Reduced Order Approximations in Uncertainty Analysis of Nuclear Engineering Applications

Oleg Roderick, Mihai Anitescu, Zhu Wang

Argonne National Laboratory, 9700 S. Cass Ave., Argonne, IL 60439
roderick@mcs.anl.gov, anitescu@mcs.anl.gov, wangzhu@vt.edu

INTRODUCTION

Uncertainty analysis of complex simulation models plays an important role in nuclear engineering, where better understanding of uncertainty leads to greater confidence in the models and in the improved safety and efficiency of engineering projects.

It is often the case that approximation of uncertainty-induced variation in the outputs of a model requires extensive sampling. At the same time, running a computationally expensive simulation model more than a few times is impractical. The contradiction may be resolved if a complex model has a simplified, lower-quality version that runs much faster. Order reduction of the model equations based on proper orthogonal decomposition is an attractive choice for this simplification, due to its applicability to nonlinear systems, straightforward implementation, and availability of an a posteriori error estimate [1]. If the reduced model is very good, it replaces the full model for all purposes. In a more general case, the error can be described by a stochastic process with the covariance function fitted to the available training data [2].

The idea of uncertainty analysis on a combination of perfect and imperfect data is not completely new [3]. Our work is distinguished by its emphasis on model order reduction, and also by its relationship with our ongoing work on the use of gradient information for uncertainty quantification [4,5]. Gradient-enhanced automatic learning used in combination with learning on imperfect data allows us to construct models of uncertainty in high dimension, using very little sampling.

DESCRIPTION OF THE WORK

In our work, we use a combination of three techniques: evaluation of a reduced-order model to *create* the imperfect training data, Gaussian-processes based learning to *correct* the imperfection, and multivariate polynomial regression on the corrected training data to create the *surrogate model* of uncertainty.

For model reduction, we use a proper-orthogonal decomposition based technique known as the method of snapshots [6]. Given a model based on differential-algebraic equations $f(u,x)=0$, with the solution $u \in R^n$ dependent on the uncertain parameters $x \in R^m$, we collect observations $U=[u(t_1),u(t_2),...,u(t_N)]$ from a full model solution trajectory (based on a single instance of values of parameters with uncertainty).

The reduced-order subspace (of dimension $k << n$) is defined as the dominant eigenspace of the empirical correlation matrix, $C = U \cdot U^T$; the leading eigenvectors are recorded as $\Phi=[\phi_1,...,\phi_k]$. Integration of the reduced-order equations $\hat{f}(q,x)=0$ can be much faster than that of the full model.

Consider a scalar model output $J(u)$. To create a surrogate model of its response uncertainty, we attribute variability in an output of interest to a set of stochastic parameters (uncertainty quantifiers) [4]. Our surrogate model is a deterministic multivariate polynomial expansion. Given imperfect training data, the expansion acquires an additional stochastic error term $Y(x)$:

$$J(u) = J(u(x)) = \sum_i a_i \Psi_i(x) + Y(x) \qquad (1)$$

We can describe $Y(x)$ by a Gaussian process with a covariance function of a particular algebraic form, e.g. a Matern function:

$$\mathrm{cov}(x,x';\theta) = \sum_{i=1}^{m} (1+\sqrt{3}\left|\frac{x_i - x'_i}{\theta_i}\right|) \cdot e^{(-\sqrt{3}\left|\frac{x_i - x'_i}{\theta_i}\right|)} \qquad (2)$$

The covariance function is specified by a set of hyper-parameters $\theta_1,\theta_2,...,\theta_m$, estimated by maximizing a (logarithmic) marginal likelihood function on the training set $Y=\{Y(x): x \in X\}$:

$$\log(\Pr[Y \mid X,\theta]) = \frac{1}{2} Y^T \mathrm{cov}(X,X)^{-1} Y - \frac{1}{2}\log(\mathrm{cov}(X,X)) - \frac{n}{2}\log(2\pi) \qquad (3)$$

We use the following options:

(I) Train the covariance function (2) on the explicitly known errors: $Y_{(I)} = \{J(u(x)) - J(\hat{u}(x)\}$.

(II) Train the covariance function on errors inferred from any lower-quality approximation of the full model:

$Y_{(II)} = \{R(x) - J(\hat{u}(x))\}$, $R(x) \approx J(u(x))$. Here, $R(x)$ can be a linear approximation of $J(u(x))$.

(III) Train on a weighted combination of training sets $Y_{(I)}, Y_{(II)}$.

The error term is computed by Kriging. For a set of uncertainty quantifiers X_V,

$$Y(X_V) = (\mathrm{cov}(X_V, X_V)) \cdot (\mathrm{cov}(X, X))^{-1} \cdot Y(X). \quad (4)$$

The variance of the error is expressed as

$$\mathrm{var}[Y(X_V)] = \mathrm{var}[Y(X)] \cdot (\mathrm{cov}(X_V, X_V) - (\mathrm{cov}(X_V, X_V))^T \cdot (\mathrm{cov}(X, X))^{-1} \cdot (\mathrm{cov}(X_V, X_V)) \quad (5)$$

Note that (5) allows us to put confidence intervals on the surrogate model of uncertainty.

RESULTS

We tested our method on simplified models of Navier-Stokes flow in 2-dimensoinal rectangular channel, with uncertainty in the shape of current at the inflow:

$$\frac{\partial u}{\partial t} + (u \cdot \nabla)u - \frac{1}{\mathrm{Re}}\Delta u = 0, \quad u_{\partial\Omega} = x \quad (6)$$

For an output of interest, we chose a fairly arbitrary quantity $J = mean(1/v^2)$; where v was the velocity component directed along the channel. Our full model would typically have dimension 100-20,000; a reduced model would have dimension 20-50. For parameterization of the inflow profile with 5-10 independent uncertainty quantifiers, we were able to construct adequate models of uncertainty using 1-3 full model runs (and 100-200 reduced model runs).

In Table 1 we report a few metrics of the observed and predicted responses to uncertainty for a flow model with uncertainty dimension 7. Covariance function was constructed using option (III), with a training set of *2 full model evaluations* (and 100 reduced model evaluations at a total computational cost less than 1% of the full model run).

We stress that even for this relatively simple problem, predictions such as above would not be possible to obtain by sampling the reduced model outputs. At the same time, large-scale sampling of full model outputs would require magnitudes more computational effort. Considering the popularity and straightforward implementation of POD-based model reduction, our approach looks very attractive in comparison with other intrusive-analysis based techniques.

Table 1. Surrogate model of uncertainty

Metric	Observed on 100 full model runs	Predicted
Mean	10065	9998
Range	8562 - 11259	7900 - 11259
St. deviation	1081	1012

In our ongoing work, we are applying our approach to the Naiver-Stokes flow modeled by a high-performance fluid dynamics solver Nek5000, which has reduced-order solver implemented [7], with runtime on the order of seconds, as opposed to hours. We obtained our first results for the case with a single uncertain parameter (Reynolds umber), and are now working to demonstrate the performance for higher-dimensional uncertainty.

Our current goal is to also characterize the class of models for which the covariance structure of the model can be recovered by (3).

ACKNOWLEDGMENTS

This work was supported by the Office of Advanced Scientific Computing Research, Office of Science, U.S. Department of Energy, under Contract DE-AC02-06CH11357.

REFERENCES

1. L. PETZOLD and C. YANG, “A posteriori error estimation and global error control for ordinary differential equations by the adjoint method”, SIAM Journal on Sci Comp, 26(2), 359-374, (2004).
2. C. RASUMSSEN and C. WILLIAMS, “Gaussian Processes for Machine Learning”, MIT Press, (2006).
3. D. HIGDON, H. LEE, and B. ZHUOXIN, “A Bayesian approach to characterizing uncertainty in inverse problems using coarse and fine-scale information”, IEEE Trans. Signal Processing, 50(2), 398-399, (2002).
4. O. RODERICK, M. ANITESCU, and P. FISCHER, “Polynomial regression approaches using derivative information for uncertainty quantification,” Nuclear Science and Engineering, 164(2): 122-138 (2010).
5. B. LOCKWOOD and M. ANITESCU, “Gradient-enhanced universal Kriging for uncertainty propagation”, Preprint ANL/MCS-P1808-1110 (2011).
6. S. VOLKWEIN, “Proper orthogonal decomposition: applications in optimization and control” CEA-EDF-INRIA Numerical Analysis Summer School (2007).
7. E. MERZARI, P. FISCHER, and W. POINTER,“A POD-based solver for the advection-diffusion equation”, Proc. ASME-JSME-KSME Joint Fluids Engineering Conference, (2011).