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Adaptive-sparse polynomial dimensional decomposition methods for high-dimensional stochastic computing ☆

Vaibhav Yadav, Sharif Rahman *

College of Engineering, The University of Iowa, Iowa City, IA 52242, USA

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ABSTRACT

This article presents two novel adaptive-sparse polynomial dimensional decomposition (PDD) methods for solving high-dimensional uncertainty quantification problems in computational science and engineering. The methods entail global sensitivity analysis for retaining important PDD component functions, and a full- or sparse-grid dimension-reduction integration or quasi Monte Carlo simulation for estimating the PDD expansion coefficients. A unified algorithm, endowed with two distinct ranking schemes for grading component functions, was created for their numerical implementation. The fully adaptive-sparse PDD method is comprehensive and rigorous, leading to the second-moment statistics of a stochastic response that converges to the exact solution when the tolerances vanish. A partially adaptive-sparse PDD method, obtained through regulated adaptivity and sparsity, is economical and is, therefore, expected to solve practical problems with numerous variables. Compared with past developments, the adaptive-sparse PDD methods do not require their truncation parameter(s) to be assigned *a priori* or arbitrarily. The numerical results reveal that an adaptive-sparse PDD method achieves a desired level of accuracy with considerably fewer coefficients compared with existing PDD approximations. For a required accuracy in calculating the probabilistic response characteristics, the new bivariate adaptive-sparse PDD method is more efficient than the existing bivariately truncated PDD method by almost an order of magnitude. Finally, stochastic dynamic analysis of a disk brake system was performed, demonstrating the ability of the new methods to tackle practical engineering problems.

1. Introduction

Uncertainty quantification, an emerging multidisciplinary field blending physical and mathematical sciences, characterizes the discrepancy between model-based simulations and physical reality in terms of the statistical moments, probability law, and other relevant properties of a complex system response. For practical applications, encountering a large number of input random variables is not uncommon, where an output function of interest, defined algorithmically via expensive finite-element analysis (FEA) or similar numerical calculations, is all too often expensive to evaluate. The most promising stochastic methods available today are perhaps the collocation [6,10] and polynomial chaos expansion (PCE) [14,39] methods, including sparse-grid techniques [18], which have found many successful applications. However, for truly high-dimensional

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* Corresponding author. Tel.: +1 3193355679.
E-mail addresses: vaibhav-yadav@uiowa.edu (V. Yadav), rahman@engineering.uiowa.edu (S. Rahman).

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systems, they require astronomically large numbers of terms or coefficients, succumbing to the curse of dimensionality [1]. Therefore, alternative computational methods capable of exploiting low effective dimensions of multivariate functions, such as the polynomial dimensional decomposition (PDD) method, are most desirable. Readers, not familiar with but interested in PDD, are referred to the authors' past works [25–27,32].

For practical applications, the PDD must be truncated with respect to S and m, where S and m define the largest degree of interactions among input variables and largest order of orthogonal polynomials, respectively, retained in a concomitant approximation. These truncation parameters depend on the dimensional structure and nonlinearity of a stochastic response. The higher the values of S and m, the higher the accuracy, but also the computational cost that is endowed with an Sth- or mth-order polynomial computational complexity. However, the dimensional hierarchy or nonlinearity, in general, is not known *a priori*. Therefore, indiscriminately assigning the truncation parameters is not desirable, nor is it possible to do so when a stochastic solution is obtained via complex numerical algorithms. In which case, one must perform these truncations automatically by progressively drawing in higher-variate or higher-order contributions as appropriate. Furthermore, all S-variate component functions of PDD may not contribute equally or even appreciably to be considered in the resulting approximation. Hence, a sparse approximation, expelling component functions with negligible contributions, should be considered as well.

Addressing some of the aforementioned concerns have led to adaptive versions of the cut-high-dimensional model representation (cut-HDMR) [20] and the anchored decomposition [43], employed in conjunction with the sparse-grid collocation methods, for solving stochastic problems in fluid dynamics. Several adaptive variants of the PCE [2,19,37] method have also appeared. It is important to clarify that the cut-HDMR and anchored decompositions are the same as the referential dimensional decomposition (RDD) [28,30]. Therefore, both adaptive methods essentially employ RDD for multivariate function approximations, where the mean values of random input are treated as the reference or anchor point – a premise originally proposed by Xu and Rahman [41]. The developments of these adaptive methods were motivated by the fact that an RDD approximation requires only function evaluations, as opposed to high-dimensional integrals required for an ANOVA Dimensional Decomposition (ADD) approximation. However, a recent error analysis [30] reveals sub-optimality of RDD approximations, meaning that an RDD approximation, regardless of how the reference point is chosen, cannot be better than an ADD approximation for identical degrees of interaction. The analysis also finds ADD approximations to be exceedingly more precise than RDD approximations at higher-variate truncations. In addition, the criteria implemented in existing adaptive methods are predicated on retaining higher-variate component functions by examining the second-moment properties of only univariate component functions, where the largest degree of interaction and polynomial order in the approximation are still left to the user's discretion, instead of being determined automatically based on the problem being solved. Therefore, more intelligently derived adaptive-sparse approximations and decompositions rooted in ADD or PDD should be explored by developing relevant criteria and acceptable error thresholds. These enhancements, some of which are indispensable, should be pursued without sustaining significant additional cost.

This paper presents two new adaptive-sparse versions of the PDD method – the fully adaptive-sparse PDD method and a partially adaptive-sparse PDD method – for solving high-dimensional stochastic problems commonly encountered in computational science and engineering. The methods are based on (1) variance-based global sensitivity analysis for defining the pruning criteria to retain important PDD component functions; (2) a full- or sparse-grid dimension-reduction integration or quasi Monte Carlo simulation (MCS) for estimating the PDD expansion coefficients. Section 2 briefly describes existing dimensional decompositions, including PDD and its S-variate, mth-order approximation, to be contrasted with the proposed methods. Two adaptive-sparse PDD methods are formally presented in Section 3, along with a computational algorithm and a flowchart for numerical implementation of the methods. Two different approaches for calculating the PDD coefficients, one emanating from dimension-reduction integration and the other employing quasi MCS, are explained in Section 4. Section 5 presents three numerical examples for probing the accuracy, efficiency, and convergence properties of the proposed methods, including a comparison with the existing PDD methods. Section 6 reports a large-scale stochastic dynamics problem solved using a proposed adaptive-sparse method. Finally, conclusions are drawn in Section 7.

2. Dimensional decompositions

Let $\mathbb{N}, \mathbb{N}_0, \mathbb{R}$, and $\mathbb{R}_0^+$ represent the sets of positive integer (natural), non-negative integer, real, and non-negative real numbers, respectively. For $k \in \mathbb{N}$, denote by $\mathbb{R}^k$ the k-dimensional Euclidean space, by $\mathbb{N}_0^k$ the k-dimensional multi-index space, and by $\mathbb{R}^{k\times k}$ the set of $k \times k$ real-valued matrices. These standard notations will be used throughout the paper.

Let $(\Omega, \mathcal{F}, P)$ be a complete probability space, where Ω is a sample space, $\mathcal{F}$ is a σ-field on Ω, and $P : \mathcal{F} \to [0, 1]$ is a probability measure. With $\mathcal{B}^N$ representing the Borel σ-field on $\mathbb{R}^N, N \in \mathbb{N}$, consider an $\mathbb{R}^N$-valued random vector $\mathbf{X} := (X_1, \ldots, X_N) : (\Omega, \mathcal{F}) \to (\mathbb{R}^N, \mathcal{B}^N)$, which describes the statistical uncertainties in all system and input parameters of a high-dimensional stochastic problem. The probability law of $\mathbf{X}$ is completely defined by its joint probability density function $f_{\mathbf{X}} : \mathbb{R}^N \to \mathbb{R}_0^+$. Assuming independent coordinates of $\mathbf{X}$, its joint probability density $f_{\mathbf{X}}(\mathbf{x}) = \Pi_{i=1}^{i=N} f_i(x_i)$ is expressed by a product of marginal probability density functions f_i of $X_i, i = 1, \ldots, N$, defined on the probability triple $(\Omega_i, \mathcal{F}_i, P_i)$ with a bounded or an unbounded support on $\mathbb{R}$. For a given $u \subseteq \{1, \ldots, N\}$, $f_{\mathbf{X}_{-u}}(\mathbf{x}_{-u}) := \prod_{i=1, i\notin u}^{N} f_i(x_i)$ defines the marginal density function of $\mathbf{X}_{-u} := \mathbf{X}_{\{1,\ldots,N\}\setminus u}$.