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Global Sensitivity Analysis for Stochastic Collocation

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Non-intrusive stochastic expansion methods for uncertainty quantication (UQ) has received a great deal of attention the past decade because of their rigorous mathematical foundations and their ability to efficiently accurately characterize the probablilistic metrics of complex engineering systems. Furthermore, their formulations are especially amenable to variance-based global sensitivity analysis, and in this paper, we describe a novel method to obtain variance-based sensitivity information as a post-processing procedure to the construction of these stochastic expansion models.

I. Introduction

Modern analysis and design of engineering systems are typically performed with the use of large-scale computer simulations. As a part of understanding model behavior, the ability to characterize relationships between the inputs (whose values are often uncertain) and the output is important. Because of model complexity and implementation nuance this relationship, commonly known as output sensitivity or simply sensitivity, is often obscured. The goal of sensitivity analysis is precisely to identify the most significant factors or variables affecting the model predictions or results. This is not to be confused with uncertainty analysis, which is to quantify the uncertainty in model results due to the uncertainty in the inputs; for sensitivitiy analysis, inputs need not be uncertain. The greatest barrier to conducting either of these analyses is the computational cost to run the simulations. In fact, the popularity of stochastic expansion methods can be attributed almost entirely to their ability to accurately quantify system uncertainty with much fewer function evaluations than traditional sampling methods. Following variance-based approaches to global sensitivity analysis, we present an effective strategy for computing input sensitivities that does not require additional function evaluations beyond those needed to construct the stochastic expansion. In this paper, we focus on the stochastic collocation (SC) class of expansion models.

The remaining sections of this paper outline the basics of variance-based sensitivity analysis and stochastic collocation followed by the specific formulation of sensitivity indices for a stochastic collocation representation. In particular, Section II presents the notation and formulation used for variance-based decomposition and definitions for the sensitivity metrics. Section III discusses the fundamentals of SC for uncertainty quantification (UQ) and includes a detailed derivation for the sensitivity metrics within the machinery of SC. Finally, Section IV provides results for a variety of response functions which compare this paper's formulation with analogous work in polynomial chaos expansion[1] and Latin Hypercube sampling. Section V concludes with some suggestions for future work that can further couple the relationship between SA and UQ.

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II. Variance-Based Sensitivity Analysis

Traditional sensitivity analysis examines the local influence of a parameter x_j to a response $Y(\mathbf{x})$ by its partial derivative at a single point in the parameter space. Alternatively, global sensitivity analysis (GSA) captures the effect of a parameter by measuring some aggregate contribution over the entire space. Using variance as an indicator for importance is not new and can be shown to underlie the regression based methods[2,3,7] for sensitivity analysis. This section begins with some general concepts to variance-based GSA and concludes with the definitions for sensitivity as defined in the method of Sobol'. For details on other variance based methods, the authors refer readers to the literature.[8]

A. Notation

Here, we introduce some notation that will be used in the rest of the paper. Let u be a multi-index such that $u \subseteq \mathcal{U}$, where $\mathcal{U} = \{1, 2, \ldots, d\}$. Let us also define $x_u = \{x_i \,|\, \forall i \in u\}$ as the set of variables whose indices lies in u, and $\hat{f}_u$ to be a basis function that depends only on x_u. Furthermore, let u' be the complement of u and defined such that $\{u \bigcup u'\} = \mathcal{U}$ and $\{u \bigcap u'\} = \emptyset$. Finally, define the collection of all u to be the power set $\mathcal{F} = \mathcal{P}(\mathcal{U})$.

B. ANOVA Decomposition

Consider a square-integrable function $f(\mathbf{x}) : \Omega \mapsto \mathbb{R}$, where $\mathbf{x} = (x_1, x_2, \ldots x_d)$ is decomposed in the form:

$$f(\mathbf{x}) = \sum_{\mathcal{F}} \hat{f}_u(x_u) \tag{1}$$

The decomposition is of analysis-of-variance (ANOVA) type if it satisfies the following properties:

$$\begin{aligned} \int \hat{f}_u(x_u) d\mu(x_u) &= 0 \quad \text{for} \quad u \neq \emptyset & (2) \\ \int \hat{f}_u(x_u) \hat{f}_v(x_v) d\mu(\mathbf{x}) &= 0 \quad \text{for} \quad u \neq v & (3) \\ \mathrm{Var}[f] &= \sum_{u \in \mathcal{F} \neq \emptyset} \mathrm{Var}[\hat{f}_u] & (4) \end{aligned}$$

It is simple to show that these properties are satisfied when the basis function $\hat{f}_u$ is defined as

$$\hat{f}_u = \begin{cases} \int f(\mathbf{x}) d\mu(x_{u'}) - \sum_{w \subset u} \hat{f}_w(x_w) & \text{for} \quad u \neq \emptyset \\ \int f(\mathbf{x}) d\mu(\mathbf{x}) & \text{for} \quad u = \emptyset \end{cases} \tag{5}$$

C. Global Sensitivity Analysis via Method of Sobol'

In GSA, the general approach to measuring the importance of a parameter x_i is to compare its variance of the conditional expectation, $\mathrm{Var}_{X_i}[\mathrm{E}(Y \,|\, x_i)]$, against the total variance, $\mathrm{Var}[Y]$. Sobol'[12] generalized this idea to the ANOVA decomposition, which allows one to measure the importance of x_u via the variance of $\hat{f}_u$; namely, its contribution to the total variance of f. These sensitivity measures, collectively known as Sobol' indices, are called main effect indices S_u and total effect indices S_{T_u} respectively defined to be:

$$\begin{aligned} S_u &= \frac{D_u}{D} & (6) \\ S_{T_u} &= \sum_{\{v \in \mathcal{F} \,|\, u \subseteq v\}} \frac{D_v}{D} & (7) \end{aligned}$$

where

$$D = \mathrm{Var}[f] \tag{8}$$

$$\begin{aligned} D_{u\neq\emptyset} &= \mathrm{Var}[\hat{f}_u] \\ &= \int \hat{f}_u^2 d\mu(x_u) - \left(\int \hat{f}_u d\mu(x_u)\right)^2 \\ &= \int \hat{f}_u^2 d\mu(x_u) \end{aligned} \tag{9}$$

Using the orthogonality property of the ANOVA decomposition in Equation 3 we can show that the partial variance D_u simplifies to

$$D_u = \int \left(\int f(\mathbf{x}) d\mu(x_{u'})\right)^2 d\mu(x_u) - \sum_{w\subset u} \int \left(\hat{f}_w(x_w)\right)^2 d\mu(x_u) \tag{10}$$

where the details can be found in Appendix A.

These indices have very intuitive interpretations. S_u measures the main effect of x_u by evaluating the variance contribution of the basis function $\hat{f}_u$ that depends *strictly* on the set of variables in x_u. Similarly, S_{T_u} measures the total effect of x_u by evaluating the variance contribution of *all* basis functions $\hat{f}_v$ whose dependencies include x_u. In practice, we are typically concerned only with the total effect of sets u which have a cardinality of one, and thus, henceforth we will denote the total effect to be S_{T_j} for $j = 1, 2, \ldots, d$.

III. Stochastic Collocation Expansion

The stochastic collocation (SC) method is an attractive technique for uncertainty quantification (UQ) due to its strong mathematical basis and ability to produce functional representations of stochastic variability. Moreover, because the probability space is merely an extension of the existing parameter space, SC has the flexibility to expand over non-probabilistic variables as well.[15] SC forms interpolation functions by evaluating the model at prescribed collocation point sets derived from tensor product or sparse grids. More specifically, the SC expansion is formed as a weighted tensor product of one-dimensional Lagrange polynomials l_j^i. Because l_j^i has the feature of being equal to 1 at its particular collocation point j and 0 at all other points, the coefficients, or weights, of the expansion are just the corresponding response values $f(x_j^i)$. For d variables and m_{i_k} collocation points in dimension i_k the multi-dimensional expansion can be written as:

$$f(\mathbf{x}) \approx \sum_{j_1=1}^{m_{i_1}} \cdots \sum_{j_d=1}^{m_{i_d}} f(x_{j_1}^{i_1}, \ldots, x_{j_d}^{i_d})(l_{j_1}^{i_1} \otimes \cdots \otimes l_{j_d}^{i_d}) \tag{11}$$

The key to maximizing performance with this approach is to use the appropriate abscissas defined by Gauss quadrature rules. Greater theoretical detail on this topic can be found in the literature[9,10] so we only present the most salient result relevant to this paper: the weighted integral of a polynomial of up to order $2n-1$ can be computed exactly using an n term summation when the abscissas are appropriately chosen. More accurately, the abscissas are chosen to the n zeros $\{\xi_i\}_{i=1}^n$ of the n^{th} order polynomial ψ_n^p belonging to the family of polynomials $\{\psi_i^p\}_{i=0}^\infty$ that are optimal for a given weight function $p(x)$.

$$\int g(x)p(x)dx = \sum_{i=1}^n w_i g(\xi_i),\ g \in \mathbb{P}^m,\ m \leq 2n-1 \tag{12}$$

$$\psi_n^p(\xi_i) = 0, \quad i = 1, 2, \ldots n \tag{13}$$

Following these rules, it can be shown[11] that the stochastic expansion converges exponentially in L_2. Once the optimal polynomial basis is determined, the set of $(m_{i_k}-1)^{th}$ order, one-dimensional Lagrange polynomials can be constructed by the expression

$$l_{j_k}^{i_k}(x^{i_k}) = \prod_{s=1\neq j_k}^{m_{i_k}-1} \frac{x^{i_k} - \xi_s^{i_k}}{\xi_{j_k}^{i_k} - \xi_s^{i_k}}, \quad j = 1, 2, \ldots, m_{i_k} \tag{14}$$

where ξ^{i_k} represents the m_{i_k} zeros of the $\psi^{p_{i_k}}_{m_{i_k}}$. Finally, Equation 11 is obtained by taking the tensor product over each dimension $i_k = 1, 2, \ldots, d$. Note that the analytic moments (e.g. mean and variance) and the sensitivity indices can be computed without actually constructing these interpolants.

A. Computing the Sobol' Indices

We assume that a set of abscissa and related function evaluations have been performed. The most critical part of computing the Sobol' indices is evaluating the nested integral in Equation 10. Let's first evaluate the inner integral with our interpolatory representation of f.

$$\int f(\mathbf{x}) d\mu(x_{u'}) = \int \sum_{j_1=1}^{m_{i_1}} \cdots \sum_{j_d=1}^{m_{i_d}} f(x^{i_1}_{j_1}, \ldots, x^{i_d}_{j_d})(l^{i_1}_{j_1} \otimes \cdots \otimes l^{i_d}_{j_d}) d\mu(x_{u'}) \tag{15}$$

For notational consistency, let's separate those interpolants that are dependent on x_u from those that are dependent on $x_{u'}$ and integrate over $x_{u'}$ using Gauss quadrature rules. Consider some $u \in \mathcal{F}$ with cardinality k

$$\begin{aligned}
\int f(\mathbf{x}) d\mu(x_{u'}) &= \sum_{j_1=1}^{m_{i_1}} \cdots \sum_{j_d=1}^{m_{i_d}} f(x^{i_1}_{j_1}, \ldots, x^{i_d}_{j_d}) \int (\mathbf{l}^{u'} \otimes \mathbf{l}^u) d\mu(x_{u'}) \\
&= \sum_{j_1=1}^{m_{i_1}} \cdots \sum_{j_d=1}^{m_{i_d}} f(x^{i_1}_{j_1}, \ldots, x^{i_d}_{j_d})(\mathbf{w}^{u'} \otimes \mathbf{l}^u) \qquad (16)
\end{aligned}$$

where

$$\begin{aligned}
u &= \{u_1, \ldots, u_k\} && (17)\\
\mathbf{w}^u &= w^{i_{u_1}}_{j_{u_1}} \otimes \cdots \otimes w^{i_{u_k}}_{j_{u_k}} && (18)\\
\mathbf{l}^u &= l^{i_{u_1}}_{j_{u_1}} \otimes \cdots \otimes l^{i_{u_k}}_{j_{u_k}} && (19)
\end{aligned}$$

We can simplify the form of Equation 16 by combining the tensor product of weights $\mathbf{w}^{u'}$ with the coefficients $f(x^{i_1}_{j_1}, \ldots, x^{i_d}_{j_d})$ to form new weighted coefficients $h(x^{i_{u_1}}_{j_{u_1}}, \ldots, x^{i_{u_k}}_{j_{u_k}})$.

$$\begin{aligned}
\sum_{j_1=1}^{m_{i_1}} \cdots \sum_{j_d=1}^{m_{i_d}} f(x^{i_1}_{j_1}, \ldots, x^{i_d}_{j_d})(\mathbf{w}^{u'} \otimes \mathbf{l}^u) &= \sum_{j_{u_1}=1}^{m_{i_{u_1}}} \cdots \sum_{j_{u_k}=1}^{m_{i_{u_k}}} \left(\sum_{j_{u'_1}=1}^{m_{i_{u'_1}}} \cdots \sum_{j_{u'_{d-k}}=1}^{m_{i_{u'_{d-k}}}} f(x^{i_1}_{j_1}, \ldots, x^{i_d}_{j_d}) \mathbf{w}^{u'} \right) (\mathbf{l}^u) \\
&= \sum_{j_{u_1}=1}^{m_{i_{u_1}}} \cdots \sum_{j_{u_k}=1}^{m_{i_{u_k}}} h(x^{i_{u_1}}_{j_{u_1}}, \ldots, x^{i_{u_k}}_{j_{u_k}})(\mathbf{l}^u) \qquad (20)
\end{aligned}$$

Now, let us evaluate the outer integral. Following the aforementioned result from Gauss quadrature that states an m_{i_k} term summation can exactly integrate any univariate polynomial of degree less than $2m_{i_k}$, we can *exactly* integrate the square of Equation 20 since its highest order univariate polynomial is of degree $2(m_{i_k} - 1)$. Furthermore, if we note the one-dimensional Lagrangian interpolants, l^i_j, to have the property

$$l^q_r(x^q_p) \cdot l^q_s(x^q_p) = \begin{cases} 1 & p = s = r \\ 0 & \text{otherwise} \end{cases} \tag{21}$$

the outer integral can be simplified to

$$\int \left(\sum_{j_{u_1}=1}^{m_{i_{u_1}}} \cdots \sum_{j_{u_k}=1}^{m_{i_{u_k}}} h(x^{i_{u_1}}_{j_{u_1}}, \ldots, x^{i_{u_k}}_{j_{u_k}})(\mathbf{l}^u) \right)^2 d\mu(x_u) = \sum_{j_{u_1}=1}^{m_{i_{u_1}}} \cdots \sum_{j_{u_k}=1}^{m_{i_{u_k}}} h^2(x^{i_{u_1}}_{j_{u_1}}, \ldots, x^{i_{u_k}}_{j_{u_k}}) \otimes \mathbf{w}^u \tag{22}$$

and when substituted back into Equation 10 we obtain the final result

$$D_u = \sum_{j_{u_1}=1}^{m_{i_{u_1}}} \cdots \sum_{j_{u_k}=1}^{m_{i_{u_k}}} h^2(x_{j_{u_1}}^{i_{u_1}}, \ldots, x_{j_{u_k}}^{i_{u_k}}) \otimes \mathbf{w}^u - \sum_{w \subset u} D_w \tag{23}$$

Clearly, the evaluation of D_u is simply a recursive computation of Equation 22. To minimize computational effort, it is recommended to solve for the partial variances of u in order of increasing cardinality. The total effect indices S_{T_j} can be trivially computed by summing over the corresponding main effect indices S_u.

This result shows that D_u, and by virtue S_u, can be evaluated without any additional function evaluations or the need to solve for additional weights/abscissas. Moreover, this methodology extends to sparse grids, which are merely linear combinations of tensor product grids, provided that the abscissas of the tensor product grids follow Gauss quadrature rules.

IV. Implementation and Results

The analytic expressions for sensitivity presented in this paper were implemented and verified in Sandia National Labs' software framework DAKOTA (Design and Analysis Toolkit for Terascale Applications),[13] and the source code can be obtained from the version of the day release.

A series of tests were conducted to compare the method in this paper with existing approaches for GSA. For the first four tests, the test functions were chosen to be simple polynomials whose sensitivities could be obtained analytically. The remaining three functions are common for testing sensitivity methods.[7] For each test, we compare the performance of our approach to traditional Latin Hypercube sampling (LHS) and to an analogous implementation for generalized polynomial chaos expansion[1] (PCE) on a variety of tensor (tr[order]) and sparse (sp[level]) grids.

The results show that GSA via stochastic expansion methods dramatically outperforms LHS and highlights the excellent convergence rates when the functions are of sufficient regularity. While this trend is unlikely to extend to higher dimensional problems where expansion methods suffer from the curse of dimensionality, this problem may be mitigated with the use of anisotropic grids.[15] For nearly all the cases, we see identical results for PCE and SC when the abscissas are chosen from tensor grids, which is consistent with their behavior in computing analytic moments.[14] The exception can be found in Table 7 but this is likely a consequence of computational roundoff as opposed to solution disagreement. A related consequence is the possibility of negative sensitivity indices; the specific formulation to the PCE approach does not require subtraction and eliminates the possibility of castastrophic cancellation. As mentioned in Section A, the evaluation of the Sobol' Indices are exact with respect to the SC representation presented in this paper; therefore, the accuracy and convergence behavior of the stochastic expansion models are transferred, without loss, to the sensitivity analysis. It follows that performing GSA, like solving for mean or variance, will converge at a reduced rate for non-smooth functions in L_2. An example of reduced performance can be seen in Table 6 for the non-smooth Sobol' g-Function.

Table 1: Sobol' Indices for Rosenbrock function $f = 100(x_2 - x_1^2)^2 + (1 - x_1)^2$

Approach	Func Eval	Grid Type	S_1	S_2	S_{T_1}	S_{T_2}
LHS	400	-	4.06127e-01	3.72295e-01	5.83464e-01	8.63159e-01
LHS	2000	-	2.84753e-01	3.72392e-01	6.24346e-01	7.86900e-01
LHS	4000	-	1.37274e-01	3.12069e-01	7.15033e-01	8.58973e-01
LHS	20000	-	1.73756e-01	2.82603e-01	7.09529e-01	8.58973e-01
LHS	40000	-	1.53909e-01	3.03002e-01	7.02275e-01	8.34521e-01
LHS	200000	-	1.47978e-01	2.79160e-01	7.21528e-01	8.46659e-01
PCE	4	tr2	2.09627e-01	1.97593e-01	8.02407e-01	7.90373e-01
PCE	9	tr3	1.20599e-01	2.93134e-01	7.06866e-01	8.79401e-01
PCE	25	tr5	1.53198e-01	2.82267e-01	7.17733e-01	8.46802e-01
PCE	36	tr6	1.53198e-01	2.82267e-01	7.17733e-01	8.46802e-01
PCE	13	sp2	2.84129e-01	7.15871e-01	2.84129e-01	7.15871e-01
PCE	65	sp4	1.52832e-01	2.82389e-01	7.17611e-01	8.47168e-01
PCE	321	sp6	1.53198e-01	2.82267e-01	7.17733e-01	8.46802e-01
PCE	1537	sp8	1.53198e-01	2.82267e-01	7.17733e-01	8.46802e-01
SC	4	tr2	2.09627e-01	1.97593e-01	8.02407e-01	7.90373e-01
SC	9	tr3	1.20599e-01	2.93134e-01	7.06866e-01	8.79401e-01
SC	25	tr5	1.53198e-01	2.82267e-01	7.17733e-01	8.46802e-01
SC	36	tr6	1.53198e-01	2.82267e-01	7.17733e-01	8.46802e-01
SC	13	sp2	1.54653e-01	2.90070e-01	7.09930e-01	8.45347e-01
SC	65	sp4	1.53198e-01	2.82267e-01	7.17733e-01	8.47802e-01
SC	321	sp6	1.53198e-01	2.82267e-01	7.17733e-01	8.46802e-01
SC	1537	sp8	1.53198e-01	2.82267e-01	7.17733e-01	8.46802e-01
TRUE	-	-	1.53198e-01	2.82267e-01	7.17733e-01	8.46802e-01

Table 2: Sobol' Indices for $f = (x_1 - 1)^4 + (x_2 - 1)^4$

Approach	Func Eval	Grid Type	S_1	S_2	S_{T_1}	S_{T_2}
LHS	400	-	4.64092e-01	5.41070e-01	5.41070e-01	4.95429e-01
LHS	2000	-	4.76199e-01	5.24702e-01	5.24412e-01	5.04126e-01
LHS	4000	-	4.87648e-01	5.12858e-01	4.91029e-01	5.12199e-01
LHS	20000	-	5.02428e-01	4.97679e-01	5.09053e-01	5.02952e-01
LHS	40000	-	4.89737e-01	5.10320e-01	4.93644e-01	4.91893e-01
LHS	200000	-	4.95960e-01	5.04051e-01	4.99884e-01	4.97408e-01
PCE	4	tr2	5.00000e-01	5.00000e-01	5.00000e-01	5.00000e-01
PCE	9	tr4	5.00000e-01	5.00000e-01	5.00000e-01	5.00000e-01
PCE	25	tr6	5.00000e-01	5.00000e-01	5.00000e-01	5.00000e-01
PCE	36	tr8	5.00000e-01	5.00000e-01	5.00000e-01	5.00000e-01
PCE	17	sp2	4.95299e-01	4.95299e-01	5.04701e-01	5.04701e-01
PCE	97	sp4	4.99964e-01	4.99964e-01	5.00036e-01	5.00036e-01
PCE	305	sp6	4.99964e-01	2.82267e-01	5.00036e-01	5.00036e-01
PCE	705	sp8	4.99985e-01	4.99985e-01	5.00015e-01	5.00015e-01
SC	4	tr2	5.00000e-01	5.00000e-01	5.00000e-01	5.00000e-01
SC	9	tr4	5.00000e-01	5.00000e-01	5.00000e-01	5.00000e-01
SC	25	tr6	5.00000e-01	5.00000e-01	5.00000e-01	5.00000e-01
SC	36	tr8	5.00000e-01	5.00000e-01	5.00000e-01	5.00000e-01
SC	17	sp2	5.28463e-01	5.28463e-01	4.81537e-01	4.81537e-01
SC	97	sp4	4.98911e-01	4.98911e-01	5.01089e-01	5.01089e-01
SC	305	sp6	5.00132e-01	5.00132e-01	4.99868e-01	4.99868e-01
SC	705	sp8	4.99987e-01	4.99987e-01	5.00013e-01	5.00013e-01
TRUE	-	-	5.00000e-01	5.00000e-01	5.00000e-01	5.0000e-01

Table 3: Sobol' Indices for $f = x_1^2 - \frac{x_2}{2}$

Approach	Func Eval	Grid Type	S_1	S_2	S_{T_1}	S_{T_2}
LHS	400	-	8.11961e-01	1.88291e-01	8.21556e-01	1.73615e-01
LHS	2000	-	8.21845e-01	1.78386e-01	8.24890e-01	1.84108e-01
LHS	4000	-	8.05006e-01	1.95046e-01	7.98831e-01	1.99964e-01
LHS	20000	-	8.16281e-01	1.83728e-01	8.01936e-01	1.90491e-01
LHS	40000	-	8.09067e-01	1.90941e-01	8.11791e-01	1.86326e-01
LHS	200000	-	8.10709e-01	1.89293e-01	8.09960e-01	1.87076e-01
LHS	400000	-	8.09877e-01	1.90123e-01	8.09727e-01	1.91407e-01
PCE	4	tr2	8.00000e-01	2.00000e-01	8.00000e-01	2.00000e-01
PCE	16	tr4	8.10127e-01	1.89873e-01	8.10127e-01	1.89873e-01
PCE	36	tr6	8.10127e-01	1.89873e-01	8.10127e-01	1.89873e-01
PCE	64	tr8	8.10127e-01	1.89873e-01	8.10127e-01	1.89873e-01
PCE	13	sp2	8.00000e-01	2.00000e-01	8.00000e-01	2.00000e-01
PCE	65	sp4	8.10127e-01	1.89873e-01	8.10127e-01	1.89873e-01
PCE	321	sp6	8.10127e-01	1.89873e-01	8.10127e-01	1.89873e-01
PCE	1537	sp8	8.10127e-01	1.89873e-01	8.10127e-01	1.89873e-01
SC	4	tr2	8.00000e-01	2.00000e-01	8.00000e-01	2.00000e-01
SC	16	tr4	8.10127e-01	1.89873e-01	8.10127e-01	1.89873e-01
SC	36	tr6	8.10127e-01	1.89873e-01	8.10127e-01	1.89873e-01
SC	64	tr8	8.10127e-01	1.89873e-01	8.10127e-01	1.89873e-01
SC	13	sp2	8.10127e-01	1.89873e-01	8.10127e-01	1.89873e-01
SC	65	sp4	8.10127e-01	1.89873e-01	8.10127e-01	1.89873e-01
SC	321	sp6	8.10127e-01	1.89873e-01	8.10127e-01	1.89873e-01
SC	1537	sp8	8.10127e-01	1.89873e-01	8.10127e-01	1.89873e-01
TRUE	-	-	8.10127e-01	1.89873e-01	8.10127e-01	1.89873e-01

Table 4: Sobol' Indices for $f = x_2^2 - \frac{x_1}{2}$

Approach	Func Eval	Grid Type	S_1	S_2	S_{T_1}	S_{T_2}
LHS	400	-	1.67513e-01	8.33176e-01	1.61058e-01	8.13480e-01
LHS	2000	-	1.79156e-01	8.21072e-01	1.91097e-01	8.34315e-01
LHS	4000	-	1.77226e-01	8.22785e-01	1.82247e-01	8.31742e-01
LHS	20000	-	1.98623e-01	8.01388e-01	1.89664e-01	8.11840e-01
LHS	40000	-	1.82394e-01	8.17612e-01	1.82364e-01	8.14272e-01
LHS	200000	-	1.88671e-01	8.11330e-01	1.87260e-01	8.08251e-01
LHS	400000	-	1.91731e-01	8.08270e-01	1.91781e-01	8.11015e-01
PCE	4	tr2	2.00000e-01	8.00000e-01	2.00000e-01	8.00000e-01
PCE	16	tr4	1.89873e-01	8.10127e-01	1.89873e-01	8.10127e-01
PCE	36	tr6	1.89873e-01	8.10127e-01	1.89873e-01	8.10127e-01
PCE	64	tr8	1.89873e-01	8.10127e-01	1.89873e-01	8.10127e-01
PCE	13	sp2	2.00000e-01	8.00000e-01	2.00000e-01	8.00000e-01
PCE	65	sp4	1.89873e-01	8.10127e-01	1.89873e-01	8.10127e-01
PCE	321	sp6	1.89873e-01	8.10127e-01	1.89873e-01	8.10127e-01
PCE	1537	sp8	1.89873e-01	8.10127e-01	1.89873e-01	8.10127e-01
SC	4	tr2	2.00000e-01	8.00000e-01	2.00000e-01	8.00000e-01
SC	16	tr4	1.89873e-01	8.10127e-01	1.89873e-01	8.10127e-01
SC	36	tr6	1.89873e-01	8.10127e-01	1.89873e-01	8.10127e-01
SC	64	tr8	1.89873e-01	8.10127e-01	1.89873e-01	8.10127e-01
SC	13	sp2	1.89873e-01	8.10127e-01	1.89873e-01	8.10127e-01
SC	65	sp4	1.89873e-01	8.10127e-01	1.89873e-01	8.10127e-01
SC	321	sp6	1.89873e-01	8.10127e-01	1.89873e-01	8.10127e-01
SC	1537	sp8	1.89873e-01	8.10127e-01	1.89873e-01	8.10127e-01
TRUE	-	-	1.89873e-01	8.10127e-01	1.89873e-01	8.10127e-01

Table 5: Sobol' Indices for $f = \frac{(x_2+0.5)^4}{(x_1+0.5)^2}$

Approach	Func Eval	Grid Type	S_1	S_2	S_{T_1}	S_{T_2}
LHS	400	-	6.22785e-01	6.56084e-01	2.07789e-01	9.07812e-01
LHS	2000	-	3.29550e-01	5.28888e-01	4.88533e-01	7.41134e-01
LHS	4000	-	2.45757e-01	5.12369e-01	5.00761e-01	8.04966e-01
LHS	20000	-	2.65514e-01	4.98655e-01	5.14580e-01	7.86911e-01
LHS	40000	-	2.78471e-01	5.25235e-01	4.61501e-01	7.41430e-01
LHS	200000	-	2.64119e-01	5.19057e-01	4.87495e-01	7.40763e-01
PCE	4	tr2	2.43001e-00	5.89552e-01	4.10448e-01	7.56999e-01
PCE	9	tr3	2.52312e-01	5.30029e-01	4.69971e-01	7.47688e-01
PCE	25	tr5	2.61703e-01	5.11375e-01	4.88625e-01	7.38296e-01
PCE	36	tr6	2.61888e-01	5.11029e-01	4.88971e-01	7.38111e-01
PCE	13	sp2	3.29508e-01	6.70492e-01	3.29508e-01	6.70492e-01
PCE	65	sp4	2.63513e-01	5.15699e-01	4.84301e-01	7.36487e-01
PCE	321	sp6	2.61916e-01	5.10990e-01	4.89010e-01	7.38084e-01
PCE	1537	sp8	2.61914e-01	5.10983e-01	4.89017e-01	7.38086e-01
SC	4	tr2	2.43001e-00	5.89552e-16	4.10448e-01	7.56999e-01
SC	9	tr3	2.52312e-01	5.30029e-01	4.69971e-01	7.47688e-01
SC	25	tr5	2.61703e-01	5.11375e-01	4.88625e-01	7.38296e-01
SC	36	tr6	2.61888e-01	5.11029e-01	4.88971e-01	7.38111e-01
SC	13	sp2	2.48662e-01	4.28701e-01	5.71299e-01	7.51338e-01
SC	65	sp4	2.61310e-01	5.10192e-01	4.89808e-01	7.38690e-01
SC	321	sp6	2.61914e-01	5.10983e-01	4.89017e-01	7.38086e-01
SC	1537	sp8	2.61914e-01	5.10983e-01	4.89017e-01	7.38086e-01

Table 6: Sobol' Indices for the Sobol' g-Function $f = 2\prod_{j=1}^{5} \frac{|4x_j - 2| + a_j}{1 + a_j}$; $\mathbf{a} = [0, 1, 2, 4, 8]$

Approach	Func Eval	Grid Type	S_1	S_2	S_3	S_4	S_5
LHS	7000	-	5.91333e-01	1.47510e-01	6.75943e-02	3.35949e-02	-3.03280e-03
LHS	35000	-	6.12067e-01	1.59304e-01	6.93052e-02	3.49980e-02	5.59985e-03
LHS	70000	-	6.41981e-01	1.47865e-01	8.06888e-02	2.24580e-02	1.00360e-02
LHS	350000	-	6.35479e-01	1.60470e-01	6.89460e-02	2.34116e-02	7.40881e-03
LHS	700000	-	6.33740e-01	1.61268e-01	7.06319e-02	2.69095e-02	7.70250e-03
PCE	32	tr2	0.00000e-00	0.00000e-00	6.45161e-02	5.80645e-01	6.45161e-02
PCE	243	tr3	5.99272e-01	1.28220e-01	5.42446e-02	1.87888e-02	5.65402e-03
PCE	1024	tr4	6.46390e-01	1.68398e-01	7.58935e-02	2.76298e-02	8.59202e-03
PCE	3125	tr5	6.21874e-01	1.46776e-01	6.40180e-02	2.27051e-02	6.93877e-03
PCE	7776	tr6	6.40868e-01	1.63388e-01	7.30962e-02	2.64539e-02	8.19362e-03
PCE	16807	tr7	6.28497e-01	1.52461e-01	6.70901e-02	2.39619e-02	7.35684e-03
PCE	32678	tr8	6.38803e-01	1.61536e-01	7.20691e-02	2.60245e-02	8.04870e-03
PCE	61	sp2	1.00000e-00	0.00000e-00	0.00000e-00	0.00000e-00	0.00000e-00
PCE	801	sp4	8.09099e-01	1.47072e-01	3.03062e-02	3.10093e-06	1.35196e-02
PCE	6993	sp6	5.90683e-01	1.42680e-01	6.88667e-02	4.81179e-02	5.71842e-02
PCE	51713	sp8	6.33501e-01	1.56378e-01	6.71917e-02	2.25731e-02	7.56251e-03
PCE	135073	sp9	6.38484e-01	1.58953e-01	6.96320e-02	2.40071e-02	6.87157e-03
PCE	345665	sp10	6.35135e-01	1.58349e-01	6.99588e-02	2.49043e-02	7.84157e-03
SC	32	tr2	7.33333e-01	7.33333e-01	7.33333e-01	7.33333e-01	7.33333e-01
SC	243	tr3	5.99272e-01	1.28220e-01	5.42446e-02	1.87888e-02	5.65402e-03
SC	1024	tr4	6.46390e-01	1.68398e-01	7.58935e-02	2.76298e-02	8.59202e-03
SC	3125	tr5	6.21874e-01	1.46776e-01	6.40180e-02	2.27051e-02	6.93877e-03
SC	7776	tr6	6.40868e-01	1.63388e-01	7.30962e-02	2.64539e-02	8.19362e-03
SC	16807	tr7	6.28497e-01	1.52461e-01	6.70901e-02	2.39619e-02	7.35684e-03
SC	32768	tr8	6.38803e-01	1.61536e-01	7.20691e-02	2.60245e-02	8.04870e-03
SC	61	sp2	6.12891e-01	-9.96566e-02	-1.72524e-01	-1.90741e-01	-1.95295e-01
SC	801	sp4	4.90716e-01	-1.11982e-01	-2.18710e-01	-2.67265e-01	-2.83116e-01
SC	6993	sp6	5.67804e-01	1.24812e-02	-9.42399e-02	-1.50300e-01	-1.71939e-01
SC	51713	sp8	6.18682e-01	1.14612e-01	1.90377e-02	-3.11604e-02	-5.12477e-02
SC	135073	sp9	6.28501e-01	1.38023e-01	4.59513e-02	-1.93184e-03	-2.09570e-02
SC	345665	sp10	6.32966e-01	1.49798e-01	5.97042e-02	1.31964e-02	-5.12018e-03

Approach	Func Eval	Grid Type	S_{T_1}	S_{T_2}	S_{T_3}	S_{T_4}	S_{T_5}
LHS	7000	-	6.72206e-01	1.86171e-01	1.17109e-01	5.77715e-03	-9.02123e-03
LHS	35000	-	7.38654e-01	2.29849e-01	1.22343e-01	4.64609e-02	3.02973e-02
LHS	70000	-	7.40672e-01	2.40038e-01	1.11206e-01	5.98694e-02	2.47003e-02
LHS	350000	-	7.22398e-01	2.07503e-01	8.47251e-02	2.15933e-02	-4.94203e-03
LHS	700000	-	7.26557e-01	2.22900e-01	1.04010e-01	3.48873e-02	9.51685e-03
PCE	32	tr2	0.00000e-00	0.00000e-00	3.06452e-01	8.22581e-01	3.06452e-01
PCE	243	tr3	7.77373e-01	2.55631e-01	1.18106e-01	4.27975e-02	1.31030e-02
PCE	1024	tr4	7.11752e-01	2.14784e-01	9.98585e-02	3.69641e-02	1.15712e-02
PCE	3125	tr5	7.46823e-01	2.35794e-01	1.09272e-01	4.00032e-02	1.23773e-02
PCE	7776	tr6	7.19827e-01	2.19470e-01	1.01963e-01	3.76491e-02	1.17544e-02
PCE	16807	tr7	7.37548e-01	2.30066e-01	1.06711e-01	3.91829e-02	1.21614e-02
PCE	32768	tr8	7.22820e-01	2.21229e-01	1.02752e-01	3.79052e-02	1.18227e-02
PCE	61	sp2	1.00000e-00	0.00000e-00	0.00000e-00	0.00000e-00	0.00000e-00
PCE	801	sp4	8.09099e-01	1.47072e-01	3.03062e-02	3.10093e-06	1.35196e-02
PCE	6993	sp6	6.70159e-01	1.93377e-01	9.84211e-02	6.48668e-02	6.56442e-02
PCE	51713	sp8	7.30498e-01	2.21190e-01	1.02726e-01	4.15261e-02	1.91126e-02
PCE	135073	sp9	7.29110e-01	2.22165e-01	1.02688e-01	3.80657e-02	1.26439e-02
PCE	345665	sp10	7.25354e-01	2.22384e-01	1.03870e-01	4.02503e-02	1.53053e-02
SC	32	tr2	4.00000e-01	4.00000e-01	4.00000e-01	4.00000e-01	4.00000e-01
SC	243	tr3	7.77373e-01	2.55631e-01	1.18106e-01	4.27975e-02	1.31030e-02
SC	1024	tr4	7.11752e-01	2.14784e-01	9.98585e-02	3.69641e-02	1.15712e-02
SC	3125	tr5	7.46823e-01	2.35794e-01	1.09272e-01	4.00032e-02	1.23773e-02
SC	7776	tr6	7.19827e-01	2.19470e-01	1.01963e-01	3.76491e-02	1.17544e-02
SC	16807	tr7	7.37548e-01	2.30066e-01	1.06711e-01	3.91829e-02	1.21614e-02
SC	32768	tr8	7.22820e-01	2.21229e-01	1.02752e-01	3.79052e-02	1.18227e-02
SC	61	sp2	1.06778e-00	2.91470e-01	7.28675e-02	1.82169e-02	4.55422e-03
SC	801	sp4	9.89681e-01	3.25014e-01	1.54804e-01	5.61298e-02	1.61487e-02
SC	6993	sp6	8.44473e-01	2.60080e-01	1.23259e-01	4.68687e-02	1.49192e-02
SC	51713	sp8	7.58487e-01	2.31469e-01	1.08062e-01	4.02856e-02	1.27392e-02
SC	135073	sp9	7.41164e-01	2.26819e-01	1.05551e-01	3.90980e-02	1.22739e-02
SC	345665	sp10	7.32933e-01	2.24861e-01	1.04492e-01	3.85827e-02	1.20597e-02

Table 7: Sobol' Indices for the Ishigami Function
$f = \sin(2\pi x_1 - \pi) + 7\sin^2(2\pi x_2 - \pi) + 0.1(2\pi x_3 - \pi)^4 \sin(2\pi x_1 - \pi)$

Approach	Func Eval	Grid Type	S_1	S_2	S_3	S_{T_1}	S_{T_2}	S_{T_3}
LHS	5000	-	2.88446e-01	4.42871e-01	5.52915e-03	5.93029e-01	4.00977e-01	2.32240e-01
LHS	25000	-	3.05843e-01	4.37050e-01	-1.87194e-02	5.66739e-01	4.30240e-01	2.48935e-01
LHS	50000	-	3.28016e-01	4.34040e-01	-8.27517e-03	5.61866e-01	4.45603e-01	2.41798e-01
LHS	250000	-	3.15380e-01	4.42334e-01	5.15642e-03	5.55366e-01	4.43332e-01	2.46431e-01
LHS	500000	-	3.14020e-01	4.42135e-01	-9.13024e-04	5.60501e-01	4.33634e-01	2.36443e-01
PCE	8	tr2	1.00000e-00	3.62082e-32	3.62082e-32	1.00000e-00	7.01534e-32	2.12723e-31
PCE	27	tr3	4.15063e-01	4.39941e-01	2.69333e-32	5.60059e-01	4.39941e-01	1.44995e-01
PCE	64	tr4	3.99679e-01	3.15380e-01	2.17138e-32	6.84620e-01	3.15380e-01	2.84941e-01
PCE	216	tr6	4.05169e-01	2.80300e-01	1.56108e-30	7.19700e-01	2.80300e-01	3.14531e-01
PCE	25	sp2	1.00000e-00	1.36887e-31	0.00000e-00	1.00000e-00	1.36887e-31	0.00000e-00
PCE	177	sp4	6.71159e-01	4.44492e-02	1.83743e-07	9.55551e-01	9.59348e-02	2.32906e-01
PCE	1073	sp6	3.69705e-01	3.54341e-01	3.14446e-19	6.45659e-01	3.54790e-01	2.75516e-01
PCE	6017	sp8	3.16646e-01	4.37727e-01	1.91006e-31	5.62273e-01	4.37727e-01	2.45627e-01
PCE	32001	sp10	3.13906e-01	4.42411e-01	2.04501e-30	5.57589e-01	4.42411e-01	2.43684e-01
SC	8	tr2	1.00000e-00	0.00000e-00	-1.73938e-15	1.00000e-00	0.00000e-00	1.73938e-15
SC	27	tr3	4.15063e-01	4.39941e-01	9.02345e-17	5.60059e-01	4.39941e-01	1.44995e-01
SC	64	tr4	3.99679e-01	3.15380e-01	-4.35361e-16	6.84620e-01	3.15380e-01	2.84941e-01
SC	216	tr6	4.05169e-01	2.80300e-01	1.65375e-16	7.19700e-01	2.80300e-01	3.14531e-01
SC	25	sp2	6.46098e-02	9.35390e-01	0.00000e-00	6.46098e-02	9.35390e-01	0.00000e-00
SC	177	sp4	3.38208e-01	3.53492e-01	-5.12588e-16	6.46508e-01	3.53492e-01	3.08299e-01
SC	1073	sp6	3.13909e-01	4.42416e-01	1.53970e-15	5.57584e-01	4.42416e-01	2.43675e-01
SC	6017	sp8	3.13905e-01	4.42411e-01	-1.41137e-15	5.57589e-01	4.42411e-01	2.43684e-01
SC	32001	sp10	3.13905e-01	4.42411e-01	1.59101e-14	5.57589e-01	4.42411e-01	2.43684e-01

V. Conclusions

This paper presented a computationally effective approach to global sensitivity analysis on stochastic collocation models. Retaining the high levels of accuracy and exponential rates of convergence that have made stochastic expansion methods preferred over their counterparts, this approach allows sensitivity indices to be computed as a simple post-processing procedure to the construction of the expansion. Furthermore, inexpensive availability of this information presents an attrative route to adaptive grid refinement, helping to ameliorate the curse of dimensionality and subequently improving the efficacy of stochastic expansions methods.

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VII. Appendix

A. Derivation for Result in Equation 10

Firstly, expand the square of the integrand

$$
\begin{aligned}
\hat{f}_u^2 &= \left(\int f(\mathbf{x}) d\mu(x_{u'}) - \sum_{w \subset u} \hat{f}_w(x_w) \right)^2 \\
&= \left(\int \sum \hat{f}_u d\mu(x'_u) - \sum_{w \subset u} \hat{f}_w(x_w) \right)^2 \\
&= \left(\int \sum \hat{f}_u d\mu(x'_u) \right)^2 - 2 \int \sum \hat{f}_u d\mu(x'_u) \sum_{w \subset u} \hat{f}_w(x_w) + \left(\sum_{w \subset u} \hat{f}_w(x_w) \right)^2 \\
\int \hat{f}_u^2 d\mu(x_u) &= \int \left(\int \sum \hat{f}_u d\mu(x'_u) \right)^2 d\mu(x_u) - 2 \int \left(\int \sum \hat{f}_u d\mu(x'_u) \sum_{w \subset u} \hat{f}_w(x_w) \right) d\mu(x_u) \\
&\quad + \int \left(\sum_{w \subset u} \hat{f}_w(x_w) \right)^2 d\mu(x_u)
\end{aligned}
$$

Now applying the orthogonality property on the second term on the right hand side

$$
\begin{aligned}
2 \int \left(\int \sum_{\mathcal{F}} \hat{f}_u d\mu(x'_u) \sum_{w \subset u} \hat{f}_w(x_w) \right) d\mu(x_u) &= 2 \int \int \sum_{\mathcal{F}} \hat{f}_u(x_u) \sum_{w \subset u} \hat{f}_w(x_w) d\mu(x'_u) d\mu(x_u) \\
&= 2 \int \int \sum_{\mathcal{F}} \sum_{w \subset u} \hat{f}_u(x_u) \hat{f}_w(x_w) d\mu(\mathbf{x}) \\
&= 2 \int \sum_{w \subset u} \left(\hat{f}_u(x_u) \right)^2
\end{aligned}
$$

and similarly for the third term

$$
\int \left(\sum_{w \subset u} \hat{f}_w(x_w) \right)^2 d\mu(x_u) = \sum_{w \subset u} \int \left(\hat{f}_w(x_w) \right)^2 d\mu(x_u)
$$

Finally, substituting back into Equation 9

$$
\begin{aligned}
\int \hat{f}_u^2 d\mu(x_u) &= \int \left(\int \sum \hat{f}_u d\mu(x'_u) \right)^2 d\mu(x_u) - \int \sum_{w \subset u} \left(\hat{f}_w(x_w) \right)^2 d\mu(x_u) \\
&= \int \left(\int f(\mathbf{x}) d\mu(x'_u) \right)^2 d\mu(x_u) - \sum_{w \subset u} \int \left(\hat{f}_w(x_w) \right)^2 d\mu(x_u)
\end{aligned}
$$

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