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Enhancing adaptive sparse grid approximations and improving refinement strategies using adjoint-based a posteriori error estimates

J.D. Jakeman *, T. Wildey

Sandia National Laboratories, Albuquerque, NM 87185, United States

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ABSTRACT

In this paper we present an algorithm for adaptive sparse grid approximations of quantities of interest computed from discretized partial differential equations. We use adjoint-based a posteriori error estimates of the physical discretization error and the interpolation error in the sparse grid to enhance the sparse grid approximation and to drive adaptivity of the sparse grid. Utilizing these error estimates provides significantly more accurate functional values for random samples of the sparse grid approximation. We also demonstrate that alternative refinement strategies based upon a posteriori error estimates can lead to further increases in accuracy in the approximation over traditional hierarchical surplus based strategies. Throughout this paper we also provide and test a framework for balancing the physical discretization error with the stochastic interpolation error of the enhanced sparse grid approximation.

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Partial differential equations (PDE) are used to simulate a wide range of phenomenon and are often used to inform design decisions and to estimate risk in systems with large human and/or financial impact but with limited capacity for experimentation. Given the importance of these applications the ability to accurately quantify uncertainty in model predictions is essential.

Most uncertainty quantification (UQ) studies focus on estimating parametric uncertainty. In such analysis, the uncertainty in the input data, such as model coefficients, forcing terms etc., is usually represented through a finite number of random variables with a known probability distribution. The goal of the study is then to compute the effect of the varying input data on the system response, and in many cases, to calculate the statistics of the response.

The accuracy to which uncertainty can be quantified is limited by the computational resources available to resolve the governing equations. Many models require vast amounts of computational effort and thus the number of model evaluations that can be used to interrogate the uncertainty in the system behavior is limited. Consequently a significant portion of methods developed for uncertainty quantification (UQ) in recent years have focused on constructing surrogates of expensive simulation models using only a limited number of model evaluations.

The most widely adopted approximation methods are based on generalized polynomial chaos (PC) expansions [14,26], sparse grid interpolation [19,20] and Gaussian process (GP) models [24]. The performance of these methods is problem

* Corresponding author.
E-mail address: jdjakem@sandia.gov (J.D. Jakeman).

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dependent and in practice it is difficult to estimate the accuracy of the approximation constructed. Cross-validation is one means of estimating the accuracy of the approximation, however the accuracy of the cross-validation prediction of the error is limited. Moreover, cross validation is not readily applied for approximation methods which require structured model samples, such as sparse grid interpolation and many forms of pseudo-spectral projection.

In this paper we utilize sparse grid interpolation to approximate model responses. Sparse grids can be built using local or global basis functions and have well established and effective adaptivity procedures which can be leveraged in conjunction with good error estimates to concentrate computational effort to resolving important dimensions and/or regions of the random parameter space. Unlike regression based PCE or Gaussian process models, sparse grids can be used regardless of the computational budget of the UQ analysis. For example sparse grids can be used to approximate a model response using tens to millions of model runs, whereas the aforementioned alternatives have upper limits in the low thousands imposed by the need to solve large linear systems.

Throughout this paper, we will use $J(\boldsymbol{\xi})$ to denote the exact response (quantity of interest) from a partial differential equation that depends on the unknown variable $\boldsymbol{\xi}$. When solving PDEs using techniques such as the finite element method the physical discretization error will be non-zero. We use $J_h(\boldsymbol{\xi})$ to denote the response from the discretized model. As previously mentioned, solving the discretized model is often computationally expensive and therefore we need to consider a surrogate approximation of $J_h(\boldsymbol{\xi})$, which we denote $J_{h,n}(\boldsymbol{\xi})$. Given these approximations, the error in the response can be decomposed into two components

$$\left\| J(\boldsymbol{\xi}) - J_{h,n}(\boldsymbol{\xi}) \right\| \leq \underbrace{\left\| J(\boldsymbol{\xi}) - J_h(\boldsymbol{\xi}) \right\|}_{I} + \underbrace{\left\| J_h(\boldsymbol{\xi}) - J_{h,n}(\boldsymbol{\xi}) \right\|}_{II} \tag{0.1}$$

where: *I* is the finite element *physical discretization* error; and *II* is the *stochastic approximation* error introduced by approximating the quantity of interest by a sparse grid interpolant.

Recently, a posteriori error estimation has arisen as a promising approach to estimate the error in approximate input–output relationships. Adjoint-based a posteriori error estimation was originally developed to estimate error in numerical approximations of deterministic partial differential equations (PDE) [2,10,15,23], but recent modifications allow similar ideas to be used to estimate error in approximations of quantities of interest from PDEs with uncertain parameters. This relatively new approach, introduced in [7] and further analyzed in [6,8], is based on goal-oriented adjoint-based error estimates and is used to predict error in samples of a response surface approximation of a specific quantity of interest. Similar to standard adjoint-based error estimation procedures, this new approach includes the physical discretization error if the adjoint problem is approximated in a higher-order discretization space. However, the error estimate from this new approach also contains an approximation of the error in the stochastic discretization due to the evaluation of the response surface model rather than the PDE. In [6,8], it was shown that, for spectral and pseudo-spectral Galerkin approximations, this estimate of the stochastic interpolation error is higher-order even if a low order approximation of the adjoint is used for the stochastic approximation.

In general, it is inefficient to reduce the stochastic error to a level below the error introduced by the deterministic discretization. Much of the existing literature focuses on minimizing the stochastic approximation error, however only a few attempts have been made to discuss or account for the combined effect of deterministic and stochastic approximation error. Error bounds for the stochastic approximation error for isotropic sparse grid approximations of elliptic PDEs using Clenshaw–Curtis or Gaussian abscissa are given in [21]. In this paper, we use adjoint-based error estimates to ensure that the error in the stochastic approximation is never significantly less than the physical discretization error.

Our goal in this paper is to utilize adjoint-based a posteriori error estimates to efficiently compute pointwise approximations of specific quantities of interest, usually computed from PDE solutions, using adaptive sparse grid approximations. Specifically, we aim to

- Provide theoretical bounds on the error in a posteriori enhanced Clenshaw–Curtis sparse grids.
- Numerically demonstrate the enhancement results in [6] extend to adaptive sparse grid approximations.
- Present new refinement strategies for sparse grids based on a posteriori error estimates.
- Present a strategy for reducing the cost of computing a posteriori error estimates.
- Provide a criterion to stop sparse grid refinement when the stochastic approximation error of the sparse grid is approximately equal to the physical discretization error.

The remainder of this paper is organized as follows. Section 1 introduces the general model problem we are interested in. Sparse grid approximation is reviewed in Section 2 and we recall the standard adjoint-based posteriori error analysis for deterministic PDEs in Section 3. In Section 4 we formulate an a posteriori error estimate for samples of a sparse grid surrogate and derive theoretical bounds on the error in the a posteriori error estimate. Section 5, presents new adaptive strategies for sparse grid refinement that leverage a posteriori error estimates and Section 6 introduces the sparse grid approximation of the error estimate and our stopping criteria based on an estimate the physical discretization error. Numerical results are presented in Section 7 and our conclusions are presented in Section 8.

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