Advanced Methods in Stochastic Collocation for Polynomial Chaos in RAVEN

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Outline

Discussion Points

Outline

Background

Terminology

- Model - Mathematical representation
- Simulation/Code - Algorithms to Solve Model
- Output - Solution to Model

- Input Space - Space Spanning Possible Input Values
- Response - Map of Input Space to Output Space

Background

UQ

Understanding Simulations

Background

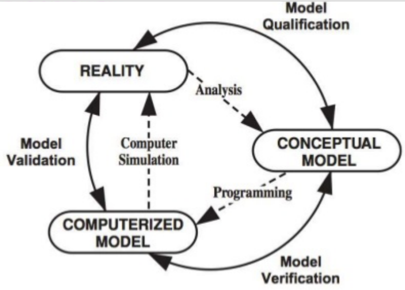
UQ

Understanding Simulations

- Verification - Is the code consistent?
  - Spatial, Temporal Convergence
- Validation - Does it match experiment?
  - Fitting, Extrapolation
- Uncertainty Quantification - Behavior of Response
  - Response Surface Characterization

Background

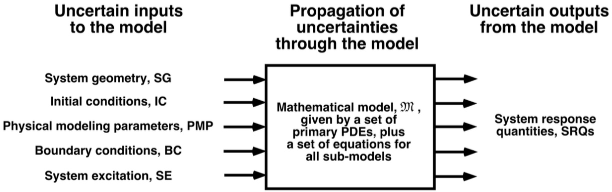
Verification and Validation



The role of verification and validation (Schlesinger, 1979, as cited in Oberkampf & Roy, 2010, p.23)

Background

Uncertainty Quantification



Oberkampf and Roy, 2010

Background

RAVEN

- (R)isk (A)nalysis (V)irtual (EN)vironment
- Verification and Validation
- Uncertainty Quantification
- Response Surfaces, Risk
- Reduced-Order Models
- Operates on Black-box Models

Goal: Add New UQ Methods to RAVEN

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Background

Intrusiveness

Two approaches to UQ:

- Intrusive
  - Interacts with Simulation Algorithms
  - Examples: Stochastic Galerkin, Adjoint-Based
- Non-Intrusive
  - Agnostic of Code
  - Example: Monte Carlo, Stochastic Collocation

For RAVEN, need non-intrusive algorithms

Sampling Strategies

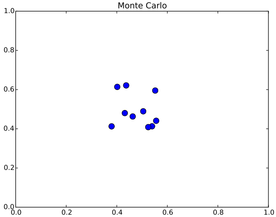
Non-Intrusive Sampling Strategies

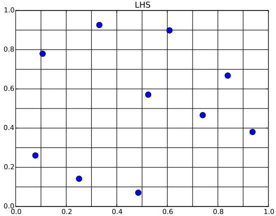
Monte Carlo

- Generate independent, identically-distributed samples
- Derive mean, variance, response surface

Latin Hypercube

- Distributed Monte Carlo





Sampling Strategies

Limitations

Monte Carlo common choice for UQ

- Pro: Convergence agnostic of dimensionality
- Con: Convergence can take many, many samples

Outline

Definitions

- $N \in \mathbb{N}^+$ - Cardinality of Input Space
- Probabilty Space (Ω, Θ, ρ), $Y : \Theta \to \mathbb{R}^N$
- $Y = (y_1, \cdots, y_N)$ - Uncertain Input Parameter Vector
- Subspaces $(\Omega_n, \Theta_n, \rho_n)$
- $Y \in \mathbb{R}^N$, $y_n \in \mathbb{R} \forall n \leq N, n \in \mathbb{N}^+$
- Members of Y are uncorrelated
- $\rho(Y) = \prod_{n=1}^{N} \rho_n(y_n)$ - Joint Probability Density Function
- $u(Y)$ - QoI as a function of Input Parameters Y

Generalized Polynomial Chaos

gPC

$$u(Y) = \sum_{k\in\Lambda} c_k \Phi_k(Y),$$

- Λ - a finite set of polynomial indices,
- $k = (k_1, \cdots, k_N)$ indexes Λ, $k_n \in \mathbb{N}^0$,
- $c_k \in \mathbb{R}$ - scalar coefficients,
- $\phi_{k_n}(y_n)$ - Gauss polys order k_n orthonormal w.r.t $\rho_n(y_n)$,
- $\Phi_k(Y) = \prod_{n=1}^N \phi_{k_n}(y_n)$,
- $\Phi_k(Y)$ orthonormal w.r.t $\rho(Y)$ over Ω.

Generalized Polynomial Chaos

Truncated

In practice, truncate to some gPC level $L \in \mathbb{N}^+$,

$$u(Y) \approx G_L[u](Y) \equiv \sum_{k \in \Lambda(L)} c_k \Phi_k(Y).$$

Error is of order equal to the polynomial terms removed by truncation.

Generalized Polynomial Chaos

Constructing $\Lambda(L)$

$\Lambda(L)$ is list of multidimensional polynomial indices k

For example, $N = 3$:

$$k = (3, 1, 2) \quad \rightarrow \quad \Phi_k(Y) = \phi_3(y_1)\phi_1(y_2)\phi_2(y_3).$$

Generalized Polynomial Chaos

Constructing $\Lambda(L)$

Naïve choice for $\Lambda(L)$ is tensor product of all polynomials of order less than or equal to L,

$$\Lambda_{\text{TP}}(L) = \Big\{ k = (k_1, \cdots, k_N) : \max_{1 \le n \le N} k_n \le L \Big\}.$$

Size of Index Set: $|\Lambda_{\text{TP}}(L)| = (L+1)^N$.

(3,0)	(3,1)	(3,2)	(3,3)
(2,0)	(2,1)	(2,2)	(2,3)
(1,0)	(1,1)	(1,2)	(1,3)
(0,0)	(0,1)	(0,2)	(0,3)

Table: Tensor Product Index Set, $N = 2, L = 3$

Generalized Polynomial Chaos

Constructing $\Lambda(L)$

Common choice for $\Lambda(L)$: Total Degree of all polynomials of order less than or equal to L,

$$\Lambda_{\mathrm{TD}}(L) = \left\{ \bar{p} = (p_1, \cdots, p_N) : \sum_{n=1}^{N} p_n \leq L \right\}.$$

Size of Index Set: $|\Lambda_{\mathrm{TD}}(L)| = \binom{L+N}{N}$.

(3,0)			
(2,0)	(2,1)		
(1,0)	(1,1)	(1,2)	
(0,0)	(0,1)	(0,2)	(0,3)

Table: Total Degree Index Set, $N = 2$, $L = 3$

Generalized Polynomial Chaos

Constructing $\Lambda(L)$

Hyperbolic Cross: Limited by product of all polynomial orders,

$$\Lambda_{HC}(L) = \left\{ \bar{p} = (p_1, \ldots, p_N) : \prod_{n=1}^{N} p_n + 1 \leq L + 1 \right\}.$$

Index Set Bound: $|\Lambda_{HC}(L)| \leq (L+1)(1+\log(L+1))^{N-1}$.

(3,0)			
(2,0)			
(1,0)	(1,1)		
(0,0)	(0,1)	(0,2)	(0,3)

Table: Hyperbolic Cross Index Set, $N = 2, L = 3$

Generalized Polynomial Chaos

Constructing $\Lambda(L)$

Anisotropic Rules using weights $\alpha = (\alpha_1, \cdots, \alpha_N)$

$$\tilde{\Lambda}_{\text{TD}}(L) = \Big\{\bar{p} = (p_1, \cdots, p_N) : \sum_{n=1}^{N} \alpha_n p_n \leq |\alpha|_1 L\Big\},$$

$$\tilde{\Lambda}_{\text{HC}}(L) = \Big\{\bar{p} = (p_1, \cdots, p_N) : \prod_{n=1}^{N} (p_n + 1)^{\alpha_n} \leq (L + 1)^{|\alpha|_1}\Big\}.$$

$$|\alpha|_1 \equiv \frac{\sum_{n=1}^{N} \alpha_n}{N}.$$

Generalized Polynomial Chaos

Sparse Grid Quadrature

Generalized Polynomial Chaos

Sparse Grid Quadrature

Necessary to find coefficients c_k,

$$G[u](Y) = \sum_{k\in\Lambda(L)} c_k\Phi_k(Y).$$

Using orthonormality of $\Phi_k(Y)$,

$$c_k = \langle u(Y)\Phi_k(Y)\rangle = \int_\Omega \rho(Y)u(Y)\Phi_k(Y)dY$$

Generalized Polynomial Chaos

Sparse Grid Quadrature

The quadrature and polynomials to use depends on the distribution $\rho_n(y_n)$,

PDF Kind	Polynomials / Quadrature
Uniform	Legendre
Normal	Hermite
Gamma	Laguerre
Beta	Jacobi

Generalized Polynomial Chaos

Order of Quadrature

Determine order of quadrature

$$\int_{\Omega_x} f(x)\rho(x)dx = \sum_{\ell=1}^{\infty} w_\ell f(x_\ell).$$

If $f(x)$ is a polynomial of order $2m-1$,

$$\int_{\Omega_x} f(x)\rho(x)dx = \sum_{\ell=1}^{m} w_\ell f(x_\ell).$$

Let

$$q^m[f(x)] \equiv \sum_{\ell=1}^{m} w_\ell f(x_\ell).$$

In our case (let N=1),

$$c_k = \int u(Y)\Phi(Y)\rho(Y)dY = q^m[u(Y)\Phi(Y)].$$

Generalized Polynomial Chaos

Order of Quadrature

$$c_k = \int_\Omega u(Y)\Phi(Y)\rho(Y)dY = q^m[u(Y)\Phi_k(Y)].$$

To determine m, replace $u(Y) = G[u](Y)$:

$$\begin{aligned} c_k &= q^m\left[\Phi_k(Y)\sum_{k'\in\Lambda(L)} c_{k'}\Phi_{k'}(Y)\right], \\ &= q^m\left[c_k\Phi_k(Y)^2\right], \\ &= q^m\left[\mathcal{O}(k^2)\right], \end{aligned}$$

so

$$2m+1 = 2k \quad \rightarrow \quad m = k+\frac{1}{2} \approx m = k+1.$$

Generalized Polynomial Chaos

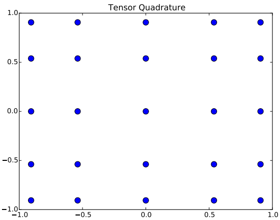
Sparse Grid Quadrature

Multidimensional Quadrature

- Each point needs N quadrature sets
- Ex. $N = 2$, k=(4,4), need (5,5) quadratures
- Needed for each k in Λ

Tensor quadrature

$$Q^M = q_1^{m_1} \otimes q_2^{m_2} \otimes \cdots \otimes q_N^{m_N},$$
$$= \bigotimes_{n=1}^{N} q_n^{m_n}.$$



Generalized Polynomial Chaos

Sparse Grid Quadrature

Smolyak sparse grids $S[u](Y)$:

$$\text{Let } \Delta_k^m[f(x)] \equiv \left(q_k^m - q_{k-1}^m\right)[f(x)].$$

$$S_{\Lambda,N}^M[u(Y)\Phi_k(Y)] = \sum_{k\in\Lambda(L)} \left(\Delta_{k_1}^{m_1} \otimes \cdots \otimes \Delta_{k_N}^{m_N}\right)[u(Y)\Phi_k(Y)].$$

Generalized Polynomial Chaos

Sparse Grid Quadrature

Equivalently,

$$S^M_{\Lambda,N}[u(Y)\Phi_k(Y)] = \sum_{k\in\Lambda(L)} s(k) \bigotimes_{n=1}^{N} q^{m_n}_n[u(Y)\Phi_k(Y)],$$

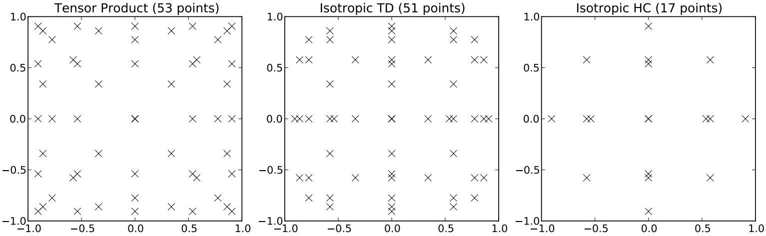
$$s(k) = \sum_{\substack{j=\{0,1\}^N,\\ k+j\in\Lambda}} (-1)^{|j|_1}, \quad |j|_1 \equiv \sum_{p\in j} p.$$

$$\begin{aligned} c_k &= \langle u(Y)\Phi_k(Y)\rangle, \\ &\approx S^M_{\Lambda,N}[u(Y)\Phi_k(Y)]. \end{aligned}$$

Generalized Polynomial Chaos

Sparse Grid Quadrature

Comparison, $N = 2$, $L = 4$



Generalized Polynomial Chaos

Adaptive Index Sets

Generalized Polynomial Chaos

Adaptive Index Sets

Special property of gPC:

$$G[u](Y) = \sum_{k\in\Lambda} c_k \Phi_k(Y),$$

$$\text{mean} = \langle G[u](Y) \rangle = c_{\{0\}^N},$$

$$\begin{aligned}\text{var} &= \langle G[u](Y)^2 \rangle - c_{\{0\}^N}^2,\\ &= \sum_{k\in\Lambda} c_k^2 - c_{\{0\}^N}^2.\end{aligned}$$

Generalized Polynomial Chaos

Adaptive Index Sets

Adaptive Index Set construction using ANOVA

$$\text{Impact Parameter } \eta_k = \frac{c_k^2}{\text{var}\left\{G[u](Y)\right\}}, \quad 0 \leq \eta_k \leq 1$$

$$\text{Est. Impact Parameter } \tilde{\eta}_k = \prod_{n=1,k_n>0}^{N} \eta_{(k_1,\cdots,k_n-1,\cdots,k_N)}$$

Example,

$$\tilde{\eta}_{(2,1,3)} = \eta_{(1,1,3)} \cdot \eta_{(2,0,3)} \cdot \eta_{(2,1,2)}$$

Generalized Polynomial Chaos

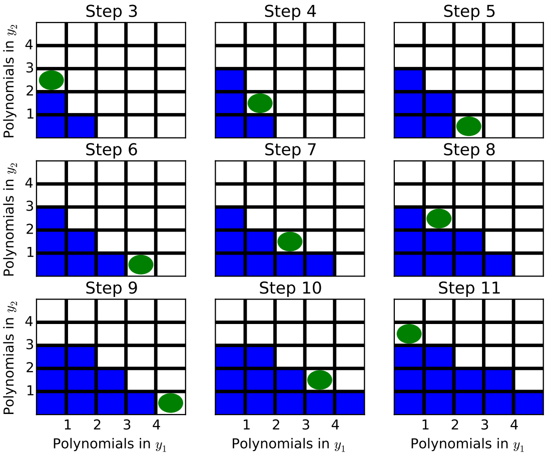
Adaptive Index Sets

Adaptive Index Set Algorithm

- Calculate mean (zeroth-order) polynomial expansion
- While not converged:
  - Collect list of indices whose predecessors are in Λ
  - Using existing impacts, predict impact of each potential index
  - If total of impacts is less than tolerance, convergence is reached
  - Otherwise, add highest-impact index and construct new expansion

Generalized Polynomial Chaos

Adaptive Index Sets



Physical Models

Physical Models

Efficiency of gPC compared to Monte Carlo depends on

- Regularity of response surface
- Dimensionality of input space

Demonstrate using three models

- Tensor Polynomial
- Attenuation
- Neutron Diffusion

Physical Models

Tensor Polynomial

From Ayres and Eaton, 2015

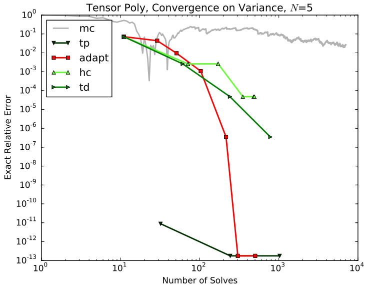
$$u(Y) = \prod_{n=1}^{N} (y_n + 1), \quad y_n \sim \mathcal{U}[-1, 1]$$

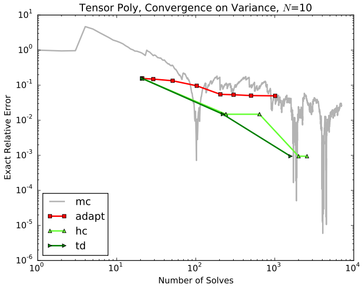
Features:

- Analytic mean, variance
- Regularity
- Exact in finite polynomial space

Tensor Polynomials

Results





Physical Models

Attenuation

Exit strength of beam incident on discrete absorbing material

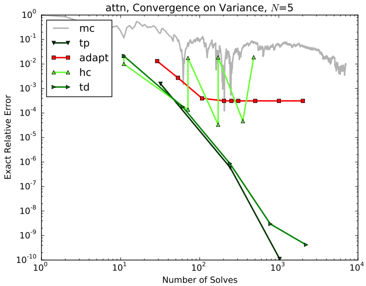
$$u(Y) = \prod_{n=1}^{N} e^{-y_n/N}, \quad y_n \sim \mathcal{U}[0,1]$$

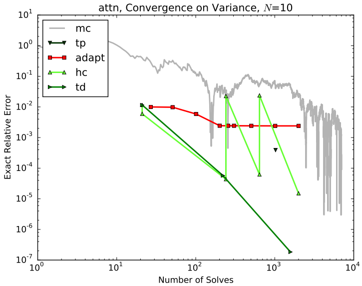
Features:

- Analytic mean, variance
- Regularity
- Inexact in finite polynomial space
- Taylor expansion is tensor high-order polynomials

Attenuation

Results





Physical Models

Neutron Diffusion

Quarter-core 2-group steady state reactor benchmark
165x165 cm domain

$$-\nabla\cdot(D_1(\bar{x})\nabla\phi_1(\bar{x}))+\left(\Sigma_a^{(1)}(\bar{x})+\Sigma_s^{(1\to 2)}(\bar{x})\right)\phi_1(\bar{x})=\frac{1}{k(\phi)}\sum_{g'=1}^{2}\nu_{g'}\Sigma_f^{(g')}(\bar{x})\phi_{g'}(\bar{x}),$$

$$-\nabla\cdot(D_2(\bar{x})\nabla\phi_2(\bar{x}))+\Sigma_a^{(2)}(\bar{x})\phi_2(\bar{x})=\Sigma_s^{(1\to 2)}(\bar{x})\phi_1(\bar{x})$$

QoI: $k(\phi)$

Neutron Diffusion

Geometry

5	5	5	5	5	5	5	5	5	5	5
5	5	5	5	5	5	5	5	5	5	5
3	3	3	3	3	3	3	5	5	5	5
3	3	3	3	3	3	3	4	5	5	5
2	1	1	1	1	2	2	3	3	5	5
2	1	1	1	1	2	2	3	3	5	5
1	1	1	1	1	1	1	3	3	5	5
1	1	1	1	1	1	1	3	3	5	5
1	1	1	1	1	1	1	3	3	5	5
1	1	1	1	1	1	1	3	3	5	5
2	1	1	1	1	2	2	3	3	5	5

Vacuum, Reflective boundaries

Neutron Diffusion

BCs

Boundary Conditions

$$\frac{\phi_g}{4} - \frac{D_g}{2}\frac{\partial \phi_g}{\partial x_1}\bigg|_{\partial\Omega_{\text{top}}} = 0, \quad g = 1, 2, \tag{1}$$

$$\frac{\phi_g}{4} - \frac{D_g}{2}\frac{\partial \phi_g}{\partial x_2}\bigg|_{\partial\Omega_{\text{right}}} = 0, \quad g = 1, 2, \tag{2}$$

$$-D_g\frac{\partial \phi_g}{\partial x_1}\bigg|_{\partial\Omega_{\text{bottom}}} = 0, \quad g = 1, 2, \tag{3}$$

$$-D_g\frac{\partial \phi_g}{\partial x_2}\bigg|_{\partial\Omega_{\text{left}}} = 0, \quad g = 1, 2. \tag{4}$$

Neutron Diffusion

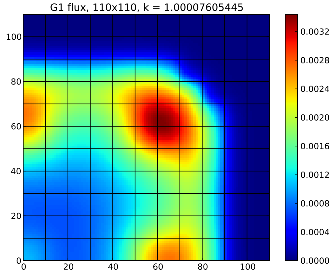
Input Space

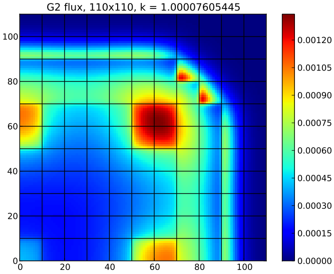
Region	Group	D_g	$\Sigma_{a,g}$	$\nu\Sigma_{f,g}$	$\Sigma_s^{1,2}$
1	1	1.255	8.252e-3	4.602e-3	2.533e-2
	2	2.11e-1	1.003e-1	1.091e-1	
2	1	1.268	7.181e-3	4.609e-3	2.767e-2
	2	1.902e-1	7.047e-2	8.675e-2	
3	1	1.259	8.002e-3	4.663e-3	2.617e-2
	2	2.091e-1	8.344e-2	1.021e-1	
4	1	1.259	8.002e-3	4.663e-3	2.617e-2
	2	2.091e-1	7.3324e-2	1.021e-1	
5	1	1.257	6.034e-4	0	4.754e-2
	2	1.592e-1	1.911e-2	0	

Neutron Diffusion

Reference Solution

k=1.00007605445





Neutron Diffusion

Uncertainty

5% Uncertainty in Parameters:

N=3, N=5

- $\nu\Sigma_{2,f}^{(1)}$
- $\nu\Sigma_{2,f}^{(4)}$
- $D_2^{(5)}$

- $\Sigma_{2,c}^{(1)}$
- $\Sigma_{2,c}^{(4)}$

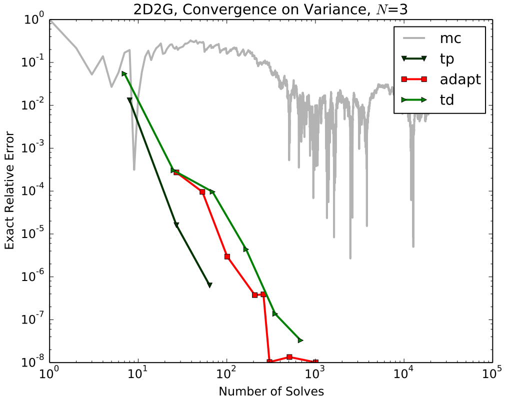
N=10

- $\Sigma_{2,c}^{(1)}$, $\nu\Sigma_{2,f}^{(1)}$
- $\Sigma_{2,c}^{(2)}$, $\nu\Sigma_{2,f}^{(2)}$
- $\Sigma_{2,c}^{(3)}$, $\nu\Sigma_{2,f}^{(3)}$
- $\Sigma_{2,c}^{(4)}$, $\nu\Sigma_{2,f}^{(4)}$, $\nu\Sigma_{1\to2}^{(4)}$
- $D_2^{(5)}$

Neutron Diffusion

Results

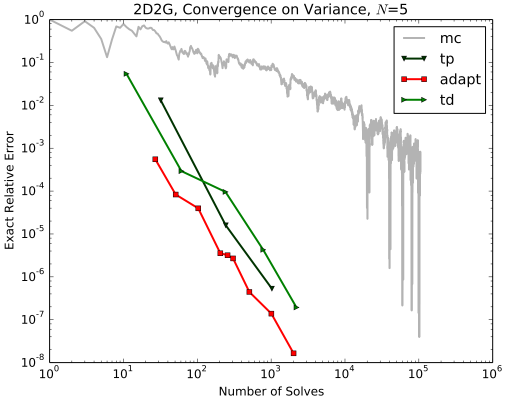
N=3



Neutron Diffusion

Results

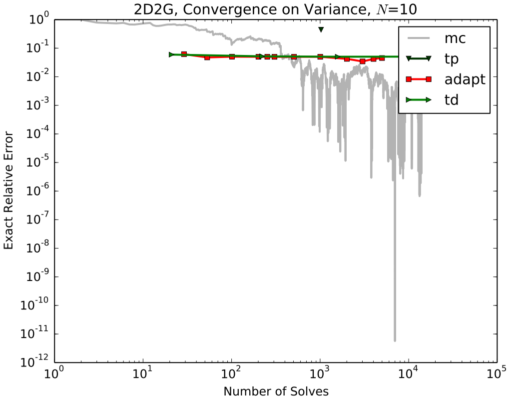
N=5



Neutron Diffusion

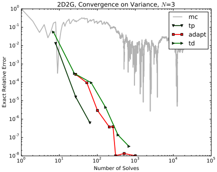
Results

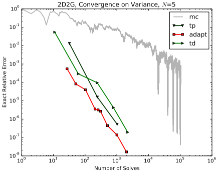
N=10

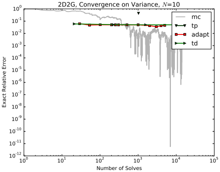


Neutron Diffusion

Results







Results

Summary

Preliminary Conclusions

- SC for gPC suffers greatly from curse of dimensionality
- Adaptive SC can help
- For 5 or less dimensions, performs well for regular responses

Outline

Proposal
HDMR

ANOVA method to decompose input space

$$\tilde{H}[u](Y) = u_0 + \sum_{i=1}^{N} u_i + \sum_{i_1=1}^{N} \sum_{i_2=1}^{i_1-1} u_{ij} + \cdots + c_{i_1,\ldots,i_N},$$

$$u_0 \equiv \int dy_1 \cdots \int dy_N u(Y),$$

$$u_i \equiv \int dy_1 \cdots \int dy_{i-1} \int dy_{i+1} \cdots \int dy_N u(Y) - u_0$$

Proposal

HDMR

Sobol' sensitivity coefficients

$$\mathcal{S}_i = \frac{\text{var}\left\{u_i\right\}}{\text{var}\left\{\tilde{H}[u](Y)\right\}}$$

$$\text{var}\left\{u(Y)\right\} = \sum_{i=1}^{N} \mathcal{S}_i + \sum_{i_1=1}^{N} \sum_{i_2=1}^{i_1-1} \mathcal{S}_{ij} + \cdots + \mathcal{S}_{i_1,\ldots,i_N}$$

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Proposal
HDMR

Problem: Costly integrals (even low-level expansion)
Solution: Cut-HDMR, reference point $\hat{Y} = (\hat{y}_1, \ldots, \hat{y}_N)$
Let $u(y_i) \equiv u(\hat{y}_1, \ldots, \hat{y}_{i-1}, \; y_i \;, \hat{y}_{i+1}, \ldots, \hat{y}_N)$

$$H[u](Y) = h_0 + \sum_{i=1}^{N} h_i + \sum_{i_1=1}^{N} \sum_{i_2=1}^{i_1-1} h_{ij} + \cdots + h_{i_1,\ldots,i_N},$$

$$\begin{aligned}
h_0 &\equiv u(\hat{Y}),\\
h_i &\equiv u(y_i) - u_0,\\
h_{ij} &\equiv u(y_i, y_j) - u_i - u_j - u_0
\end{aligned}$$

Proposal

HDMR

Problem with Cut-HDMR: Terms not orthogonal

$$\mathcal{S}_i \neq \frac{\text{var}\{h_i\}}{\text{var}\{H[u](Y)\}} \equiv \xi_{ij}$$

$$\text{var}\{u(Y)\} \neq \sum_{i=1}^{N} \xi_i + \sum_{i_1=1}^{N} \sum_{i_2=1}^{i_1-1} \xi_{ij} + \cdots + \xi_{i_1,\ldots,i_N}$$

However, no integrals!

Proposal
HDMR

Next step: HDMR terms are SCgPC

$$H[u](Y) = h_0 + \sum_{i=1}^{N} h_i + \sum_{i_1=1}^{N} \sum_{i_2=1}^{i_1-1} h_{ij} + \cdots + h_{i_1,\ldots,i_N},$$

$$\begin{aligned} h_0 &\equiv u(\hat{Y}), \\ h_i &\equiv G[u](y_i) - u_0, \\ h_{ij} &\equiv G[u](y_i, y_j) - u_i - u_j - u_0 \end{aligned}$$

Benefit: most terms low dimension, regular

Proposal

Adaptive HDMR

Better than HDMR: Adaptive HDMR with Adaptive SCgPC
Choose terms based on impact parameters ξ, η

- Evaluate the reference (all mean) case.
- Construct all HDMR first-order SCgPC models.
- While not converged:
  - Using existing subset impacts, predict importance of future subsets
  - Consider impact of adding polynomials to existing subset gPCs
  - Choose: expand existing subsets or add new subsets
  - If contribution of new HDMR expectation less than tolerance, convergence

Proposal

Adaptive HDMR

Example, $N = 3$

$H[u](Y)$	$=$	$h_0 +$	$h_1 +$	$h_2 +$	$h_3 +$	$h_{12} +$	$h_{13} +$	$h_{23} +$	h_{123}
		0	1	1	1				
SCgPC Order:		0	2	1	1				
		0	2	1	1	1			
		0	2	2	1	1			
		0	2	2	2	1			
		0	2	2	2	1	1		

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Proposal

Mammoth

Mammoth: MOOSE framework MultiApp

- RattleS$_N$ake: Neutron Transport code
  - Provides power distributions
  - Tens of thousands of inputs
- Bison: Fuel Performance code
  - Analyzes fuel: stress, temperature, displacement
  - Dozens of inputs

Goal: Demonstrate Adaptive HDMR with Adaptive SCgPC

Proposal

Special Thanks

Proposal

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