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An efficient adaptive sparse grid collocation method through derivative estimation

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ABSTRACT

For uncertainty propagation of highly complex and/or nonlinear problems, one must resort to sample-based non-intrusive approaches (Le Maître and Knio, 2010). In such cases, minimizing the number of function evaluations required to evaluate the response surface is of paramount importance. Sparse grid approaches have proven effective in reducing the number of sample evaluations. For example, the discrete projection collocation method has the notable feature of exhibiting fast convergence rates when approximating smooth functions; however, it lacks the ability to accurately and efficiently track response functions that exhibit fluctuations, abrupt changes or discontinuities in very localized regions of the input domain. On the other hand, the piecewise linear collocation interpolation approach can track these localized variations in the response surface efficiently, but it converges slowly in the smooth regions. The proposed methodology, building on an existing work on adaptive hierarchical sparse grid collocation algorithm (Ma and Zabaras, 2009), is able to track localized behavior while also avoiding unnecessary function evaluations in smoother regions of the stochastic space by using a finite difference based one-dimensional derivative evaluation technique in all the dimensions. This derivative evaluation technique leads to faster convergence in the smoother regions than what is achieved in the existing collocation interpolation approaches. Illustrative examples show that this method is well suited to high-dimensional stochastic problems, and that stochastic elliptic problems with stochastic dimension as high as 100 can be dealt with effectively.

1. Introduction

Any model consists of input parameters which are inherently random. The uncertainty in the inputs naturally leads to an uncertainty in the output. Thus a single solution for the system using a fixed set of input parameters is not sufficient to describe the system completely. Thus, given the input uncertainties, it is of real interest to understand how these uncertainties propagate through the deterministic system model and result in uncertainties in the output solution. The quantification of the output uncertainties is a much more comprehensive descriptor of the system under study.

The traditional approach is to use random sampling techniques such as Monte Carlo (MC) method. It involves generating sets of realizations of all the input parameters following their individual probability distributions and then solving the deterministic code for each set of realizations. The advantage of this method is that it is easy to implement, it has a non-intrusive nature and the convergence rate is independent of the number of stochastic dimensions. On the other hand, it suffers from the drawback that it cannot easily approximate the solution space and usually only gives the output statistics, such as the mean and the variance. The convergence rate for this method is also very slow and is given by $\epsilon = O(N^{-1/2})$, where N is the total number of points at which the deterministic model is solved. Another major issue is the lack of control of the distribution of points in the domain which causes unwanted clustering and scattering of points. For complicated deterministic models with high stochastic dimensions, the number of realizations required for a certain high level of accuracy may be unrealistic. Approaches like Latin Hypercube sampling (LHS) [1], Importance Sampling [2,3], Quasi Monte Carlo Methods (using Halton sets, Sobol sets) [4] have been used successfully to achieve better convergence rates than the conventional Monte Carlo method. Artificial Neural Networks [5], In-situ Adaptive Tabulation (ISAT) [6] and the Inverse Distance Weighted (IDW) [7] technique are some of the approaches which can be used in tandem with Monte Carlo sampling as postprocessing tools to approximate the surface and hence build a surrogate surface.

Stochastic Galerkin Method [8] is a spectral approach which is a very popular tool for uncertainty propagation. It is a non-sampling

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approach where the unknown solution is projected onto the stochastic space spanned by a set of complete orthogonal polynomials after which the Galerkin projection is applied to minimize the error due to the gPC expansion and form a coupled set of deterministic equations. Wiener's original work on polynomial chaos [9] dealt with representation of a Gaussian random process using global Hermite polynomials. Initial work on the stochastic Galerkin method was done by Ghanem and Spanos [10] using the concept of polynomial chaos by Wiener and has been subsequently applied to various practical problems [11–15]. Generalized polynomial chaos (gPC) expansion was developed by Xiu and Karniadakis [16] by including various other global polynomial-random variable combinations, with a few applications found in [17–19]. This method is known to have a very high convergence rate given the response surface is sufficiently smooth in all the stochastic dimensions. In the presence of discontinuities or highly localized variations in the response surface, this method may fail to converge due to the well-known Gibbs phenomenon. Remedies for this problem have been sought using multielement gPC [20–22], piecewise polynomial basis [23], the wavelet basis [24] and basis enrichment of polynomial chaos expansions [25]. All these methods involve solution of a coupled system of deterministic equations which may be non-trivial to solve when the original deterministic model is very complex in itself. This is the drawback of the intrusive nature of the method. A way to get around this issue is the usage of non-intrusive collocation approaches.

The basic idea of non-intrusive collocation approaches is to strategically select points in the stochastic space. A surrogate response surface is then constructed based on these points to allow for cheap extraction of more sample responses. The goal is to achieve a specified level of accuracy with an optimally small number of sample evaluations. This method solves the deterministic problem at pre-selected collocation points in the random domain, determined by using either interpolation approaches or discrete projection approaches [26]. Some of the earlier works on this method [27,28] used a tensor product of 1-D interpolation functions. This approach suffers from the so-called 'curse of dimensionality' [29] as the number of points needed for full model evaluations increases exponentially with increase in the number of dimensions. Sparse grid [30] approaches alleviate this problem to some extent as they significantly reduce the number of points in high dimensions while maintaining almost the same level of accuracy. Sparse grids are especially suitable for high dimensional problems involving numerical integration and interpolation. The interpolation approach approximates the stochastic space using multi-dimensional interpolation with the existing data such that the surrogate surface always passes through the pre-determined points [31–34]. More recent works introduce adaptivity into the sparse grid collocation interpolation approach, including dimension-adaptive sparse grid methods [35,36], Multi-Element(domain-adaptive) sparse grid interpolation [37,38], and adaptive sparse grid subset interpolation [39]. The adaptivity helps to efficiently characterize any highly localized variations and discontinuities in the response surface. The discrete gPC projection approach, also known as the pseudospectral approach [26] is a discretized version of the exact generalized Polynomial Chaos(gPC) projection method, where a multi-dimensional numerical integration is performed with the existing data to approximate the stochastic solution. The surrogate surface here is not constrained to pass through the pre-determined points. This approach is non-intrusive and has fast convergence rates for smooth stochastic domains, but it is less conducive to tackling problems with discontinuous response in the stochastic space. A global approach based on Padé-Legendre approximation [40] has also been used to track down strong non-linearities or discontinuities in the response surface. It has also been shown [41,42] that selection of input points by considering the probability structure of the input domain can lead to efficient sampling.

The present work is based on the work done by Ma and Zabaras [39] on adaptive sparse grid subset interpolation. Similar to that work, the proposed approach uses linear basis functions for the adaptive sparse grid interpolation to capture any localized variations in the response. In addition, it aims to reduce the number of function evaluations by local 1-dimensional cubic spline interpolations [43] in the smoother regions of the response domain. The smoothness is measured by successive derivative estimation along a straight line of points using finite differences of the output values in any of the input dimensions. Small changes (within a tolerance) in the derivative estimates will indicate sufficient smoothness for cubic spline interpolation along the straight line. This helps to achieve the same accuracy as in [39], but decreases the number of function evaluations, especially when the response function is widely smooth. It is worth mentioning here that the derivative information is extracted approximately from the output values without any exact knowledge about the derivative of the output of interest.

The rest of the manuscript is organized as follows: In Section 2, the general mathematical model for any physical system with uncertainties is described. In Section 3, the conventional stochastic collocation (CSC) method, the adaptive sparse grid collocation (ASGC) method and then the proposed efficient adaptive sparse grid collocation (E-ASGC) method are discussed in details. Section 4 deals with the various numerical examples to compare the performance of the proposed method with a few existing methods. Finally, the concluding remarks are given in Section 5.

2. Problem definition

Following notations in [39], we represent the complete probability space by the triplet $(\Omega, \mathcal{F}, \mathcal{P})$ where Ω corresponds to the sample space of outcomes, $\mathcal{F} \subset 2^{\Omega}$ is the sigma algebra of measurable events in Ω, and $\mathcal{P} : \mathcal{F} \to [0, 1]$ is the probability measure. Let $I(\omega) = \{I_1, I_2, I_3, \dots, I_d\}$ be the multidimensional vector of random input parameters in a problem of interest, where $I : \Omega \to \in \mathbb{R}^d$

$$Z(\omega) = f(I(\omega)), \quad \forall\, \omega \in \Omega \tag{1}$$

The goal is then to find out how the vector valued output $Z(\omega)$ varies with respect to each of the random vector components $I_i(\omega), i \in [1, 2, \dots, d]$.

3. Stochastic collocation interpolation method

3.1. Conventional sparse grid interpolation

For a function $f : [a, b] \to \mathbb{R}$, the one-dimensional interpolation formula is given by:

$$U^k(f(x)) = \sum_{x^k \in X^k} a_{x^k}(x) f(x^k) = \sum_{j=1}^{m_k} a_{x_j^k}(x) f(x_j^k), \tag{2}$$

where $x \in [a, b]$, $X^k = \{x^k | x^k \in [a, b]\}$, $a_{x_j^k}(x) \in [0, 1] \subset \mathbb{R}^1$, $a_{x_j^k}(x_i^k) = \delta_{ij}$, $\{i, j\} \in [1, 2, \dots, m_k]$, and m_k = number of points in the set X^k. For multi-dimensional interpolation, the one-dimensional case can be upgraded to obtain a tensor product formula:

$$\begin{aligned}&(U^{k_1} \otimes \cdots \otimes U^{k_d})(f(\mathbf{x})) \\ &= \sum_{j_1=1}^{m_1} \cdots \sum_{j_d=1}^{m_d} (a_{x_{j_1}^{k_1}}(\mathbf{x}) \otimes \cdots \otimes a_{x_{j_d}^{k_d}}(\mathbf{x})) f(x_{j_1}^{k_1}, \dots, x_{j_d}^{k_d})\end{aligned} \tag{3}$$

where d is the total number of dimensions and $\mathbf{x} = \{x_1, x_2, \dots, x_d\} \in \mathbb{R}^d$

The major drawback of this tensor product formula is that the total number of points required are $(m_1)(m_2)(m_3)\dots(m_d)$ which rises exponentially with increase in dimensions, leading to the curse of dimensionality. The sparse grid approach that is used in the current work mitigates this issue to quite an extent by sampling significantly fewer points which are subsets of the tensor grid structure. Though the accuracy of the algorithm is not totally dimension-independent, it gets weakened down to a logarithmic dependence.