Preprint ANL/MCS-P1833-0111

Gradient-Enhanced Universal Kriging for Uncertainty Propagation in Nuclear Engineering

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In this work, we investigate a surrogate for modeling the response of a simulated nuclear engineering system for use in uncertainty propagation. Building on our recent work using a gradient-enhanced regression approach, we examine the ability of a universal gradient-enhanced Kriging model to provide a means for inexpensive uncertainty quantification.

I. INTRODUCTION

In this work, we wish to rapidly characterize the distribution of simulation outputs based on the probability distribution of input parameters. For high-fidelity simulations, determining the output distribution based on exhaustive sampling is prohibitively expensive; hence, other methods based on an inexpensive surrogate model approximating the simulation output are often used. In previous work, a polynomial regression approach based on function and gradient observations was used to approximate the simulation outputs with a reduced number of simulations.[1] In order to improve this surrogate, the regression is used as the mean function for a universal Kriging model also incorporating gradient observations, giving rise to an approach we call gradient-enhanced universal Kriging (GEUK).[2] We demonstrate here the ability of this GEUK approach to represent nuclear engineering simulation outputs.

II. MODEL OVERVIEW

For the GEUK model, the mean behavior of the function is represented by the previously developed polynomial regression. Departures from this mean obey the following Gaussian process.

$$y(\vec{x}) = N(m(\vec{x}), K(\vec{x}, \vec{x}; \theta)) \tag{1}$$

In order to incorporate gradient observations, the covariance matrix, K, is extended to include the correlation between function and gradient terms. The covariance function is specified based on the assumed smoothness of the data, and the parameters in the covariance are determined by a maximum likelihood approach. Predictions are made by sampling from the distribution conditional on the available observations.[3]

$$y_* \left| \overrightarrow{X}, Y = m(\overrightarrow{x_*}) + k_*^T K^{-1} (Y - M(\overrightarrow{X})) \right. \tag{2}$$

III. DEMONSTRATION RESULTS

To demonstrate the utility of the GEUK model, we approximated the outputs of a Matlab model and the MATWS code. The Matlab model predicts the peak fuel pin temperature in a sodium-cooled reactor, and the MATWS code (a subset of the SAS4A/SASSYS1 code enhanced by automatic differentiation) predicts the fuel temperature for a reactor transient. A more thorough presentation of these results is found in Ref. (4).

A. Approximation Performance

With the GEUK model, the outputs of the Matlab (12 inputs) and MATWS (4 inputs) models were accurately approximated by using a handful of function/gradient evaluations, typically in the range of 8 to 20. In our tests, the GEUK model is consistently more accurate compared to regression. The GEUK surrogate also greatly benefits from the addition of gradient observations as demonstrated in Figure (1) for the Matlab data. When adjoint methods are used to calculate the gradient, the cost associated with the construction of a surrogate with a specified level of accuracy decreases dramatically.

B. Quantile Estimation

Using the GEUK surrogate, one may predict quantiles of an output. Because of the statistical nature of the GEUK surrogate, a distribution of quantile predictions can be created by repeated sampling. This distribution reflects the uncertainty of the surrogate itself, giving a basis for confidence intervals of surrogate predictions. Figure 2 shows the estimated distribution of the 95th percentile of the MATWS data using the GEUK model. As the figure shows, the 95th percentile of the validation data is within the 95% confidence interval of the GEUK prediction.

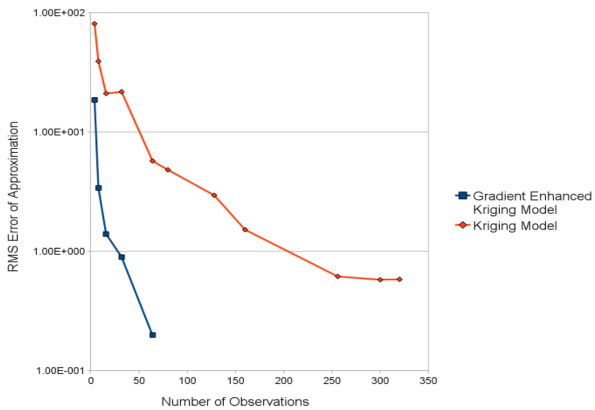

Fig. 1. RMS error based on 1,000 validation points vs. number of sample points for GEUK and Kriging model for Matlab data.

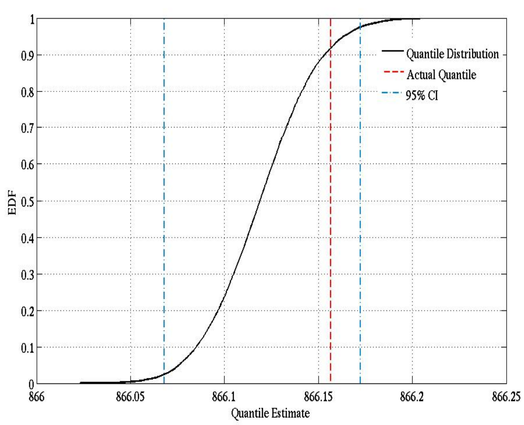

Fig. 2. Distribution of 95th temperature percentile prediction for MATWS data using the GEUK model with 50 samples.

II. CONCLUSIONS

In this work, we have demonstrated that our GEUK model consistently outperforms regression-based approaches and benefits greatly from the incorporation of gradient observations. Additionally, by using a statistical model, confidence intervals for model predictions may be estimated.

ACKNOWLEDGMENTS

This work was supported by a DOE CSGF fellowship (Brian Lockwood) and DOE Contract No. DE-AC02-06CH11357 (Mihai Anitescu).

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