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Hybrid multilevel Monte Carlo polynomial chaos method for global sensitivity analysis

Michael Merritt[1]

Gianluca Geraci, Mike Eldred, Teresa Portone[2]

NC State University, Department of Mathematics[1]
Sandia National Laboratories, Department of Optimization and Uncertainty Quantification[2]

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Sensitivity analysis for high-fidelity models

- Global sensitivity analysis (GSA) aims to quantify the importance of uncertain input parameters
- Our main tool, the Sobol' index, is a variance-based GSA metric
- There are numerous practical challenges associated with GSA:
  - Quantity of interest (QoI) may be high-dimensional in terms of inputs
  - High-fidelity (high-accuracy) QoIs are often prohibitively expensive to evaluate
  - Many GSA methods rely on repeated sampling of the QoI
- We consider hierarchies of related models, organized by fidelity and computational cost
- **Goal:** perform GSA efficiently on expensive, high-fidelity models by leveraging information from cheaper, lower-fidelity models

Polynomial chaos expansions (PCE)

- Given a scalar-valued function $Q(\boldsymbol{\xi})$ with random vector $\boldsymbol{\xi} \in \mathbb{R}^d$, the PCE of Q is

$$\tilde{Q}(\boldsymbol{\xi}) = \sum_{k=0}^{P} \beta_k \Psi_k(\boldsymbol{\xi}) \quad \text{and} \quad \beta_k = \frac{\mathbb{E}[Q(\boldsymbol{\xi})\Psi_k(\boldsymbol{\xi})]}{\mathbb{E}[\Psi_k^2(\boldsymbol{\xi})]},$$

  where $\{\Psi_k\}_{k\geq 1}$ is a family of orthogonal polynomials, β_k's are PCE coefficients, and P controls the number of expansion terms

- The choice of basis is meant to guarantee orthogonality with respect to the distribution of $\boldsymbol{\xi}$ (e.g. Legendre polynomials and uniform distribution)[1]

- The number of PCE terms (for a total order construction) is

$$P + 1 = \frac{(r+d)!}{r!d!}, \quad \text{where } r = \text{total polynomial order}$$

[1] Le Maitre and Knio, *Spectral methods for uncertainty quantification: with applications to computational fluid dynamics*, 2010.

PCE for GSA

- One can compute Sobol' indices from a PCE as a post process
- We define the Sobol' indices w.r.t. $u \subseteq \{1, \dots, d\}$ as

$$S_u(Q) = \frac{\mathbb{V}ar[\mathbb{E}[Q(\boldsymbol{\xi}) \mid \boldsymbol{\xi}_u]]}{\mathbb{V}ar[Q(\boldsymbol{\xi})]} = \frac{\mathcal{S}_u}{\mathbb{V}ar[Q(\boldsymbol{\xi})]} \quad \text{and} \quad T_i(Q) = \sum_{v \ni i} S_v(Q),$$

  where S_u is the main effect and T_i is the total index
- The Sobol' indices of $\tilde{Q}$ are computed as

$$S_u(\tilde{Q}) = \frac{\sum_{k \in K_u} \beta_k^2 \ \mathbb{E}[\Psi_k^2]}{\sum_{k=1}^{P} \beta_k^2 \ \mathbb{E}[\Psi_k^2]}$$

  where K_u denotes the set of PCE terms that only depend on the parameter subset $\boldsymbol{\xi}_u$

Computing PCE coefficients

- A variety of methods exist for computing PCE coefficients, including quadrature, sparse quadrature, regression, etc.[2]
- Recalling $\beta_k = \frac{\mathbb{E}[Q\Psi_k]}{\mathbb{E}[\Psi_k^2]}$, we estimate the spectral projection, $\mathbb{E}[Q\Psi_k]$, using Monte Carlo (MC) integration
- Consider the MC estimator,

$$\beta_k = \frac{\mathbb{E}[Q\Psi_k]}{\mathbb{E}[\Psi_k^2]} \approx \frac{1}{\mathbb{E}[\Psi_k^2]} \frac{1}{N} \sum_{i=1}^{N} Q\left(\boldsymbol{\xi}^{(i)}\right) \Psi_k\left(\boldsymbol{\xi}^{(i)}\right),$$

  where $\boldsymbol{\xi}^{(i)}$ denotes the ith realization out of N i.i.d. realizations of $\boldsymbol{\xi}$
- The variance of this estimator is proportional to N^{-1}, thus convergence will be slow

[2] Le Maitre and Knio, *Spectral methods for uncertainty quantification: with applications to computational fluid dynamics*, 2010.

Multilevel Monte Carlo (MLMC)

- Consider the hierarchy of models $Q_0, Q_1, \ldots, Q_L$ with a "level" index ℓ and respective costs $C_0 \leq C_1 \leq \cdots \leq C_L$
- We can decompose the kth spectral projection,

$$\mathbb{E}[Q\Psi_k] = \sum_{\ell=0}^{L} \mathbb{E}[(Q_\ell - Q_{\ell-1})\Psi_k] := \sum_{\ell=0}^{L} \mathbb{E}[P_{\ell,k}], \quad \text{where} \quad Q_{-1} = 0$$

- This decomposition leads to the multilevel Monte Carlo[3] (MLMC) estimator for β_k

$$\hat{\beta}_k = \frac{1}{b_k} \sum_{\ell=0}^{L} \frac{1}{N_\ell} \sum_{i=1}^{N_\ell} P_{\ell,k}^{(i)}$$

- One can then derive an optimal sample allocation by solving, for example,

$$\min_{N_0,\ldots,N_L} \mathbb{V}ar[\hat{\beta}_k] = \frac{1}{b_k^2} \sum_{\ell=0}^{L} \frac{\mathbb{V}ar[P_{\ell,k}]}{N_\ell} \quad \text{subject to} \quad C_{tot} = \sum_{\ell=0}^{L} N_\ell C_\ell \leq \bar{C}$$

[3] Giles, "Multilevel Monte Carlo methods", 2015.

Hybrid MLMC-PCE Method

- **Goal:** Optimally allocate multilevel samples $(N_\ell)_{\ell=0}^L$ in order to minimize the variance of the MLMC estimator for a Sobol' index
- We consider the target $\mathbb{V}ar[\hat{\mathcal{S}}_u]$, which we seek to minimize by means of some optimal sample allocation
- The variance of the PCE-estimated variance can be written as

$$\mathbb{V}ar\left[\sum_{k=1}^{P} b_k\ \hat{\beta}_k^2\right] = \sum_{k=1}^{P} b_k^2\ \mathbb{V}ar[\hat{\beta}_k^2] + \sum_{k\neq z} b_k b_z \mathbb{C}ov\left[\hat{\beta}_k^2, \hat{\beta}_z^2\right],$$

  where we can select the terms corresponding to any $\hat{\mathcal{S}}_u$
- We derived expressions for $\mathbb{V}ar\left[\hat{\beta}_k^2\right]$ and $\mathbb{C}ov\left[\hat{\beta}_k^2, \hat{\beta}_z^2\right]$ in terms of $(N_\ell)_{\ell=0}^L$ and the relevant statistical moments of the QoI
- From this, we can estimate $\mathbb{V}ar[\hat{\mathcal{S}}_u]$ and optimize the sample allocation, $(N_\ell)_{\ell=0}^L$

Optimal sample allocation for GSA

The optimal sample allocation problem has various formulations. Given a subset $u \subseteq \{1, \ldots, d\}$, an upper bound on cost, $\bar{C}$, and a reduction factor, ε, we have:

1. $$\min_{N_0,\ldots,N_L} \mathbb{V}ar[\mathcal{S}_u] \quad \text{s.t.} \quad C_{tot} = \sum_{\ell=0}^{L} N_\ell C_\ell \leq \bar{C}$$

2. $$\min_{N_0,\ldots,N_L} C_{tot} = \sum_{\ell=0}^{L} N_\ell C_\ell \quad \text{s.t.} \quad \mathbb{V}ar[\mathcal{S}_u] \leq \varepsilon \, (\mathbb{V}ar[\mathcal{S}_u])_0$$

- These formulations have been extended to arbitrary sets of Sobol' indices (e.g. all first order indices, all total indices, the full QoI variance)
- In practice, we compute the optimal allocation numerically using tools in SciPy
- The flexibility of the hybrid method in optimizing the allocation distinguishes it from other comparable GSA methods

Numerical results

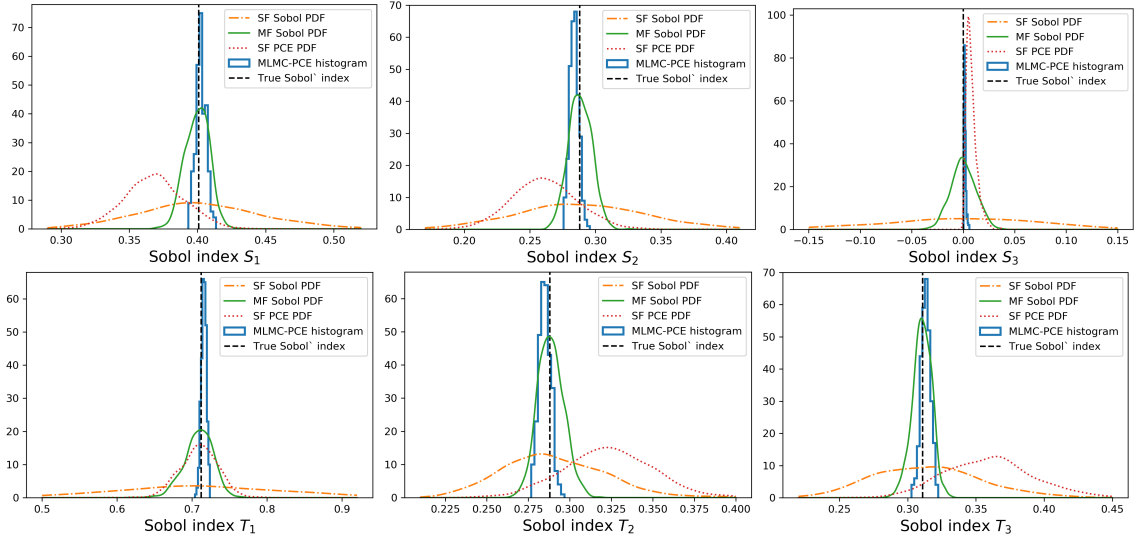
- We present a three-level version of the Ishigami function[4]:

$$
\begin{aligned}
q_0(\boldsymbol{\theta}) &= \sin(\theta_1) + (0.6)\ \ a\sin^2(\theta_2) + (9)b\theta_3^2\sin(\theta_1), \quad C_0 = 0.001 \\
q_1(\boldsymbol{\theta}) &= \sin(\theta_1) + (0.95) \qquad a\sin^2(\theta_2) + b\theta_3^4\sin(\theta_1), \quad C_1 = 0.05 \\
q_2(\boldsymbol{\theta}) &= \sin(\theta_1) + \qquad\qquad a\sin^2(\theta_2) + b\theta_3^4\sin(\theta_1), \quad C_2 = 1.0
\end{aligned}
$$

- We can compute all PCE and Sobol' terms analytically for verification
- We compare 4 competing GSA methods, using an equivalent cost for each:
  1. Our hybrid MLMC-PCE method
  2. Standard MC method ("Saltelli sampling")
  3. Single-fidelity PCE method
  4. The recent multifidelity GSA method of Qian and Willcox[4] (MF-Saltelli)

[4] Qian et al., "Multifidelity Monte Carlo estimation of variance and sensitivity indices", 2018.

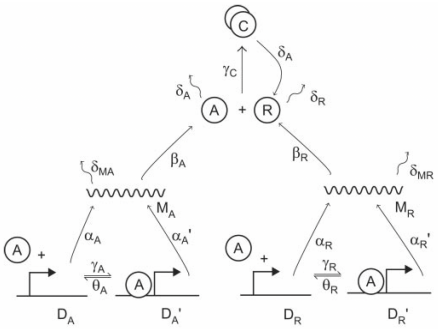
Comparison of hybrid method with other GSA methods



PDFs of first order Sobol' indices, S_i, and total Sobol' indices, T_i, $i = 1, 2, 3$.

Chemical reaction networks

- We consider an ODE model for the genetic oscillator system from chemical kinetics[5]
- The system has 16 uncertain parameters, which are the reaction rate constants



Reaction	Propensity Function
$P_a \to P_a + mRNA_a$	$\alpha_A P_a$
$P_a{-}A \to P_a{-}A + mRNA_a$	$\alpha_a \alpha_A P_a{-}A$
$P_r \to P_r + mRNA_r$	$\alpha_R P_r$
$P_r{-}A \to P_r{-}A + mRNA_r$	$\alpha_r \alpha_R P_r{-}A$
$mRNA_a \to mRNA_a + A$	$\beta_A mRNA_a$
$mRNA_r \to mRNA_r + R$	$\beta_R mRNA_r$
$A + R \to C$	$\gamma_C AR$
$P_a + A \to P_a{-}A$	$\gamma_A P_a A$
$P_a{-}A \to P_a + A$	$\theta_A P_a{-}A$
$P_r + A \to P_r{-}A$	$\gamma_R P_r A$
$P_r{-}A \to P_r + A$	$\theta_R P_r{-}A$
$A \to \emptyset$	$\delta_A A$
$R \to \emptyset$	$\delta_R R$
$mRNA_a \to \emptyset$	$\delta_{MA} mRNA_a$
$mRNA_r \to \emptyset$	$\delta_{MR} mRNA_r$
$C \to R$	$\delta_A' C$

Parameter	Value
α_A	50.0
α_R	0.01
β_A	50.0
β_R	5.0
γ_C	20.0
γ_A	1.0
θ_A	50.0
γ_R	1.0
θ_R	1.0
δ_A	1.0
δ_R	0.2
δ_{MA}	10.0
δ_{MR}	0.5
δ_A'	1.0
α_a	10.0
α_r	5000

- **Goal:** use the hybrid MLMC-PCE method with optimal sample allocation for efficient GSA. QoI: time-integrated value of the repressor protein, $R(t)$

[5] Vilar et al., "Mechanisms of noise-resistance in genetic oscillators", 2002.

Optimization results

- Setup: 3 level genetic oscillator ODE, cost: $[0.025, 0.125, 1.0]$, total order 2 PCE basis, sample profile: $[10^5, 10^4, 10^3]$
- We will solve the following problem

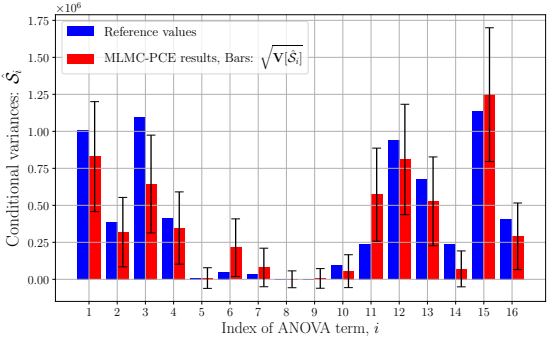
$$\min_{N_0,\ldots,N_L} \sum_u \mathbb{V}ar[\mathcal{S}_u] \quad \text{s.t.} \quad C_{tot} \leq 1000$$

- Basis reordered and truncated by choosing a threshold on $r_i = \dfrac{\sum_{k=1}^{i} b_k \ \hat{\beta}_k^2}{\widehat{\mathbb{V}ar[Q]}}$

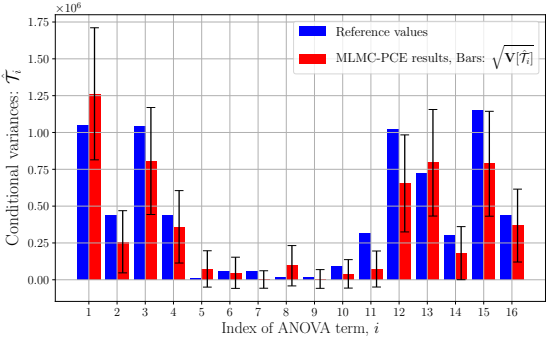
	22 PCE modes, $r = 1.0$		All 153 PCE modes	
Target	Opt. profile	Opt. profile (scaled)	Opt. profile	Opt. profile (scaled)
All main	$[6727, 3726, 191]$	$[35.2, 19.5, 1]\cdot 191$	$[6717, 3726, 191]$	$[35.2, 19.5, 1]\cdot 191$
All total	$[6714, 3711, 194]$	$[34.6, 19.1, 1]\cdot 194$	$[6666, 3694, 197]$	$[33.8, 18.8, 1]\cdot 197$
$\widehat{\mathbb{V}[\mathbb{V}[Q]]}$	$[6609, 3646, 205]$	$[32.2, 17.8, 1]\cdot 205$	$[9748, 3325, 180]$	$[54.2, 18.5, 1]\cdot 180$

Chemical reaction network results

- We compute all first order and all total indices (using optimal sampling) and report confidence intervals computed from $\mathbb{V}ar[\hat{\mathcal{S}}_i]$ and $\mathbb{V}ar[\hat{\mathcal{T}}_i], i = 1, \ldots, 16$



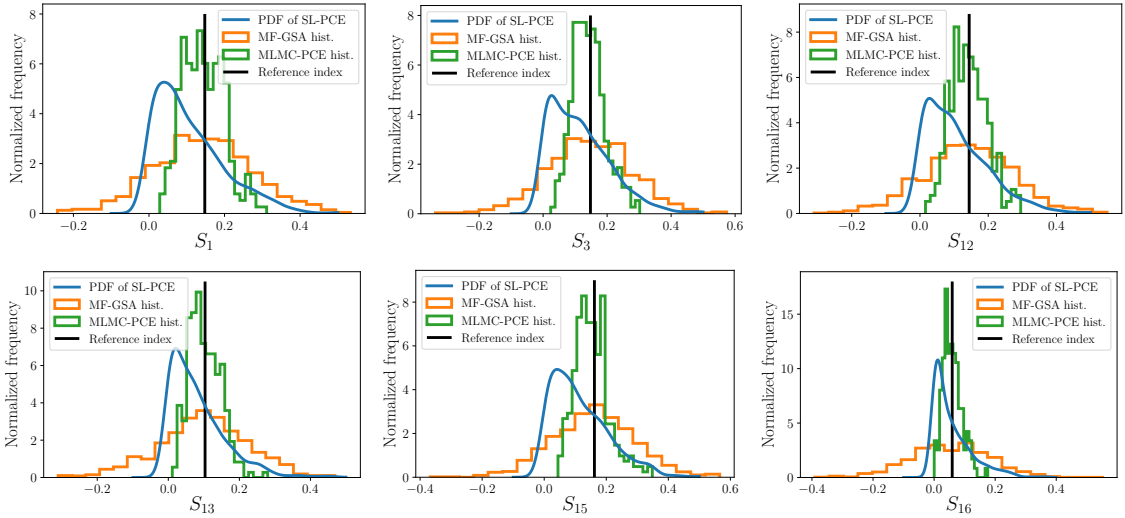
Left: first order conditional variances



Right: total order conditional variances

- Next, we compare the performance of the hybrid method against other GSA methods

Chemical reaction network results



Distributions of a few first order indices, comparing SL-PCE, MF-GSA, and the hybrid method.

Challenges/Ongoing Work

- Investigated multiple optimization frameworks for sample allocation
- Investigated the effects of using unbiased estimators and various strategies for PCE basis truncation
- Produced a library of Python tools implementing the hybrid method
- Published an early version in Sandia's CSRI Summer Proceedings:
  Michael Merritt et al. "Hybrid multilevel Monte Carlo polynomial chaos method for global sensitivity analysis". *Sandia CSRI Summer Proceedings 2020* (2020)
- A journal article is in preparation
- Future work includes extensions to the multifidelity MC and approximate control variate frameworks[6]

[6] Gorodetsky et al., "A generalized approximate control variate framework for multifidelity uncertainty quantification", 2020.

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Overview of derivation process

- Write PCE estimators as sums of MC samples
- Expand squared sums and group together terms with nonzero covariance
- Rewrite variances or covariances in terms of raw moments
- Below is an example of the single level covariance expression:

$$\mathbb{C}ov\left[(\hat{\beta}_k)^2, (\hat{\beta}_z)^2\right] = \mathbb{C}ov\left[\left(\frac{1}{\mathbb{E}[\Psi_k^2]N}\sum_{i=1}^{N} Q^i\Psi_k^i\right)^2, \left(\frac{1}{\mathbb{E}[\Psi_z^2]N}\sum_{i=1}^{N} Q^i\Psi_z^i\right)^2\right]$$
$$= \frac{1}{\mathbb{E}[\Psi_k^2]^2\mathbb{E}[\Psi_z^2]^2}\left[\frac{\mathbb{E}[Q^4\Psi_k^2\Psi_z^2] - \mathbb{E}[Q^2\Psi_k^2]\mathbb{E}[Q^2\Psi_z^2]}{N^3} + \frac{(2N-2)\ (\mathbb{E}[Q^3\Psi_k^2\Psi_z]\mathbb{E}[Q\Psi_z] - \mathbb{E}[Q^2\Psi_k^2]\mathbb{E}[Q\Psi_z]^2)}{N^3}\right.$$
$$+ \frac{(2N-2)\ \left(\mathbb{E}[Q^3\Psi_z^2\Psi_k]\mathbb{E}[Q\Psi_k] - \mathbb{E}[Q\Psi_k]^2\mathbb{E}[Q^2\Psi_z^2]\right)}{N^3} + \frac{(2N-2)\ \left(\mathbb{E}[Q^2\Psi_k\Psi_z]^2\right)}{N^3}$$
$$\left. + \frac{4(N-1)(N-2)\ (\mathbb{E}[Q^2\Psi_k\Psi_z]\mathbb{E}[Q\Psi_k]\mathbb{E}[Q\Psi_z])}{N^3} - \frac{(4N^2-10N+6)\ (\mathbb{E}[Q\Psi_k]^2\mathbb{E}[Q\Psi_z]^2)}{N^3}\right]$$

- We have derived estimators for all MLMC variances and covariances[7]

[7] Merritt et al., "Hybrid multilevel Monte Carlo polynomial chaos method for global sensitivity analysis", 2020.