Hybrid multi-level Monte Carlo polynomial chaos method for global sensitivity analysis

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Sensitivity analysis for expensive models

- We consider high-dimensional and high-fidelity models:
  - Large number of uncertain parameters
  - Model represents the system of interest with high accuracy
  - High accuracy models are often prohibitively expensive
- Sensitivity analysis allows one to characterize the uncertainty in such models
- Performing sensitivity analysis can be prohibitively expensive due to the larger number of function evaluations required
- We consider a hierarchy of related models, which are organized by fidelity/accuracy and the corresponding cost
- Our goal is to perform sensitivity analysis efficiently on a high-fidelity model by leveraging the information provided by the cheaper, lower-fidelity models

Polynomial chaos expansions - NISP

- Given a scalar-valued function $Q(\boldsymbol{\xi})$ with random vector $\boldsymbol{\xi}$, the polynomial chaos expansion (PCE) of Q is given as

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

  where $\{\Psi_k\}_{k\geq 1}$ is a family of orthogonal polynomials, the β_k's are the corresponding PCE coefficients, and P is the truncation level
- For $\boldsymbol{\xi} = (\xi_1, \ldots, \xi_d)$, the polynomial basis is a tensor product of 1D orthogonal polynomials

$$\Psi_k(\xi_1, \ldots, \xi_d) = \prod_{i=1}^{d} \psi_{a_i^k}(\xi_i), \quad a^k = (a_1^k, \ldots, a_d^k),$$

  where a_i^k is a multi-index, denoting the degree of the ith 1D polynomial for the kth multivariate polynomial

Polynomial chaos expansions

- The choice of polynomial basis is made to guarantee orthogonality with respect to the distribution of $\boldsymbol{\xi}$
(e.g. Normal and Hermite, Uniform and Legendre, etc.)[1]
- Computing a PCE can become prohibitively expensive for a high-dimensional Q due to the number of terms involved,

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

- PCE is also well-suited for functions with some underlying smoothness

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

PCE for GSA

- One notable benefit of PCE is the ability to compute global sensitivity analysis (GSA) indices as a post-process
- Given a square-integrable, scalar-valued $f(\boldsymbol{\xi})$ with $\boldsymbol{\xi} = (\xi_1, \dots, \xi_d)$, the ANOVA decomposition of f is defined as:

$$f(\boldsymbol{\xi}) = f_0 + \sum_{i=1}^{d} f_i(\xi_i) + \sum_{i<j}^{d} f_{i,j}(\xi_i, \xi_j) + \cdots + f_{1,\dots,d}(\boldsymbol{\xi}_{1,\dots,d})$$

where

$$\begin{aligned} f_0 &= \mathbb{E}[f(\boldsymbol{\xi})] \\ f_i(\xi_i) &= \mathbb{E}[f(\boldsymbol{\xi})|\xi_i] - f_0 \\ f_{i,j}(\xi_i, \xi_j) &= \mathbb{E}[f(\boldsymbol{\xi})|\xi_i, \xi_j] - f_i - f_j - f_0 \ \ \dots \end{aligned}$$

- For a PC expansion, computing the ANOVA decomposition simply involves summing the proper terms

PCE for GSA

- Given the ANOVA decomposition of f, one may define the Sobol' indices w.r.t. $u \subseteq \{1, \ldots, d\}$ as:

$$S_u(f) = \frac{\mathbb{V}ar[\mathbb{E}[f(\boldsymbol{\xi}) \mid \boldsymbol{\xi}_u]]}{\mathbb{V}ar[f(\boldsymbol{\xi})]} \quad \text{and} \quad T_u(f) = \sum_{v \cap u \neq \emptyset} S_v(f),$$

  where the order of S_u is $|u|$ and T_u is a total index
- In order to compute the Sobol' indices of Q_{PC}, we have

$$\mathbb{V}ar[Q_{PC}] = \mathbb{E}[Q_{PC}^2] - \mathbb{E}[Q_{PC}]^2 = \sum_{k=1}^{P} \beta_k^2 \, \mathbb{E}[\Psi_k^2]$$

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

- Here, K_u denotes the indices of the PCE terms that only depend on the parameter subset $\boldsymbol{\xi}_u$

PCE for GSA

- The limiting factors in computing GSA indices with a PCE are the error in each $\hat{\beta}_k$ and the truncation level P
- For many polynomial families, the norms $\mathbb{E}[\Psi_k^2]$ are known analytically, so the real cost in building a PCE is in computing the spectral projection, $\mathbb{E}[Q\Psi_k]$
- A variety of methods exist for this task, including quadrature methods, Galerkin projection, least squares approximations[2]
- We will estimate this expectation using Monte Carlo integration
- In the case of a high-dimensional Q, we will attempt to accelerate the estimation of $\mathbb{E}[Q\Psi_k]$ using a hierarchy of related models

[2] Crestaux, Le Maıtre, and Martinez, "Polynomial chaos expansion for sensitivity analysis".

Monte Carlo sampling

- Let $Q(\boldsymbol{\xi})$ be a scalar quantity of interest from a high-fidelity model, where $\boldsymbol{\xi}$ is a vector of uncertain parameters
- We want to compute $\mathbb{E}[Q(\boldsymbol{\xi})]$ and we define the estimator

$$\hat{Q} = \frac{1}{N}\sum_{i=1}^{N} Q(\boldsymbol{\xi}^i)$$

- If $\boldsymbol{\xi}^1, \ldots, \boldsymbol{\xi}^N$ are i.i.d., then $\hat{Q}$ is an unbiased estimator (i.e. $\mathbb{E}[\hat{Q}] = \mathbb{E}[Q]$) and the mean-squared error (MSE) is given by

$$\mathbb{E}[(\hat{Q} - \mathbb{E}[Q])^2] = \frac{\mathbb{V}ar[Q]}{N} + (\mathbb{E}[\hat{Q} - Q])^2 = \frac{\mathbb{V}ar[Q]}{N}$$

- Reducing the MSE through sampling alone can be expensive because convergence will be slow: rate $\mathcal{O}(N^{-1/2})$
- Another approach is to decrease $\mathbb{V}ar[Q]$, without changing $\mathbb{E}[Q]$
- In general, estimator bias is not guaranteed to be zero

Multi-level Monte Carlo

- Let $Q_0, Q_1, \dots, Q_L$ denote a hierarchy of models parameterized by a scalar ℓ with associated costs $C_0 \leq C_1 \leq \cdots \leq C_L$ for each "level"
  - A natural example of this is solving a differential equation on a mesh where the number of points is controlled by the index ℓ for Q_ℓ
- If we want to estimate $\mathbb{E}[Q_L]$, we can use

$$\mathbb{E}[Q_L] = \sum_{\ell=0}^{L} \mathbb{E}[Q_\ell - Q_{\ell-1}], \quad Q_{-1} = 0$$

- This defines a multi-level Monte Carlo (MLMC) estimator

$$\hat{Q}_L^{ML} = \sum_{\ell=0}^{L} Q_\ell \widehat{- Q}_{\ell-1} = \sum_{\ell=0}^{L} \frac{1}{N_\ell} \sum_{i=1}^{N_\ell} Q_\ell^i - Q_{\ell-1}^i,$$

with the associated cost $C_{tot} = \sum_{\ell=0}^{L} N_\ell (C_\ell + C_{\ell-1})$

Multi-level Monte Carlo

- The MSE of an unbiased $\hat{Q}_L^{ML}$ can be expressed as

$$\mathbb{E}\left[(\hat{Q}_L^{ML} - \mathbb{E}[Q_L])^2\right] = \mathbb{V}ar[\hat{Q}_L^{ML}] = \sum_{\ell=0}^{L} \frac{\mathbb{V}ar\left[Q_\ell - Q_{\ell-1}\right]}{N_\ell},$$

  where independent sampling among levels removes any covariance
- The goal then is to minimize $\mathbb{V}ar[\hat{Q}_L^{ML}]$ by appropriately allocating N_ℓ samples to each level
- In the case that $\mathbb{V}ar[Q_\ell - Q_{\ell-1}]$ is decreasing for $\ell \to L$, one is able to evaluate the majority of samples at the cheaper levels
- The optimization problem:

$$\min_{N_0,\dots,N_L} C_{tot} \quad \text{s.t.} \quad \mathbb{V}ar[\hat{Q}_L^{ML}] \leq \varepsilon^2$$

  can be solved in closed form for the optimal sample allocation[3]

[3] Giles, "Multilevel monte carlo methods".

MLMC for PCE formulation

- Returning to the estimation of PCE coefficients, we decompose the spectral projection as

$$\mathbb{E}[Q\Psi_k] = \sum_{\ell=0}^{L} \mathbb{E}[(Q_\ell - Q_{\ell-1})\Psi_k],$$

which leads to the multi-level estimator

$$\hat{\beta}_k = \frac{1}{\mathbb{E}[\Psi_k^2]} \sum_{\ell=0}^{L} (Q_\ell \widehat{- Q_{\ell-1}})\Psi_k = \frac{1}{\mathbb{E}[\Psi_k^2]} \sum_{\ell=0}^{L} \frac{1}{N_\ell} \sum_{i=1}^{N_\ell} (Q_\ell^i - Q_{\ell-1}^i)\Psi_k^i$$

- In this case, the variance of the estimator can be expressed as

$$\mathbb{V}ar[\hat{\beta}_k] = \frac{1}{\mathbb{E}[\Psi_k^2]^2} \sum_{\ell=0}^{L} \frac{\mathbb{V}ar[(Q_\ell - Q_{\ell-1})\Psi_k]}{N_\ell}$$

MLMC for PCE formulation

- We want to find an optimal sampling allocation scheme that balances the estimator variance and the cost of sampling the QoIs
- We have the optimization problem:

$$\min_{N_0,\dots,N_L} \sum_{\ell=0}^{L} N_\ell C_\ell + \mu^2 \left(\mathbb{V}ar[\hat{\beta}_k] - \varepsilon^2 \right),$$

where μ^2 is a Lagrange multipler and ε^2 is the target variance.
- The optimal sample allocation[4] can be shown to be

$$N_\ell = \mu \sqrt{\frac{\mathbb{V}ar[(Q_\ell - Q_{\ell-1})\Psi_k]}{\mathbb{E}[\Psi_k^2]\ C_\ell}} \quad \text{where} \tag{1}$$

$$\mu = \varepsilon^{-2} \sum_{\ell=0}^{L} \frac{\sqrt{\mathbb{V}ar[(Q_\ell - Q_{\ell-1})\Psi_k]\ C_\ell}}{\mathbb{E}[\Psi_k^2]} \tag{2}$$

[4] Giles, "Multilevel monte carlo methods".

Computing ensembles of PCE coefficients

- For the purposes of GSA, we need a set of PCE coefficients. Thus for L levels and P coefficients, we estimate

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

- Ideally, we share N_ℓ samples when estimating $\mathbb{E}[(Q_\ell - Q_{\ell-1})\Psi_k]$ for $k = 1, \ldots, P$
- We have two initial sample allocation schemes:
    1. Individual: estimate each β_k separately, each $\hat{\beta}_k$ has the target variance, with no sample sharing this is expensive
    2. Worst case: same samples at each level where N_ℓ is computed to minimize $\max_k \mathbb{V}ar[(Q_\ell - Q_{\ell-1})\Psi_k]$ - the worst case coefficient
- These schemes work for more general sets of PCE coefficients

Example algorithm - estimating a single PCE coefficient

Algorithm 1 Estimate kth PCE coefficient

Input: Multi-level model, target accuracy ε^2, number of pilot samples N, coefficient to estimate k, max iterations

Output: coefficients $\hat{\beta}_k$, estimator variance $\mathbb{V}[\hat{\beta}_k]$, function evaluations

Draw N pilot samples: $\boldsymbol{\xi}_{pilot}$ {Distribution included with the model}

Evaluate Ψ_k and $Q_\ell - Q_{\ell-1}$ for $\ell = 0, \ldots, L$ at $\boldsymbol{\xi}_{pilot}$

while $\mathbb{V}ar[\hat{\beta}_k] > \varepsilon^2$ and iteration $<$ max iterations **do**

    for $\ell = 0, \ldots, L$ **do**

        Estimate $\mathbb{V}ar[(Q_\ell - Q_{\ell-1})\Psi_k]$

        Compute N_ℓ in order to minimize $\mathbb{V}ar[\hat{\beta}_k]$ {See (1) and (2)}

        Draw additional samples of $\boldsymbol{\xi}$

        Evaluate functions Ψ_k and $Q_\ell - Q_{\ell-1}$ for $\ell = 0, \ldots, L$

    end for

    Estimate $\mathbb{E}[(Q_\ell - Q_{\ell-1})\Psi_k]$

    Compute $\mathbb{V}ar[\hat{\beta}_k]$

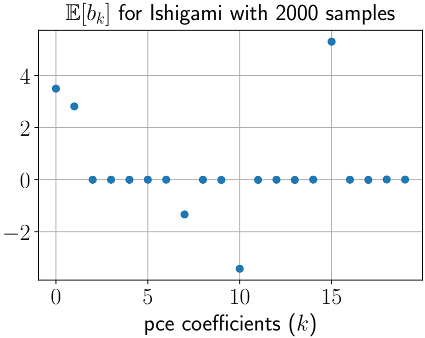
end while

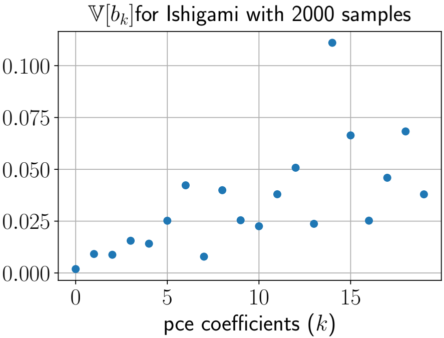
Compute final estimate of $\hat{\beta}_k$

Example with Ishigami function

$$f(\boldsymbol{\xi}) = \sin(\xi_1) + a\sin^2(\xi_2) + b\xi_3\sin(\xi_1)$$
$$\xi_i \sim \mathcal{U}[-\pi,\pi],\ i=1,2,3 \quad a=7,\ b=0.1$$

- We take the first 20 PCE modes and compute 2000 realizations of the coefficients, looking at the mean and variance of $\hat{\beta}_k$

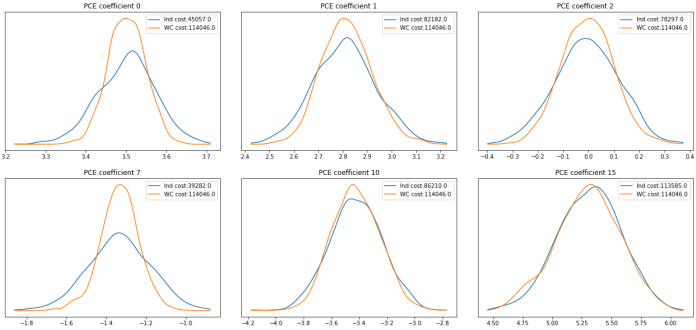




Example with multi-level Ishigami

$$
\begin{aligned}
Q &= \sin(\xi_1) + a\sin^2(\xi_2) + b\xi_3^4\sin(\xi_1) \\
Q_0 &: a = (0.6)7.0,\ \ b = (0.6)0.1,\ \ C_0 = 1 \\
Q_1 &: a = (0.8)7.0,\ \ b = (0.8)0.1,\ \ C_1 = 10 \\
Q_2 &: a = (1.0)7.0,\ \ b = (1.0)0.1,\ \ C_2 = 100
\end{aligned} \tag{3}
$$

- We compare the individual and worst-case methods for



The worst case coefficient is β_{15}. Cost is provided in the legend.

Globally optimal sample allocation scheme

- We want a sample allocation method that balances the total cost and variance for each of the estimated coefficients
- Moreover, the real goal is in targeting the Sobol' indices, minimizing the variance of $\hat{S}_u$. Thus given a PCE

$$Q_{PC} = \sum_{k=1}^{P} \hat{\beta}_k \Psi_k \quad \text{we consider} \quad \mathbb{V}ar\left[\frac{\sum_{k \in K_u} (\hat{\beta}_k)^2 \ \mathbb{E}[\Psi_k^2]}{\sum_{k=1}^{P} (\hat{\beta}_k)^2 \ \mathbb{E}[\Psi_k^2]}\right]$$

- We instead can target particular indices by subdividing

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

- Expressions are needed for $\mathbb{V}ar[\hat{\beta}_k^2]$ and $\mathbb{C}ov\left[\hat{\beta}_k^2, \hat{\beta}_z^2\right]$ in terms of moments of $Q_\ell - Q_{\ell-1}$, Ψ_k, and Ψ_z

Other concerns

- Given an unbiased estimator for β_k (i.e. $\mathbb{E}[\hat{\beta}_k] = \beta_k$), the quantity $(\hat{\beta}_k)^2$ will be a biased estimator for β_k^2, resulting in error
- This will require a bias correction to be incorporated into the estimator for each β_k^2
- This, in turn, will require unbiased estimators for the moments of the relevant $Q_\ell - Q_{\ell-1}$ and Ψ_k terms
- If $\mathbb{V}ar[\hat{\beta}_k]$ increases with k (as expected), how does one determine the appropriate truncation level?

Ongoing work

- Completed derivation of multi-level variances and covariances
- Derivation of sample allocation strategy, targeting a given accuracy for a set of GSA indices
- Rigorous evaluation of the efficiency of PCE and MLMC-PCE hybrid for GSA, considering the effects of dimension and regularity
- Extension of this hybrid MLMC-PCE method to multi-fidelity models and Approximate Control Variates[5]

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

References

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