Dimensionality Reduction for Uncertainty Quantification of Nuclear Engineering Models

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INTRODUCTION

The task of uncertainty quantification consists of relating the available information on uncertainties in the model setup to the resulting variation in the outputs of the model. Uncertainty quantification plays an important role in complex simulation models of nuclear engineering, where better understanding of uncertainty results in greater confidence in the model and in the improved safety and efficiency of engineering projects.

In our previous work, we have shown that the effect of uncertainty can be approximated by polynomial regression with derivatives (PRD): a hybrid regression method that uses first-order derivatives of the model output as additional fitting conditions for a polynomial expansion. Numerical experiments have demonstrated the advantage of this approach over classical methods of uncertainty analysis: in precision, computational efficiency, or both [1]. To obtain derivatives, we used automatic differentiation (AD) on the simulation code [2]; hand-coded derivatives are acceptable for simpler models.

We now present improvements on the method. We use a tuned version of the method of snapshots, a technique based on proper orthogonal decomposition (POD) [3], to set up the reduced order representation of essential information on uncertainty in the model inputs. The automatically obtained sensitivity information is required to set up the method.

Dimensionality reduction in combination with PRD allows analysis on a larger dimension of the uncertainty space (>100), at modest computational cost.

DESCRIPTION OF THE WORK

Given a generic model with state vector T, intermediate parameters R dependent on the state of the model and on a collection of uncertainty quantifiers x (generic quantities describing uncertainty-induced errors), and a code implementing the solution of model equations $F(T, R(T, x)) = 0$, we redefine an output of interest as a function of uncertainty quantifiers: $J(T) := \Im(x)$, and we approximate using an expansion in multivariate polynomial basis Ψ:

$$\Im(x) \approx \sum_i a_i \Psi_i(x). \qquad (1)$$

We have shown that the use of derivatives reduces the size of the sample required for regression, so that approximations of the effect of 10-50 uncertainty quantifiers can be constructed with 10 or fewer model runs. With higher dimension of the uncertainty space (100 or more), however, the size of multivariate polynomial becomes very large (10^4, with combinatorial growth) if higher-order polynomials are included; an efficient and well-conditioned regression procedure is no longer possible. We use dimensionality reduction on the uncertainty space to counter the effects of large dimension; that is, we use a reducing projection $y = \Phi x$ leading to an approximation

$$\Im(y) \approx \sum_j b_j \Psi_j(\Phi x) = \sum_j b_j \Psi_j(y), \qquad (2)$$

with the basis constructed on fewer variables.

A straightforward method of snapshots [3] applies to high-dimensional data sets as follows. Given samples of data $X = [x_1, ..., x_N]$ of vectors $x_i \in R^n$, we define the empirical correlation matrix as $C = X \cdot X^T$.

The projection $\Phi = [\phi_1, ..., \phi_k]$, $k << n$, is defined as a dominant eigenspace of C. The projected data then optimally reproduces the snapshots (in 2-norm) and is also expected to preserve the rest of the data well, provided the snapshots are representative.

Straightforward reduction, or data compression, on the uncertainty space would not have a useful effect, because in the described setup there is no interaction with the model; only the shape of the uncertainty domain is subject to compression.

We can provide the feedback from the model by defining the model output as a feature of interest and modifying the reduction technique so that this feature is best represented in model evaluations over compressed data. Two related approaches of assessing the influence of input set components on the output are available.

Approach I: dual-weighted POD

We use a dual-weighted modification of the method [4]. It is based on assigning importance measures: w_i to each of the input vectors x_i, $i = 1,2,...,N$, and λ_j to each

individual uncertainty quantifier $(x_i)_j$, $j = 1,2,...,n$. The weighted form of the correlation matrix is defined as

$$C = diag(\lambda_j) \cdot X \cdot diag(w_j) \cdot X^T . \quad (3)$$

We define the measures empirically: with derivative information already obtained, an effective scheme is

$$w_i \approx E\left[\left\|\frac{d\Im}{dx_i}\right\|\right] \quad ; \quad \lambda_j \approx 1 + const \cdot E\left[\frac{d\Im}{d(x_i)_j}\right]. \quad (4)$$

Approach II: reduction by extraction of latent factors

Suppose there exists a function f on a few variables such that

$$\Im(x) = f(\beta_1 x, \beta_2 x, ..., \beta_k x) . \quad (5)$$

Differentiation of (5) shows that

$$span(\nabla_x \Im) \approx span(\beta_i) . \quad (6)$$

The projection $\Phi := [\beta_1, ..., \beta_k]$ can then be chosen as the dominant eigenspace of the matrix that contains *gradients* of the output function at snapshot values.

In both approaches, the projected set of inputs is used to construct approximation (2) by PRD or by regression without derivative information.

Applied Example

We test the performance of the method on a simplified, three-dimensional, steady-state reactor core model with a simple heat transport description; the operational parameters chosen correspond to those of a sodium-cooled fast reactor core. The uncertainty is introduced into the dependencies of thermodynamic properties of reactor materials on temperature. We also take into account the discrepancies in the chemical composition of different fuel elements. We use a setup with 19 fuel pins; the dimension of uncertainty is 66. We choose the maximal fuel centerline temperature, measured in degrees Kelvin, as an output of interest.

RESULTS

In Table 1 we compare the performance of different approximations of the output: linear approximation, PRD approximation using polynomials of up to second order, and PRD approximation on reduced uncertainty space using approaches I and II. We show the error mean and variance on a sample of 100 points, and the number of full model runs required to construct each approximation.

Dimensionality reduction on the uncertainty space allowed using higher-order polynomials on fewer variables and gained approximately an order of magnitude improvement in precision over PRD models, for lower computational cost. Approach II is empirically the best option so far.

Table 1. Comparison of approximation methods

Method	Error mean	Error var.	# runs
Linear	-1.9045	7.2376	2
PRD	-0.2193	1.2588	68
Reduced PRD, I	-0.0148	0.4864	14
Reduced PRD, II	-0.0123	0.0878	14

With the use of advanced sampling techniques and development of error models for both PRD and POD, the results may be improved further. We note the relationship of this study with ongoing work in Gaussian-based statistical models of uncertainty that use PRD approximations as the mean of an unknown distribution [4].

Our current direction of work is to apply model reduction to automatically extracted parts of model equations, to be able to obtain sensitivity information and construct PRD approximations for high-resolution models that require extreme-scale computational resources. We hope to provide more details in our upcoming larger publication.

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