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A new algorithm for high-dimensional uncertainty quantification based on dimension-adaptive sparse grid approximation and reduced basis methods

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ABSTRACT

In this work we develop an adaptive and reduced computational algorithm based on dimension-adaptive sparse grid approximation and reduced basis methods for solving high-dimensional uncertainty quantification (UQ) problems. In order to tackle the computational challenge of "curse of dimensionality" commonly faced by these problems, we employ a dimension-adaptive tensor-product algorithm [16] and propose a verified version to enable effective removal of the stagnation phenomenon besides automatically detecting the importance and interaction of different dimensions. To reduce the heavy computational cost of UQ problems modelled by partial differential equations (PDE), we adopt a weighted reduced basis method [7] and develop an adaptive greedy algorithm in combination with the previous verified algorithm for efficient construction of an accurate reduced basis approximation. The efficiency and accuracy of the proposed algorithm are demonstrated by several numerical experiments.

1. Introduction

Many different computational methods have been proposed and developed during the last few decades to solve uncertainty quantification problems. Among the most widely used is the sampling based Monte Carlo method and its various accelerated versions [13,11], which are straightforward for implementation although they are commonly blamed for slow convergence. A fast convergent method based on the classical idea of projection has been developed under the name of stochastic Galerkin methods, for which different bases of projection can be used such as piecewise finite element and generalized polynomials [17,35,2,32]. Another efficient sampling based method, the stochastic collocation method [34,1], has been developed by taking advantage of the easy implementation of Monte Carlo method and the fast convergence of stochastic Galerkin method. In order to alleviate the computational cost, sparse grid techniques [34,24] are applied to reduce the total number of collocation samples. More recently, model order reduction techniques, including the reduced basis method [4,12,18,8] and the proper generalized decomposition method [25], have been developed. In both cases, the stochastic solution is expanded with respect to a few basis functions that are constructed offline and represent high-fidelity solutions of the underlying PDE. When the dimension of the uncertainties becomes high, the number of isotropic projection basis functions or collocation nodes may grow exponentially fast, one computational challenge known as "curse of

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dimensionality". Another computational challenge stems from the fact that when the solution of the underlying model at one sample is expensive, the available computational resource can only afford the full solve at a few tens or hundreds samples, which is far from the required number (in the order of million or beyond) involved in a high-dimensional space. Any of the two challenges makes it impossible a direct application of the stochastic computational methods introduced above in solving high-dimensional UQ problems.

A strategy to tackle the curse of dimensionality is to take advantage of the sparsity – the importance of different dimensions and their interaction/combination is very different, so that only a limited number of dimensions play an effective role [9]. This idea has led to the development of the weighted function space based quasi Monte Carlo method [11], a priori and a posteriori analysis based anisotropic sparse grid construction [23], (Sobol) decomposition of function based techniques such as ANOVA (analysis of variance) [15], HDMR (high-dimensional model representation) [22]. Another recently developed method under the name of dimension-adaptive tensor-product integration [16] uses a generalized sparse grid construction scheme and employs hierarchical surplus from the construction as error indicators to automatically detect different importance and interaction of different dimensions. Although being essentially equivalent to the anchored ANOVA approach, it is more versatile with different choices of hierarchical surpluses and suitable for interpolation problems. Still, it is to blame for the drawback of running into stagnation phenomenon, where too early stop of the grid construction in some region occurs before arriving at the desired accuracy of approximation. Another drawback is it use one higher level of grid to assess the error indicators, resulting in an unnecessarily heavy computational cost.

In this work, we adopt the more versatile dimension-adaptive algorithm based on hierarchical surpluses and generalized sparse grid construction for both integration and interpolation. Moreover, we propose two remedies in addressing the drawbacks and enhancing both its efficiency and accuracy for solving different UQ problems. As for the first drawback of running into stagnation, a balanced greedy algorithm was suggested in [16] and [21], where a purely greedy criteria of choosing the next index by hierarchical surplus for grid construction is balanced by performing the conventional sparse grid construction. However, it is neither possible to choose an optimal balance weight nor feasible to use the same weight through the whole grid construction. Rather, we propose to carry out a verification procedure in order to get rid of the stagnation phenomenon. The basic idea is that whenever the construction is stopped at some region by meeting certain criteria, we check whether it should be continued by some verification algorithms. This approach avoids the difficulty in tuning the balanced weight parameter and works efficiently to get out of the stagnation region for grid construction at the appropriate time.

The verification remedy has not yet been studied in the literature, neither applied in practice because it needs additional verification samples besides the ones used for assessing hierarchical surpluses in one higher level. This drawback is critical for large-scale UQ problems that already require large computational efforts in solving the underlying PDE model at one sample, as the second computational challenge mentioned before. In order to harness the computational burden, we employ a reduced basis method (see e.g. [30,27]), which has been used in combination with ANOVA in [19], and develop an adaptive and weighted algorithm in combination with the verified hierarchical approximation. Based on this idea and using the reduced basis method, we develop an adaptive greedy algorithm in combination with the verified dimension-adaptive hierarchical grid construction procedure to solve high-dimensional UQ problems. In order to take the arbitrary probability measure into account, we use a weighted a posteriori error bound for guiding the selection of the most representative basis functions [7]. This proves to be more efficient with much less basis functions in achieving the same approximation accuracy as the a posteriori error bound without incorporating the weight. In the end, an adaptive and reduced computational algorithm is developed in efficiently and accurately solving high-dimensional UQ problems that feature sparsity and reducibility. A series of numerical experiments featuring various properties for both functions and the underlying PDE are carried out to demonstrate the efficiency and accuracy of our method and compare its computational performance to several other techniques.

The paper is organized as follows. We briefly introduce uncertainty quantification problems in Section 2. Section 3 is devoted to the development of the verified dimension-adaptive hierarchical approximation based on generalized sparse grid construction. In Section 4, the adaptive and weighted reduced basis method is presented, where the adaptive greedy algorithm and weighted a posteriori error bound are developed in details together with the presentation of the offline–online computational decomposition for gaining computational efficiency. Numerical experiments are presented in Section 5 to demonstrate the accuracy and efficiency of the proposed computational algorithm. We close the paper by drawing some conclusions and perspectives in the last section.

2. Problem setting

Let $(\Omega, \mathfrak{F}, P)$ denote a complete probability space, where Ω is a set of outcomes $\omega \in \Omega$, $\mathfrak{F}$ is a σ-algebra of events and $P : \mathfrak{F} \to [0,1]$ with $P(\Omega) = 1$ is a probability measure. A real-valued *random variable* is defined as a measurable function $Y : (\Omega, \mathfrak{F}) \to (\mathbb{R}, \mathfrak{B})$, being $\mathfrak{B}$ the Borel σ-algebra on $\mathbb{R}$. The probability density function of a random variable $Y : \Omega \to \Gamma \subset \mathbb{R}$, being Γ the image of Y, is denoted as ρ. For any positive integer $k \in \mathbb{N}_+$, the k-th moment of Y is defined as

$$\mathbb{E}\left[Y^k\right] = \int_\Gamma y^k \rho(y) dy. \tag{1}$$

Let D be an open and bounded physical domain in $\mathbb{R}^d$ $(d = 1, 2, 3)$ with Lipschitz continuous boundary ∂D. Let $v : D \times \Omega \to \mathbb{R}$ represent a general real-valued *random field*, which is a real-valued random variable defined in Ω for each