \mathbf{U}} C_{1,il} \prod_{l \in \mathbf{U}} h_{il}(x_l)] \right\}^2 \prod_{l \in \mathbf{U}} [p_l(x_l) dx_l] - [\sum_{i=1}^{N_b} (a_i \prod_{l=1}^{M} C_{1,il})]^2$$

$$= \sum_{i_1=1}^{N_b} \sum_{i_2=1}^{N_b} \left\{ a_{i_1} a_{i_2} \prod_{l \notin \mathbf{U}} (C_{1,i_1 l} C_{1,i_2 l}) \prod_{l \in \mathbf{U}} \int h_{i_1 l}(x_l) h_{i_2 l}(x_l) dx_l \right\} - \sum_{i_1=1}^{N_b} \sum_{i_2=1}^{N_b} [a_{i_1} a_{i_2} \prod_{l=1}^{M} (C_{1,i_1 l} C_{1,i_2 l})]$$

$$= \sum_{i_1=1}^{N_b} \sum_{i_2=1}^{N_b} \left\{ a_{i_1} a_{i_2} \prod_{l=1}^{M} (C_{1,i_1 l} C_{1,i_2 l}) \{ \prod_{l \in \mathbf{U}} [C_{2,i_1 i_2 l} / (C_{1,i_1 l} C_{1,i_2 l})] - 1 \} \right\},$$

Mean of univariate basis functions

$$C_{1,il} = \int h_{il}(x_l) p_l(x_l) dx_l$$

Inner product of two univariate basis functions

$$C_{2,i_1 i_2 l} = \int h_{i_1 l}(x_l) h_{i_2 l}(x_l) p_l(x_l) dx_l$$

Derivations for Commonly Used Metamodels

- Express commonly used metamodels in the form of tensor-product function

Quadratic Polynomial:

$$f(\mathbf{x}) = \beta_0 + \sum_{0 \le i, j \le M, j \ne 0} \beta_{ij} \prod_{l=1}^{M} h_{(i,j)l}$$

$$h_{(i,j)l} = \begin{cases} 1 & \text{none of } (i, j) = l \\ x_l & \text{only one of } (i, j) = l \\ x_l^{\ 2} & \text{both of } (i, j) = l \end{cases}$$

Kriging:

$$f(\mathbf{x}) = \hat{\beta} + \sum_{i=1}^{N} \kappa_i \prod_{l=1}^{M} h_{il}(x_l)$$

$$h_{il}(x_l) = \exp\left[-\theta_l (x_l - x_{il})^2\right]$$

Gaussian RBF:

$$f(\mathbf{x}) = \beta + \sum_{i=1}^{N_\phi} [\lambda_i \prod_{l=1}^{M} h_{il}(x_l)]$$

$$h_{il}(x_l) = \exp\left[-\frac{(x_l - t_{il})^2}{2\tau_i^{\ 2}}\right]$$

MARS:

$$f(\mathbf{x}) = a_0 + \sum_{i=1}^{N_b} [a_i \prod_{l=1}^{M} h_{il}(x_l)]$$

$$h_{il}(x_l) = \begin{cases} 1 & l \notin \mathbf{K}_i \\ \left[s_{il}(x_l - t_{il})\right]_+^q & l \in \mathbf{K}_i \end{cases}$$

- Derive analytical formulations of integrals C1 and C2

Role of Sensitivity Analysis (SA) in Design under Uncertainty

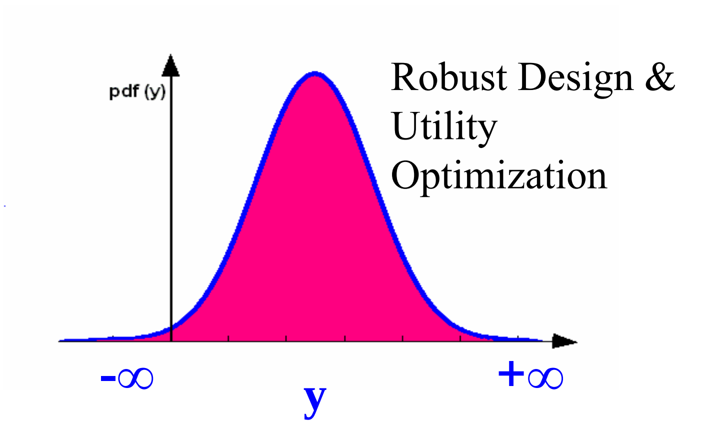
Prior-Design Stage

- **Investigate model behavior**
- **Reduce model dimension**

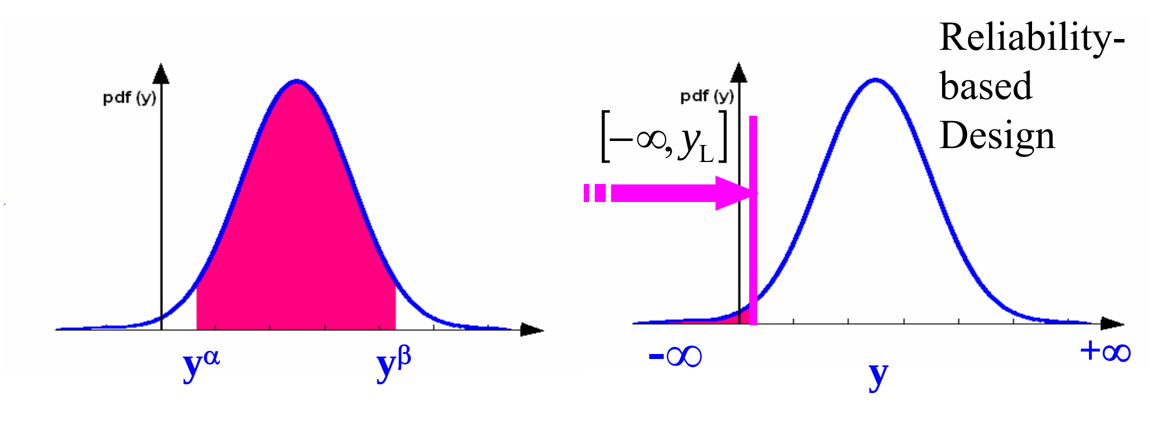
Post-Design Stage

- **Resource allocation for uncertainty reduction**
- **Improve optimality under uncertainty**

How can SA benefit design in different scenarios?



Global Response Probabilistic Sensitivity Analysis **(GRPSA)**

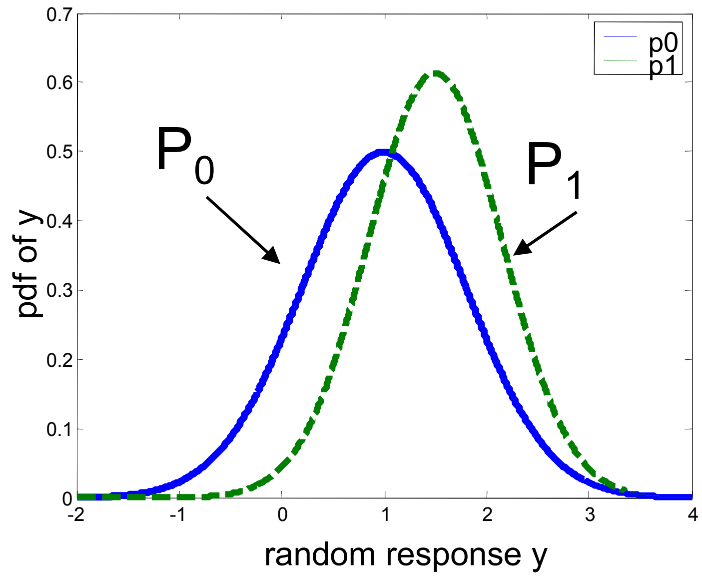


Regional Response Probabilistic Sensitivity Analysis **(RRPSA)**

Kullback-Leibler Entropy Based SSA

Limitation of Variance-Based SSA: only measure the impact on performance variance.

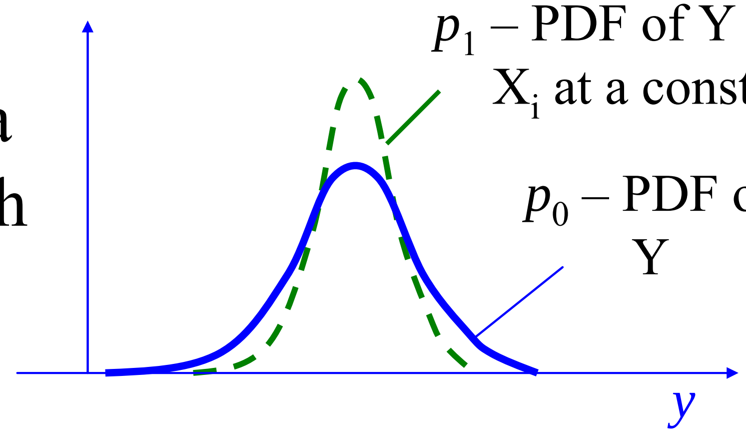
Concept of K-L Entropy Measure: measure the divergence between the change of a distribution before (P_0) and after (P_1) the elimination of a random variable



$$D_{KL}\left(p_1 \mid p_0\right) = \int_{-\infty}^{\infty} p_1(y) \cdot \log \frac{p_1(y)}{p_0(y)} dy = E_{p_1}\left[\log \frac{p_1(y)}{p_0(y)}\right]$$

Extending K-L Entropy for GRPSA and RRPSA

– The concept of "omission sensitivity" (Melchers, 1999) – impact by reducing uncertainty in a random variable or replacing it with a deterministic value.



Global Response PSA (GRPSA), Total Effect

$$D_{KL,x_i} = \int_{-\infty}^{\infty} p_1\left(y\left(x_1, \ldots \mu_{x_i}, \ldots, x_n\right)\right) \log \frac{p_1\left(y\left(x_1, \ldots \mu_{x_i}, \ldots, x_n\right)\right)}{p_0\left(y\left(x_1, \ldots x_i, \ldots, x_n\right)\right)} dy$$

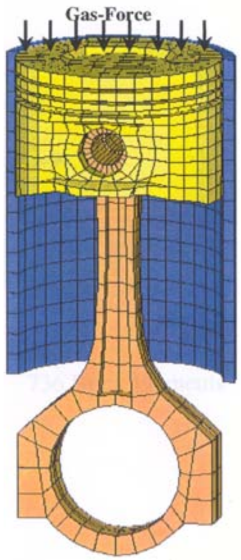
Regional Response PSA (RRPSA), Total Effect

$$D_{KL,x_i} = \int_{y_L}^{y_U} p_0\left(y\left(x_1, \ldots \mu_{x_i}, \ldots, x_n\right)\right) \left| \log \frac{p_1\left(y\left(x_1, \ldots \mu_{x_1}, \ldots, x_n\right)\right)}{p_0\left(y\left(x_1, \ldots x_i, \ldots, x_n\right)\right)} \right| dy$$

Liu, H., Chen, W., and Sudjianto, A., "Relative Entropy Based Method for Global and Regional Sensitivity Analysis in Probabilistic Design", ASME Journal of Mechanical Design, 128(2), pp1–11, 2006

Vehicle Engine Piston Design

Piston Secondary Motion



Piston Design Variables (X)

- Piston skirt profile
- Piston skirt ovality
- Piston pin offset
- Piston skirt length

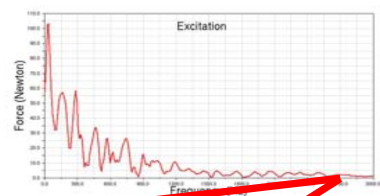
Manufacturing Noise Factor (P)

- Cylinder Block Distortion
- Piston-to-Bore Clearances

Operating Noise Factors (P)

- Spark timing variation
- Temperature
- Combustion Pressure

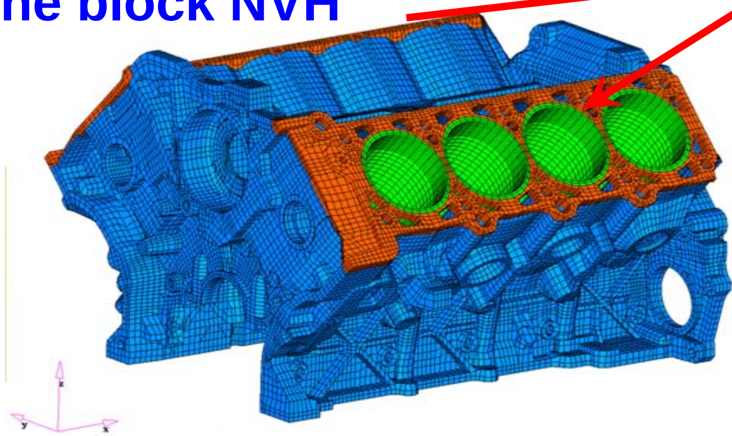
Trust Side Load



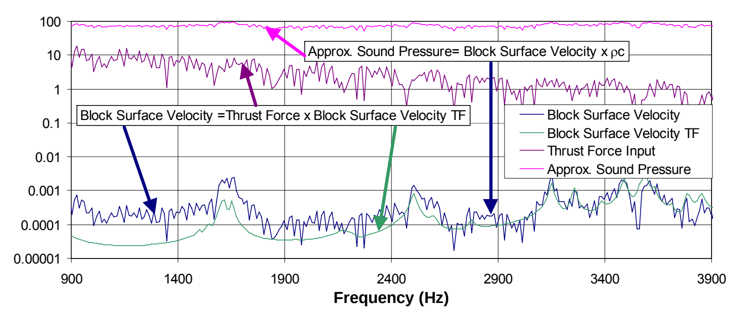
Design Performance (Y)

- Engine piston slap **noise** (**robustness**)
- Power loss due to **friction** (**reliability**)

Engine block NVH



Radiated Noise



Each simulation run takes more than 1 hour on SUN Blade.

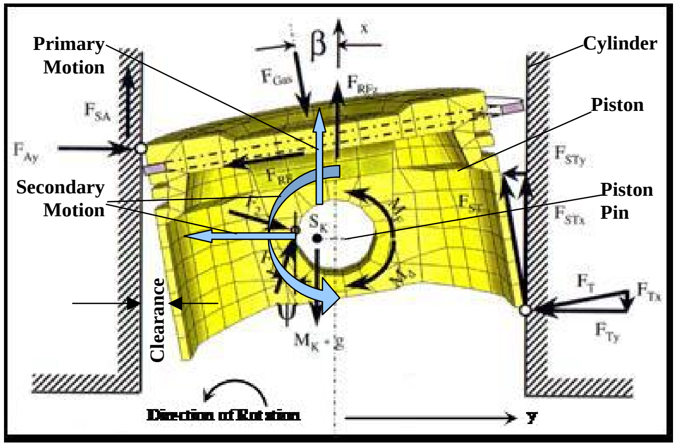
Piston Robust Design based on Secondary Motion Analysis

Responses Y

Slap noise

Piston friction

Y= f (X,P)



Design Variables X

Variable	Description	Nominal Value	Lower Bound	Upper Bound	Unit
SL	Skirt Length	23.07	21	25	millimeter
SP*	Skirt Profile	3	1	3	/
SO*	Skirt Ovality	2	1	3	/
PO	Pin Offset	0.9	0.5	1.3	millimeter

Noise Variables P

Variable	Description	Distribution	Mean	STD	Unit
CL	Piston-to-bore Clearance	Normal	50	11	micrometer
LP	Location of Combustion Peak Pressure	Normal	14.5	1	degree

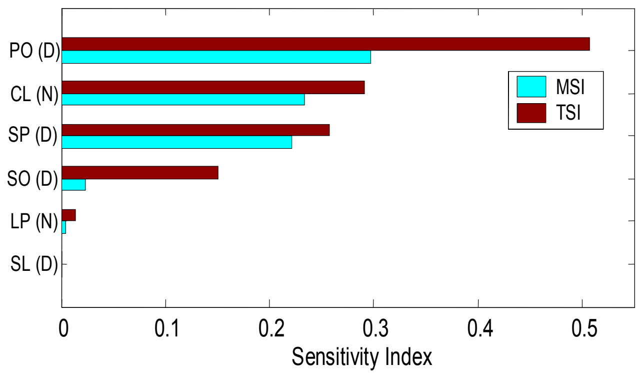
Piston Design SSA Results

Kriging model built using 30 + 30 sequential computer simulations (optimal Latin hyper cube for 4 design and 2 noise variables)

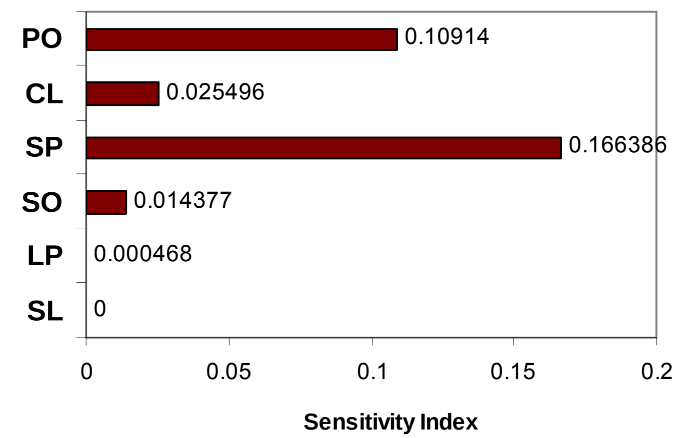
Prior Design SSA

Sobol' Method | K-L entropy based Method

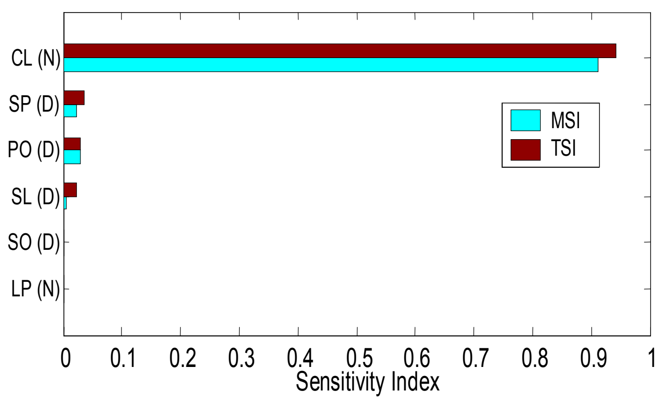
Slap Noise



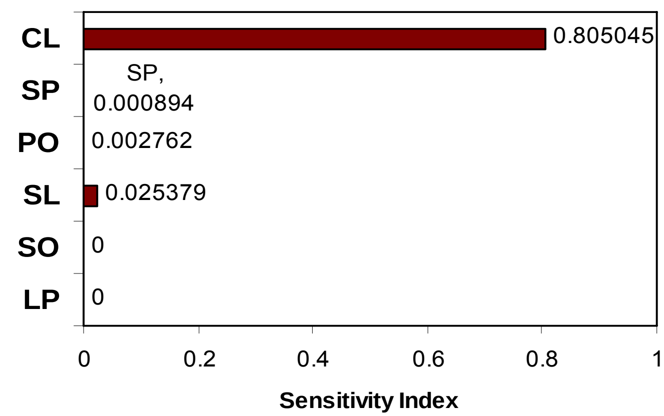
TSI (Sobol')	Importance	TSI (K-L)
PO (D)	High	SP (D)
CL (N)		PO (D)
SP (D)		CL (N)
SO (D)		SO (D)
LP (N)		LP (N)
SL (D)	Low	SL (D)



Piston Friction

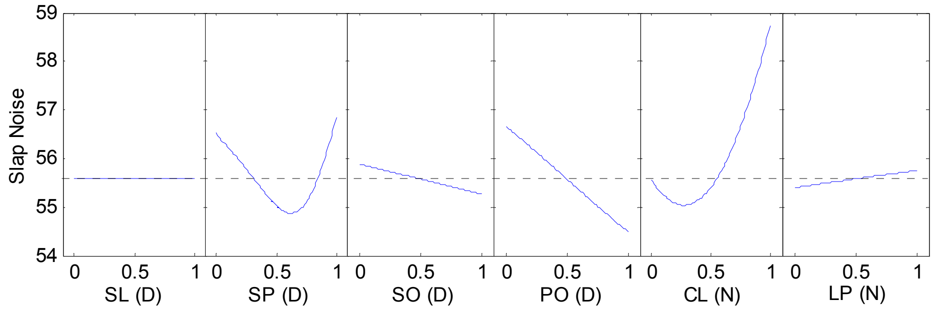


TSI (Sobol')	Importance	TSI (K-L)
CL (N)	High	CL (N)
SP (D)		SL (D)
PO (D)		PO (D)
SL (D)		SP (D)
SO (D)		SO (D)
LP (N)	Low	LP (N)

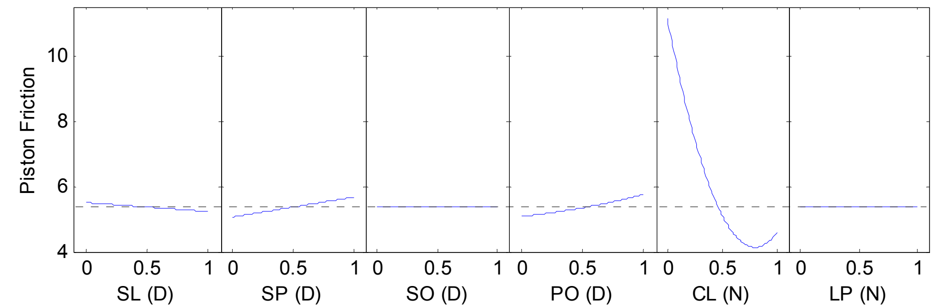


Piston Design Main & Interaction Effects

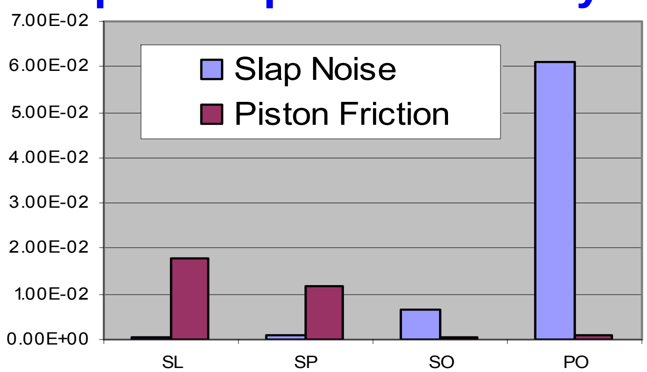
Slap noise

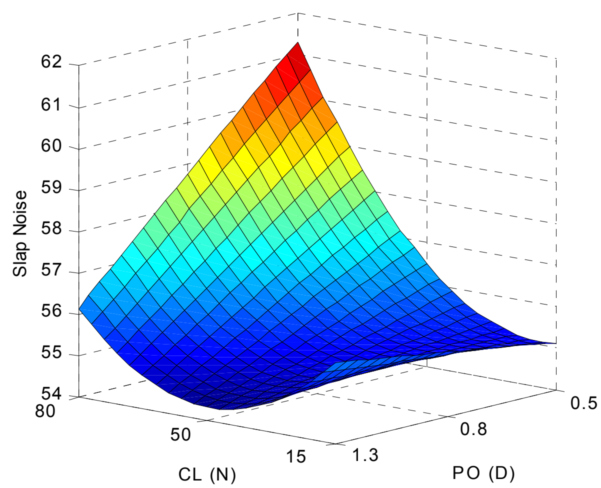


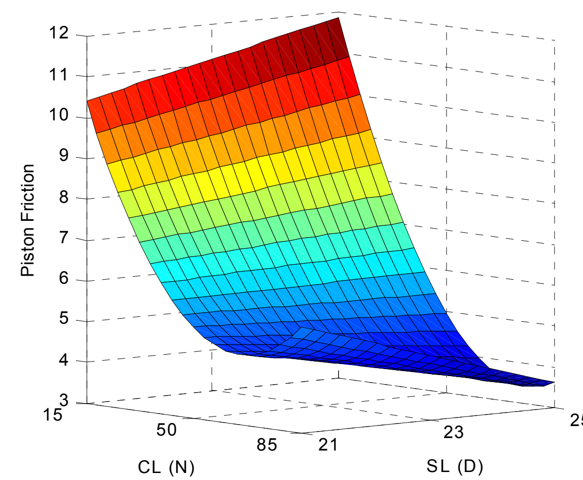
Piston Friction



Capability of a design variable to dampen output uncertainty







Clearance (N)

Pin Offset (D)

Clearance (N)

Skirt Length (D)

D – Design variable

N – Noise variable

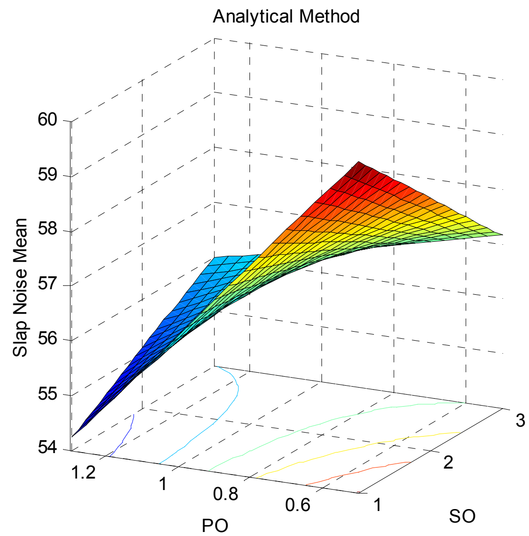
Taylor expansion is not accurate for assessing performance variance due to nonlinearity wrt the noise variable CL.

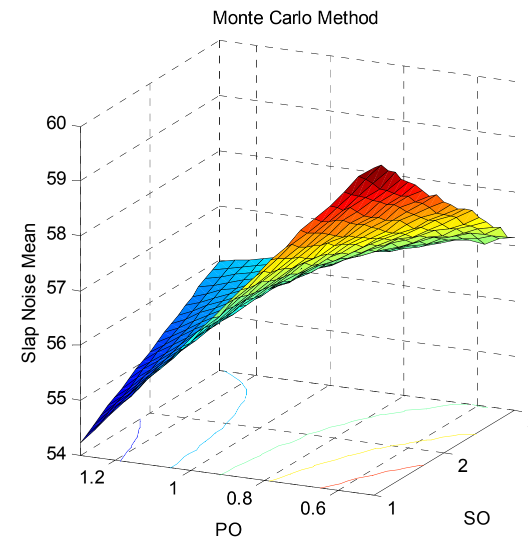
Uncertainty Propagation (Slap Noise)

Analytical

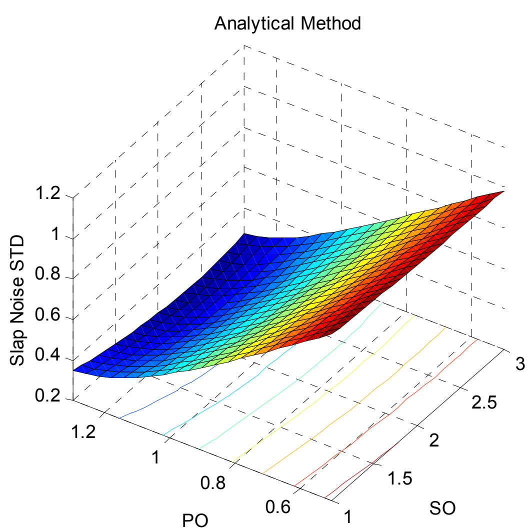
Monte Carlo

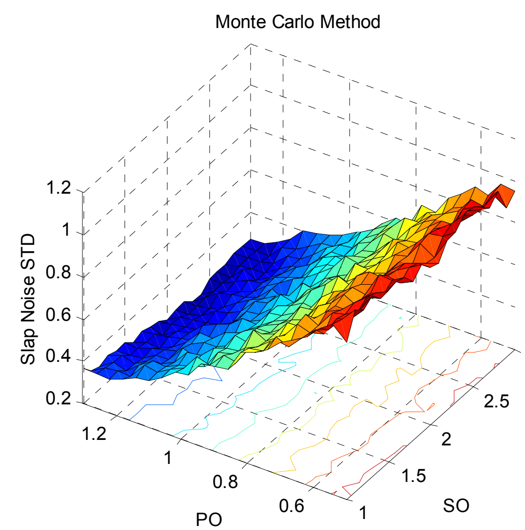
Mean





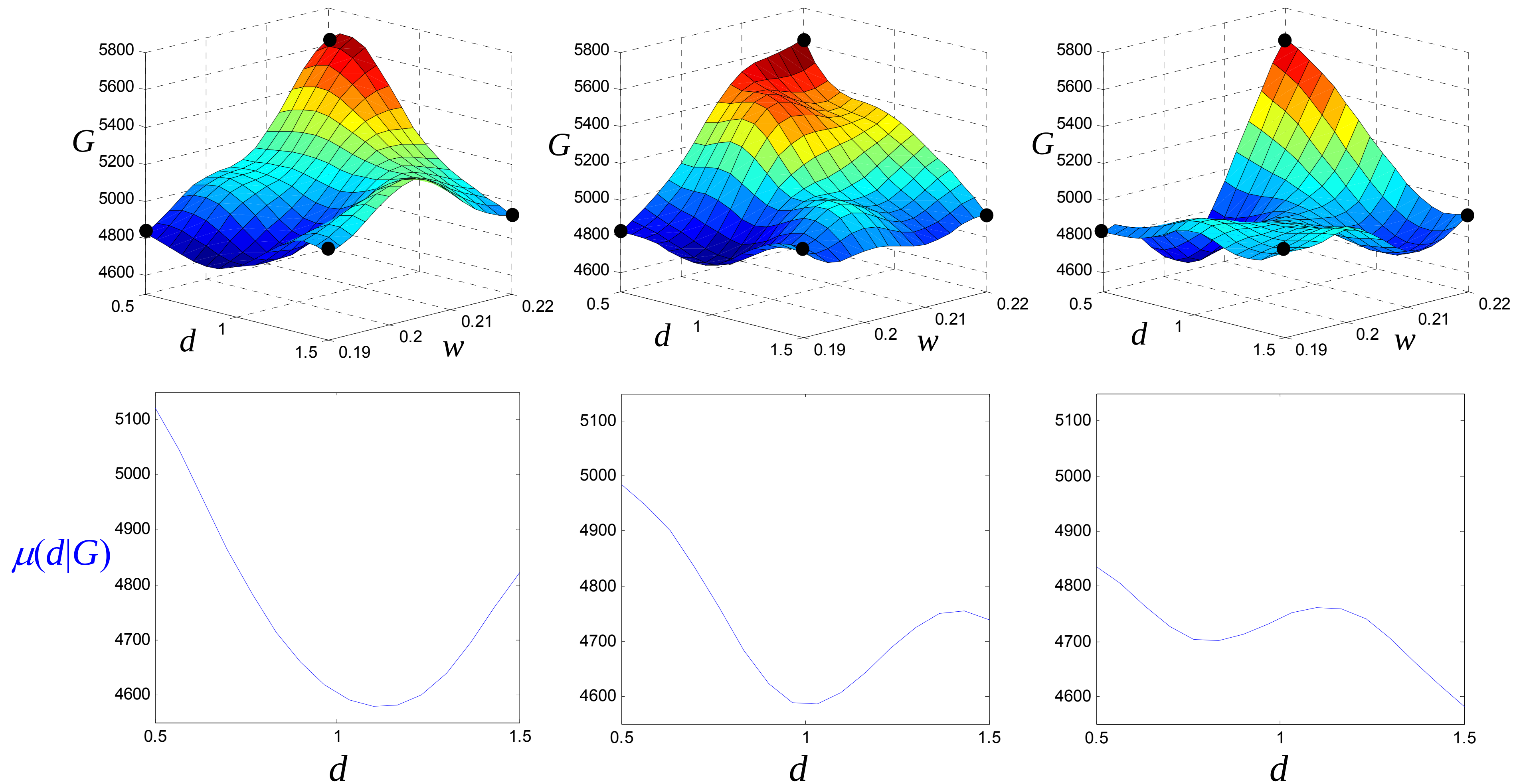
Standard Deviation





Model Uncertainty

d- design var. w-noise var.   G- possible realization of model



These are all potential response surfaces consistent with the 4 simulation results

Understanding Model Uncertainty

- How safe is it to use the metamodel in robust design? How many runs do we need?
- If we need to continue simulation, which regions shall we focus on?
- If an immediate design decision is needed, how to ensure it is robust to both metamodel uncertainty and noise uncertainty?
- How to design efficient simulation strategy to effectively reduce model uncertainty and achieve optimal design?

Bayesian Analysis of Gaussian Random Process

- The true response surface is viewed as a realization of Gaussian Random Process $G(\bullet)$
- The sampled sites are viewed as observations of the GRP $G(\bullet)$
- To represent interpolation uncertainty between the sampled sites, calculate the posterior distribution given the observations and a prior for the GRP
  - Prior mean $E[G(\boldsymbol{x})] = \boldsymbol{h}^T(\boldsymbol{x})\boldsymbol{\beta}$
  - Prior covariance $Cov[G(\boldsymbol{x}), G(\boldsymbol{x}')] = \alpha^2 R_\phi(\boldsymbol{x}, \boldsymbol{x}')$

Reference: Sacks, et.al. 1989; Currin, et.al., 1991; Kennedy and O'Hagan, 2001; Handcock, et.al., 1993

Quantification of Model Uncertainty

– Posterior mean (best Bayesian prediction)

$$\hat{y}(\boldsymbol{x}) \equiv E_{G|\boldsymbol{w},\boldsymbol{y}^N}[Y(G,\mathbf{d},\boldsymbol{w})|\ \boldsymbol{w},\boldsymbol{y}^N]$$
$$= \boldsymbol{h}^T(\boldsymbol{x})\hat{\beta} + \boldsymbol{r}^T(\boldsymbol{x})\mathbf{R}^{-1}\left(\boldsymbol{y}^N - \mathbf{H}\hat{\beta}\right)$$

– Posterior covariance

$$Cov[Y(G,\mathbf{d},\boldsymbol{w}),Y(G,\mathbf{d}',\boldsymbol{w}')|\ \boldsymbol{y}^N] = \alpha^2\{R\phi(\boldsymbol{x},\boldsymbol{x}') - \boldsymbol{r}^{\mathrm{T}}(\boldsymbol{x})\mathbf{R}^{-1}\boldsymbol{r}(\boldsymbol{x}') + [\boldsymbol{h}(\boldsymbol{x}) - \mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\boldsymbol{r}(\boldsymbol{x})]^{\mathrm{T}}[\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}]^{-1}[\boldsymbol{h}(\boldsymbol{x}') - \mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\boldsymbol{r}(\boldsymbol{x}')]\},$$

Reference: Sacks, et.al. 1989; Currin, et.al., 1991; Kennedy and O'Hagan, 2001; Handcock, et.al., 1993

Analytical Derivation of Prediction Intervals of Robust Design Objective

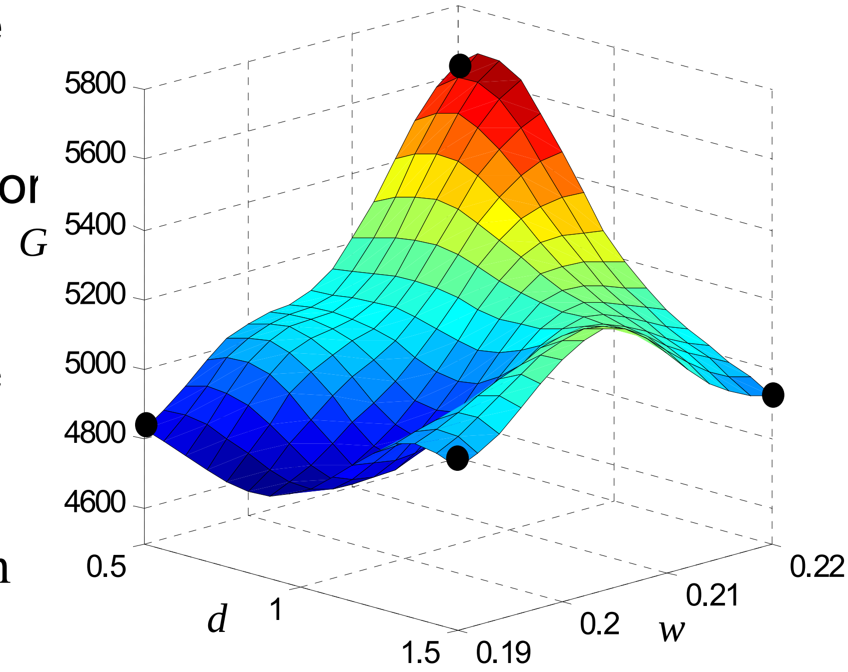
- For robust design $\sigma(\mathbf{d}|G)$ is also of interest
  - Consider more general objective $f(\mathbf{d}|G) \equiv \mu(\mathbf{d}|G) + c\sigma(\mathbf{d}|G)$
- Similar but much more complicated derivation can be applied to $\sigma(\mathbf{d}|G)$ to obtain $\mu_\sigma(\mathbf{d})$ and $\sigma_\sigma^2(\mathbf{d})$
- With some more assumptions, closed-form approximate can be obtained for the $(1-p)$ PI of f

$$f(\mathbf{d}|\,G) \in \mu_f(\mathbf{d}) \pm z_{p/2}\sigma_f(\mathbf{d})$$

Apley, D., Liu, J., and Chen, W., “Understanding the Effects of Model Uncertainty in Robust Design With Computer Experiments”, in press, *ASME Journal of Mechanical Design*, accepted in December 2005.

Computational Advantage

- Monte Carlo method to estimate the PI require prohibitive amount of computation
- For instance, to estimate $\mu_f(\boldsymbol{d})$ and $\sigma_f(\boldsymbol{d})$ used for PI, one needs to
  - Generate realizations of GRP G
  - For each G, one needs to numerically integrate over $\boldsymbol{W}$ for all $\boldsymbol{d}$ to obtain one realization of $f(\boldsymbol{d}|G)$
  - Repeat, e.g., 10,000 times to estimate the mean and variance of $f(\boldsymbol{d}|G)$



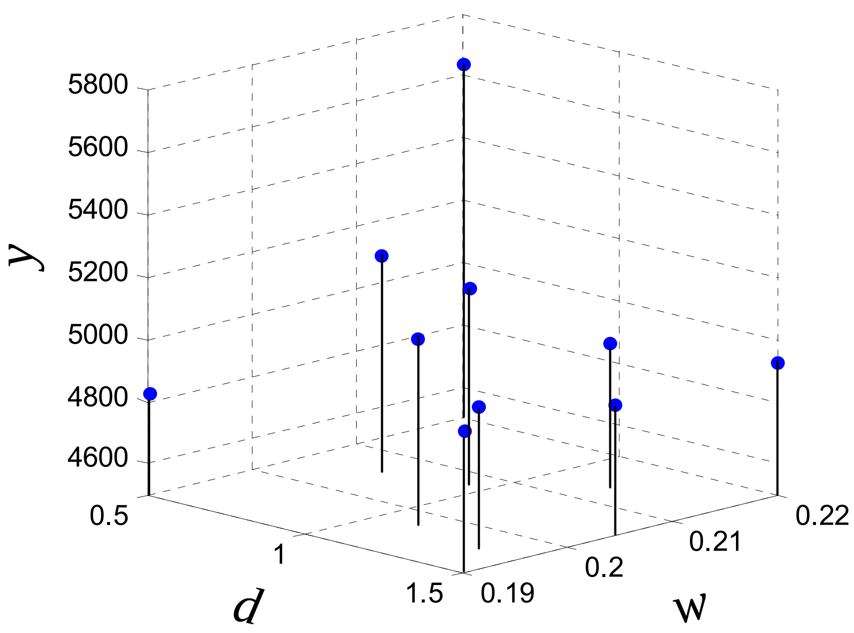
A single realization of G

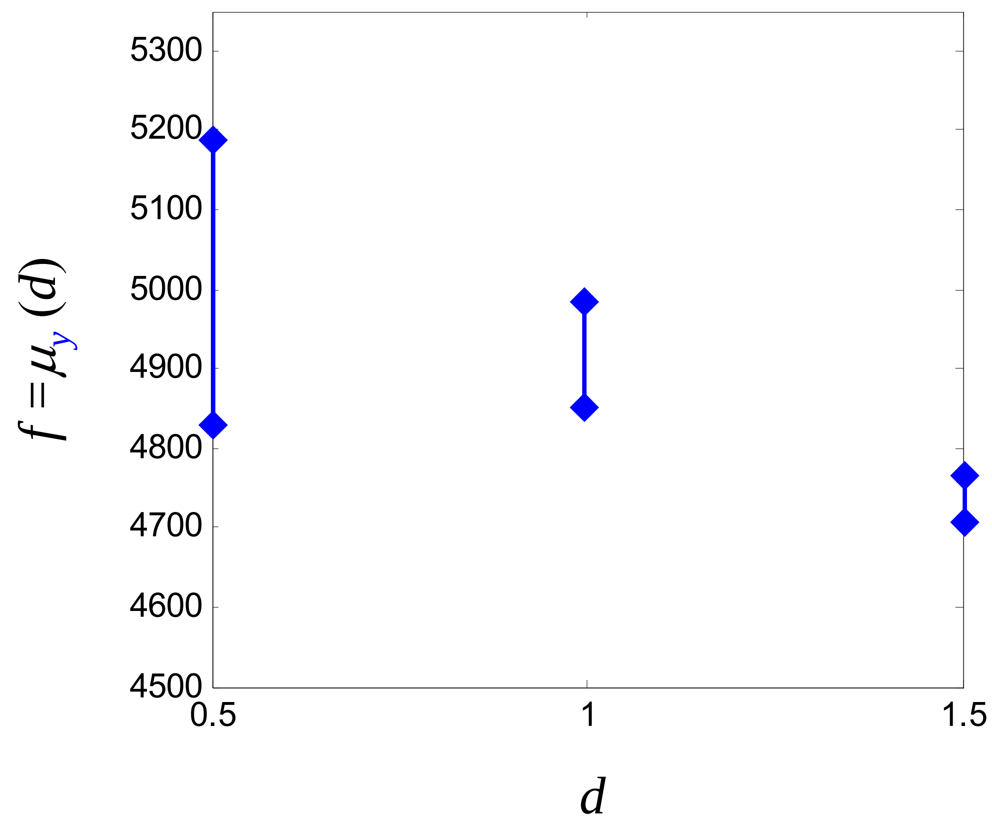
A 10 input variable case requires $20^{10}\times20^{10}$ covariance matrix to generate multivariate normal variates plus numerical integrations for each of the 10,000 replicates

Our analytical approximations provide computationally feasible approach to high-dimensional robust design problems

Comparison of Design Alternatives

After 4+6 runs of simulation



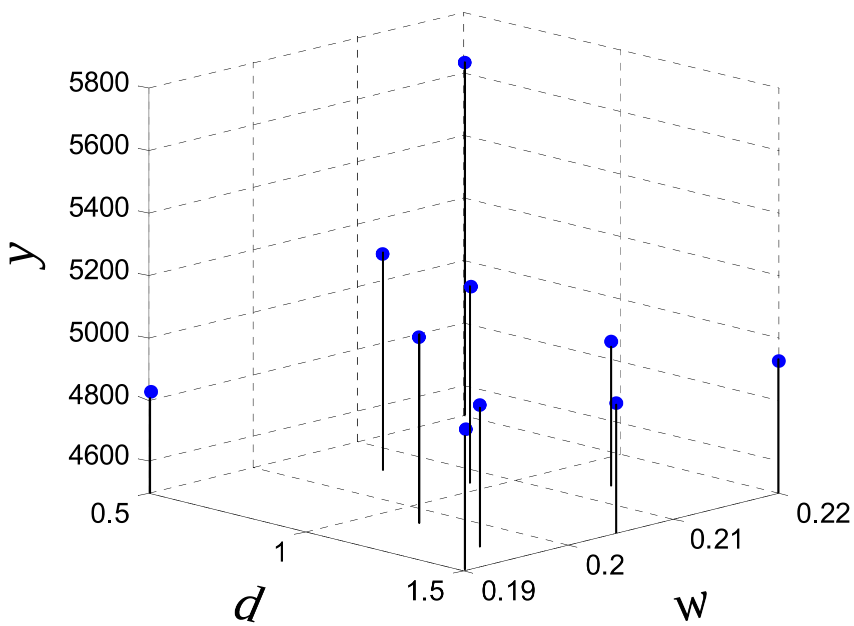


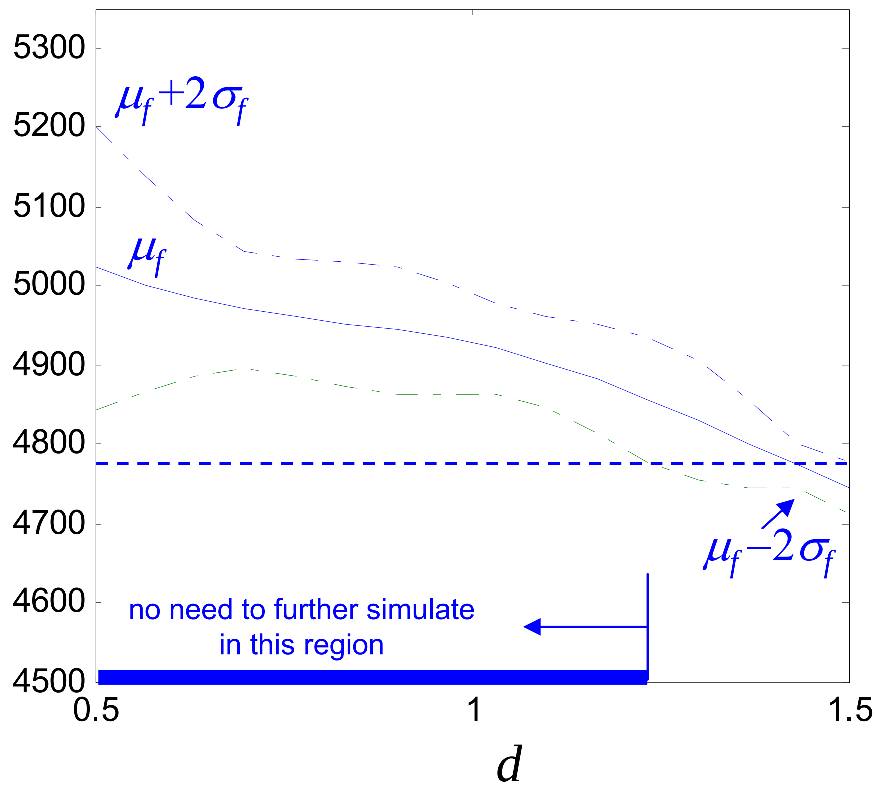
d=1.5 seems to be the best candidate among the three

Non-overlapping prediction intervals, conclude *d* =1.5 is the best among the three candidates (with approximately 95% confidence)

PI Plots for Guiding Further Simulation

All 10 simulation results



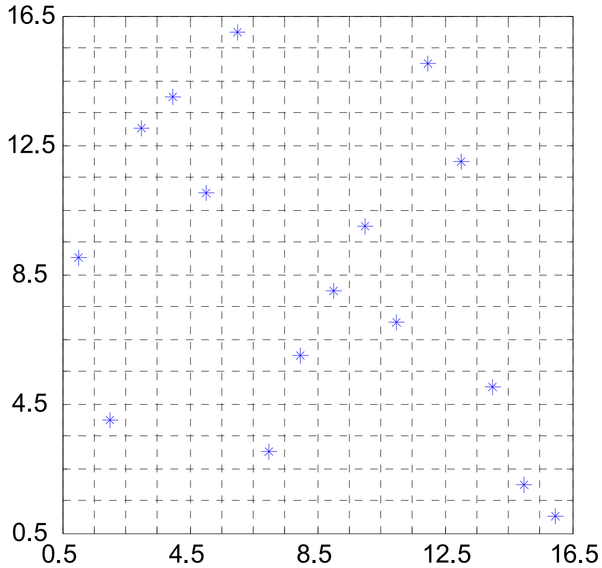


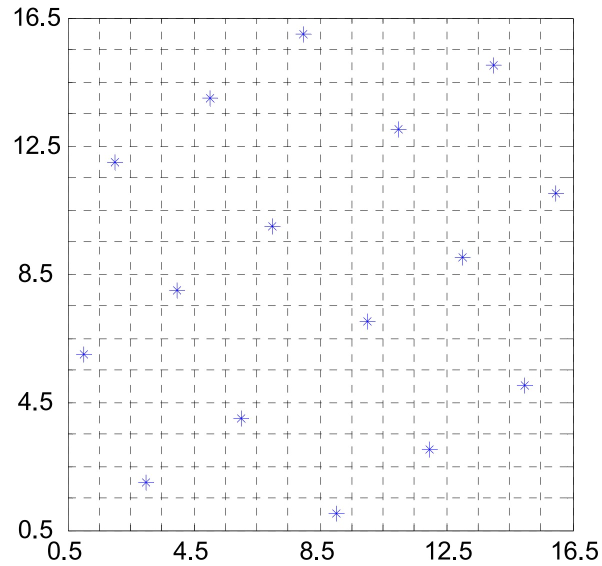
Significant portion of the design space can be ruled out as inferior, resulting in more efficient simulation

Constructing Optimal Design of Computer Experiments (Jin et al. JSPI 2005)

Integrated in iSIGHT 9.0

Before Optimization **LHD (16×2)** **After Optimization**





$$\max_{\mathbf{x}} \left[\min_{1 \le i < j \le n} \left(d(\mathbf{x}_i, \mathbf{x}_j) \right) \right] \qquad d_{ij} = d(\mathbf{x}_i, \mathbf{x}_j) = \left[\sum_{k=1}^{m} \left| x_{ik} - x_{jk} \right|^t \right]^{1/t}$$

- **Element-Exchange Operations:** to perturb the current design without changing the special structure
- **Enhanced Stochastic Evolutionary (ESE) Search Algorithm:** to efficiently search optimal experimental designs
- **Fast-updating methods:** to efficiently evaluate the value of an uniformity criterion

Closure

- The metamodeling-based techniques play an important role in simulation-based design under uncertainty.
- Efficient statistical sensitivity analysis methods are needed to enable designers to make informed decisions under uncertainty.
- Uncertainty of model uncertainty due to metamodeling needs to be considered in decision making and sequential sampling.
- How to handle both model uncertainty and parameter uncertainty needs to be studied.

Definition of Optimal Experimental Design

- Search an optimal design according to a given optimality criterion

$$\min_{\mathbf{X} \in \boldsymbol{Z}} \ f(\mathbf{X})$$

- **X**: experimental design matrix
- *Z*: A particular class of designs with special structural properties
- *f*: Optimality criterion (to measure space-filling property of **X**): e.g.,
  - Maximin -ϕ_p criterion (Johnson et al; Morris and Mitchell)
  - Centered L_2 Discrepancy Criterion (Fang et al.)
  - Entropy criterion (Shewry and Wynn, Currin et al.)

Optimality Criteria

Let $\mathbf{X}$ be the design matrix

- Entropy (Shewry and Wynn, Currin et al.)

$$\min_{\mathbf{X}}\left(-\log|\mathbf{R}|\right) \qquad R_{ij}=\exp\left(-\sum_{k=1}^{m}\theta_k\left|x_{ik}-x_{jk}\right|^{t}\right), 1\le i,j\le n; 1\le t\le 2$$

- MAXIMIN – ϕ_p (Johnson et al., Morris and Mitchell)

$$\max_{\mathbf{X}}\left[\min_{1\le i<j\le n}\left(d(\mathbf{x}_i,\mathbf{x}_j)\right)\right] \qquad d_{ij}=d(\mathbf{x}_i,\mathbf{x}_j)=\left[\sum_{k=1}^{m}\left|x_{ik}-x_{jk}\right|^{t}\right]^{1/t}$$

$$\phi_p=\left[\sum_{i=1}^{s}J_i d_i^{-p}\right]^{1/p}$$

$d_1<d_2<\ldots<d_s$; $(J_1, J_2,\ldots, J_s)$, J_i # of pairs separated by d_i.

- Centered-L_2 Discrepancy (Fang et al.)

$$\min \quad CL_2(\mathbf{X})^2=\left(\frac{13}{12}\right)^2-\frac{2}{n}\sum_{i=1}^{n}\prod_{k=1}^{m}\left(1+\frac{1}{2}\left|x_{ik}-0.5\right|-\frac{1}{2}\left|x_{ik}-0.5\right|^2\right)$$
$$+\frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}\prod_{k=1}^{m}\left(1+\frac{1}{2}\left|x_{ik}-0.5\right|+\frac{1}{2}\left|x_{jk}-0.5\right|-\frac{1}{2}\left|x_{ik}-x_{jk}\right|\right)$$

Updating Operations for Constructing New Experimental Matrix

- Columnwise Element-Exchange Operation

1	2	4	0
3	**4**	0	3
2	1	3	4
4	**0**	1	2
0	3	2	1

Exchange two elements in the second column

1	2	4	0
3	**0**	0	3
2	1	3	4
4	**4**	1	2
0	3	2	1

Preserves design matrix structure such as balance property, Latin Hypercube, etc. Extensions can be made to OA and OA-based LHD

Comparison of Acceptance Criteria

- Column Pairwise (Li and Wu, 1997)

$$p\left(T, f\left(\mathbf{X}^{\text{new}}\right), f\left(\mathbf{X}\right)\right) = \begin{cases} 1 & \text{for } f\left(\mathbf{X}^{\text{new}}\right) - f\left(\mathbf{X}\right) < T \text{ where } T = 0 \\ 0 & \text{otherwise} \end{cases}$$

- Threshold Acceptance (Winker and Fang, 1997)

$$p\left(T, f\left(\mathbf{X}^{\text{new}}\right), f\left(\mathbf{X}\right)\right) = \begin{cases} 1 & \text{for } f\left(\mathbf{X}^{\text{new}}\right) - f\left(\mathbf{X}\right) < T^i \\ 0 & \text{otherwise} \end{cases}$$

$T^i = \alpha T$; $(0 \leq \alpha < 1)$

- Simulated Annealing (Morris and Mitchell, 1995)

$$p\left(T, f\left(\mathbf{X}^{\text{new}}\right), f\left(\mathbf{X}\right)\right) = \exp\left\{-\left[f\left(\mathbf{X}^{\text{new}}\right) - f\left(\mathbf{X}\right)\right] / T^i\right\}$$

$T^i = \alpha T$; $(0 \leq \alpha < 1)$

- Enhanced Stochastic Evolutionary (ESE)

$$p\left(T, f\left(\mathbf{X}^{\text{new}}\right), f\left(\mathbf{X}\right)\right) = \begin{cases} 1 & \text{for } f\left(\mathbf{X}^{\text{new}}\right) - f\left(\mathbf{X}\right) < 0 \\ 1 - \left[f\left(\mathbf{X}^{\text{new}}\right) - f\left(\mathbf{X}\right) / T^i\right] & \text{for } f\left(\mathbf{X}^{\text{new}}\right) - f\left(\mathbf{X}\right) < T^i \\ 0 & \text{otherwise} \end{cases}$$

Temp decrease $T^i = \alpha_1 T$ and
Temp increase $T^i = T / \alpha_2$
where α_j $(0 \leq a_j < 1, j = 1,2)$

Fast Updating Calculation of Criteria

After k^{th}-column element exchange, $x_{i_1 k} \leftrightarrow x_{i_2 k}$

Re-using most of the matrix elements and updating limited-number of elements when necessary

- Entropy

$$-\log |\mathbf{R}| \qquad \mathbf{R} = [r_{ij}]_{n\times n}$$

$$r_{i_2 j}' = r_{j i_2}' = r_{i_2 j} s(i_1, i_2, k, j)$$

$$r_{i_1 j}' = r_{j i_1}' = r_{i_1 j} / s(i_1, i_2, k, j)$$

$$s(i_1, i_2, k, j) = \exp\left[\theta_k \left(\left|x_{i_2 k} - x_{jk}\right|^t - \left|x_{i_1 k} - x_{jk}\right|^t \right)\right]$$

- ϕ_p-MAXIMIN

$$\phi_p' = \left[\phi_p + \sum_{1\le j\le n, j\ne i_1, i_2} \left[(d_{i_1 j}')^{-p} - d_{i_1 j}^{\ -p} \right] + \sum_{1\le j\le n, j\ne i_1, i_2} \left[(d_{i_2 j}')^{-p} - d_{i_2 j}^{\ -p} \right] \right]^{1/p}$$

$$\mathbf{D} = [d_{ij}]_{n\times n} \qquad d_{ij} = d(\mathbf{x}_i, \mathbf{x}_j) = \left[\sum_{k=1}^{m} \left| x_{ik} - x_{jk} \right|^t \right]^{1/t}$$

$$d_{i_1 j}' = d_{j i_1}' = \left[d_{i_1 j}^{\ t} + s(i_1, i_2, k, j) \right]^{1/t} \quad d_{i_2 j}' = d_{j i_2}' = \left[d_{i_2 j}^{\ t} - s(i_1, i_2, k, j) \right]^{1/t} \quad s(i_1, i_2, k, j) = \left|x_{i_2 k} - x_{jk}\right|^t - \left|x_{i_1 k} - x_{jk}\right|^t$$

- Centered-L_2 Discrepancy

$$(CL_2^{\ 2})' = CL_2^{\ 2} + c_{i_1 i_1}' - c_{i_1 i_1} + c_{i_2 i_2}' - c_{i_2 i_2} + 2 \times \sum_{1\le j\le n, j\ne i_1, i_2}^{n} (c_{i_1 j}' - c_{i_1 j} + c_{i_2 j}' - c_{i_2 j})$$

$$\mathbf{C} = [c_{ij}]_{n\times n} \qquad c_{ij} = \begin{cases} \dfrac{1}{n^2} \displaystyle\prod_{k=1}^{m} \dfrac{1}{2} (2 + |z_{ik}| + |z_{jk}| - |z_{ik} - z_{jk}|) & \text{if } i \ne j \\ \dfrac{1}{n^2} \displaystyle\prod_{k=1}^{m} (1 + |z_{ik}|) - \dfrac{2}{n} \prod_{k=1}^{m} (1 + \dfrac{1}{2} |z_{ik}| - \dfrac{1}{2} z_{ik}^{\ 2}) & \text{otherwise} \end{cases}$$

Computational Saving of the New Criterion Evaluation Algorithms

Computational Complexity (*n*: number of runs, *m*: number of variables)

	ϕ_p	CL_2	Entropy
Re-evaluating Algorithms	$O(mn^2)+O(n^2\log_2(n))+O(s^2\log_2(p))$	$O(mn^2)$	$O(n^3)+O(mn^2)$
New Algorithms	$O(n)+O(n\log_2(p))$	$O(n)$	$O(n^2)+O(n) \sim O(n^3)+O(n)$

ESE vs. CP for Constructing Optimal 25×4 LHDs Based on ϕ_p Criterion (p = 50 and t = 1)

	Exchanges Number	Min L_1 Distance	Computing Time
CP¶	2,241,900 (100)	0.8750	10.63 hr
ESE*	120,000	0.9167	2.5 sec

¶ Tested on Sun SPARC 20 Workstation.

* Tested on a PC with a Pentium III 650 MHZ CPU.

– The results of CP algorithm were reported in literature (Ye et al, 2000) in the form of the minimum *L*1 distance (the larger the better).

Examples of Derivations (Kriging)

- Uniform distributions of input variables

$$C_{1,il} = \frac{1}{2\delta_l}\sqrt{\frac{\pi}{\theta_l}}\left\{\Phi\left(a_{il}\sqrt{2\theta_l}\right) - \Phi\left(b_{il}\sqrt{2\theta_l}\right)\right\}$$

$$C_{2,i_1i_2l} = \frac{1}{2\delta_l}\sqrt{\frac{\pi}{2\theta_l}}\exp\left[-\theta_l(x_{i_1l} - x_{i_2l})^2/2\right]\times\left(\Phi\left[\sqrt{\theta_l}(a_{i_1l} + a_{i_2l})\right] - \Phi\left[\sqrt{\theta_l}(b_{i_1l} + b_{i_2l})\right]\right)$$

Where $a_{il} = \mu_l + \delta_l - x_{0il}$ $\quad b_{il} = \mu_l - \delta_l - x_{0il}$

$\Phi(.)$ -CDF of standard normal distribution

- Normal distributions of input variables

$$C_{1,il} = \frac{1}{\sqrt{2\sigma_l^2\theta_l + 1}}\exp\left[-\frac{\theta_l}{2\sigma_l^2\theta_l + 1}(\mu_l - x_{il})^2\right]$$

$$C_{2,i_1i_2l} = \frac{1}{\sqrt{4\sigma_l^2\theta_l + 1}}\exp\left\{-\frac{\theta_l}{4\sigma_l^2\theta_l + 1}\left[(\mu_l - x_{i_1l})^2 + (\mu_l - x_{i_2l})^2 + 2\sigma_l^2\theta_l(x_{i_1l} - x_{i_2l})^2\right]\right\}$$

Bayesian Prediction Intervals for Quantifying Interpolation Uncertainty

- The robust design objective is now a function of the random process $G(\bullet)$

$$f(\mathbf{d}|G) \equiv \mu(\mathbf{d}|G) + c\,\sigma(\mathbf{d}|G)$$

  - Special case: $f(\mathbf{d}|G) \equiv \mu(\mathbf{d}|G)$

- Note $\mu(\mathbf{d}|G)$ follows Gaussian distribution with
  - Mean $\mu_\mu(\mathbf{d}) = \int \hat{y}(\mathbf{d},\mathbf{w})\, p_{\mathbf{w}}(\mathbf{w})d\mathbf{w}$
  - Variance $\sigma_\mu^2(\mathbf{d}) = \iint Cov[Y(G,\mathbf{d},\mathbf{w}),Y(G,\mathbf{d},\mathbf{w}')|\mathbf{y}^N]\,p_{\mathbf{w}}(\mathbf{w})d\mathbf{w}\,p_{\mathbf{w}}(\mathbf{w}')d\mathbf{w}'$
  - Thus $\mu(\mathbf{d}|G) \in \mu_\mu(\mathbf{d}) \pm z_{p/2}\sigma_\mu(\mathbf{d})$ with $(1-p)$ confidence