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Goal-oriented adaptive surrogate construction for stochastic inversion

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Abstract

For computationally expensive models, surrogate response surfaces are often employed to increase the number of samples used in approximating the solution to a stochastic inverse problem. The result is generally a trade-off in errors where the stochastic error is reduced at the cost of an increase in deterministic/discretization errors in the evaluation of the surrogate. Such stochastic errors pollute predictions based on the stochastic inverse. In this work, we formulate a method for adaptively creating a special class of surrogate response surfaces with these sources of error in mind. Adjoint techniques are used to enhance the local approximation properties of the surrogate allowing the construction of a higher-level enhanced surrogate. Using these two levels of surrogates, appropriately derived local error indicators are computed and used to guide refinement of both levels of the surrogates. Three types of refinement strategies are presented and combined in an iterative adaptive surrogate construction algorithm. Numerical examples, including a complex vibroacoustics application, demonstrate how this adaptive strategy allows for accurate predictions under uncertainty for a much smaller computational cost than uniform refinement.

Keywords: Uncertainty quantification; Bayesian inversion; Adaptive methods; Error estimation; Computational engineering

1. Introduction

Efficient and accurate methods for uncertainty quantification (UQ) are topics of much interest in the field of computational mathematics and engineering. While there are many UQ methods that solve a variety of stochastic inverse problems, the most commonly used methods (Bayesian inversion [1,2] and ensemble Kalman filtering [3,4]) use Monte Carlo [5,6] or Markov Chain Monte Carlo [7,8] sampling techniques to evaluate a Quantity of Interest (QoI) map, which introduces error due to finite sampling. This error is exacerbated because numerical techniques are used to solve the model instead of solving it exactly.

A common strategy for reducing the effect of finite sampling error is to construct a surrogate to the QoI response surface. Evaluating the surrogate is done at a greatly reduced computational cost. Surrogate modeling is a large

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topic, so a full review of such techniques is not possible. A widely used class of surrogate approaches involve global polynomial approximations based on stochastic spectral methods [9–17]. Another popular approach is using tensor grid and sparse grid stochastic collocation methods for building surrogates [18,19], including adaptive methods [20]. There are also approaches using stochastic optimization to construct global polynomial [21] and local [22] approximations over sequences of distributions adaptively determined from the data. The surrogate modeling approach considered in this work most closely resembles techniques that exploit derivative information for building piecewise low-order surrogate approximations to improve pointwise accuracy in propagations of uncertainties [13,23].

The surrogate response surface is polluted by two sources of error affecting local accuracy [14–17]. First, there is approximation error introduced by the type of surrogate response surface and how it is constructed. Second, there is numerical error in the evaluation of the numerical model used to construct the surrogate. Both of these are types of discretization errors. Thus, using a surrogate can represent a trade-off between the reduction in finite sampling error at the expense of an overall increase in the discretization error. The end result is that our ability to accurately quantify uncertainties by solution of a stochastic inverse problem may be compromised by the use of surrogates unless additional steps are taken to reduce the discretization errors.

Adjoint techniques for finding computable and accurate a posteriori estimates of discretization errors have existed for decades [24–27]. Such techniques have served as the basis of the error estimates for polynomial chaos and pseudospectral based surrogates derived in [14]. Subsequently, in [15,16], such error estimates were used as part of a Bayesian inference to quantify uncertainties on parameters to evolutionary partial differential equations where QoI response surfaces were approximated with polynomial chaos techniques and enhanced by the error estimates.

We present an adaptive method for updating the surrogate to accurately make predictions under uncertainty in a stochastic inverse problem setting. This adaptivity includes increasing the local polynomial order of the approximation, adding more sample points, and increasing the fidelity of the model for certain samples. The refinement is guided by two levels of surrogate models, with one incorporating adjoint-based a posteriori error estimates to reduce the effect of numerical errors. The method is designed to simultaneously decrease the effects of both types of discretization errors on the prediction at each iteration.

This paper is organized as follows. We provide some general notation, terminology, and assumptions used in this work in Section 2, as well as a brief summary of the theory behind stochastic inversion and the various contributions of errors. In Section 3, we describe the abstract process of constructing surrogate approximations, identify the various sources of error in the surrogate, and describe the implicit construction of a general piecewise low-order surrogate. We subsequently provide the conditions relating the exact and surrogate response surfaces for which the approximate solution to the stochastic inverse problem is in fact exact. A brief review of adjoint based a posteriori error and derivative estimates along with a list of useful references are provided. In Section 4, we also describe how we use such error estimates to enhance surrogates by correcting for persistent local biases due to discretization errors. Such enhanced surrogates are used to derive local error indicators which can be used for local refinement in a variety of ways. The enhanced surrogates, error indicators, and refinement strategies are combined in an adaptive strategy for surrogate construction. In Section 5, the method is applied to a number of example problems of varying complexity, including realistic engineering problems. Conclusions are discussed in Section 6.

2. Notation, terminology, and assumptions

We present some notation, terminology, and general assumptions for stochastic inversion of a physical system. Suppose there is a model $\mathcal{M}(u; \lambda) = 0$ of the system, where u denotes a vector of state variables determined by the solution of the model for a specified vector of parameters λ. These parameters may include coefficients, initial conditions, boundary conditions, source terms, etc. We assume the space of possible parameters, denoted by $\boldsymbol{\Lambda}$, is known, and these parameters explicitly determine the solution to the model.

A QoI map, Q, is defined as a vector of linear functions on the model solution, $Q(u(\lambda))$ for given parameters λ. We then write $Q(\lambda) := Q(u(\lambda))$ to emphasize both the dependence of the output data on the model parameters and the fact that in an experimental setting we may be able to control λ to observe $Q(\lambda)$ without fully observing $u(\lambda)$. Let $\boldsymbol{\mathcal{D}} := Q(\boldsymbol{\Lambda})$ denote the space of model QoI. In general, $\boldsymbol{\Lambda}$ and $\boldsymbol{\mathcal{D}}$ should be Banach spaces. Assume that the QoI map defined by Q is piecewise smooth. The QoI map is used to define a stochastic inverse problem which has a solution $P_{\boldsymbol{\Lambda}}$, a probability measure on $\boldsymbol{\Lambda}$.

Normally, the model is solved using a numerical approximation, resulting in an approximate solution $u_h(\lambda)$ to the model. Using the approximate solution $u_h(\lambda)$ introduces error into the computation of QoI. There may be other