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KRIGING-BASED DYNAMIC ADAPTIVE SAMPLING FOR EFFECTIVE UNCERTAINTY QUANTIFICATION

Koji Shimoyama[1] and Soshi Kawai[2]

[1] Institute of Fluid Science, Tohoku University
Sendai 980-8577, Japan, shimoyama@edge.ifs.tohoku.ac.jp
[2] Institute of Space and Astronautical Science, Japan Aerospace Exploration Agency
Sagamihara 252-5210, Japan, kawai@flab.isas.jaxa.jp

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A conventional simulation model is assumed to output an unique value of solution $f(\boldsymbol{x})$ at fixed values of input parameters $\boldsymbol{x}$ in a deterministic way. On the other hand, a simulation coupled with *uncertainty quantification (UQ)* considers the model, which assumes that input parameters $\boldsymbol{x}$ are affected by some uncertainties, represented as random variables $\boldsymbol{\xi}$, and an output solution $f(\boldsymbol{x})$ fluctuates under the input parameter uncertainties $\boldsymbol{\xi}$, i.e., $f(\boldsymbol{x}(\boldsymbol{\xi})) = f(\boldsymbol{\xi})$. Using this model in a stochastic manner, UQ helps to provide a solution in a more realistic environment.

There are several UQ methods to approximate a stochastic behavior of output solution $f(\boldsymbol{\xi})$ against input parameter uncertainties $\boldsymbol{\xi}$ as a mathematical form and predict the solutions at unknown conditions. *Polynomial chaos expansion (PCE)* formulates the stochastic behavior as a linear combination of orthogonal polynomials. However, when the stochastic behavior includes a non-smooth response, conventional PCE approach often induces approximation errors and deteriorates accuracy and efficiency of predicting the stochastic behavior. Different from polynomial functions used in PCE, the *Kriging model* approximates the stochastic behavior based on Bayesian statistics. As illustrated in Fig. 1, the Kriging model can adapt well to a nonlinear function $f(\boldsymbol{\xi})$ to be approximated, and estimates not only the function values $\hat{f}(\boldsymbol{\xi})$ but also their fit uncertainties $\hat{s}(\boldsymbol{\xi})$.

The present paper proposes to use the Kriging model for determining effective criteria for adaptive sampling and also detecting discontinuities, and thus reducing errors in UQ. In the past, Dwight and Han [1] proposed Kriging-based adaptive sampling method that is based on the product of the fit uncertainty in the Kriging predictor ($\hat{s}(\boldsymbol{\xi})$) and the probability density function of input parameter uncertainties (PDF($\boldsymbol{\xi}$)) as an adaptive sampling criterion (named criterion 1 in this paper). However, as we will show in this paper the criterion 1 is not still sufficient in terms of accuracy and efficiency in the UQ

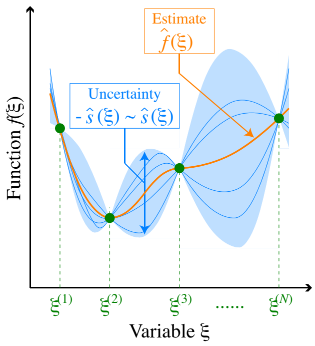

Figure 1: Kriging model.

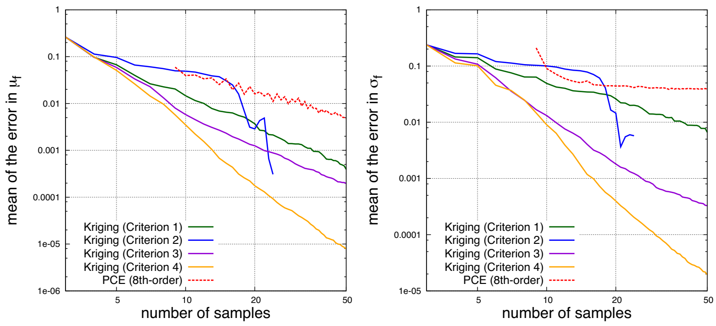

Figure 2: Errors in the statistics (left: mean, right: standard deviation) of one-dimensional non-smooth test functions estimated by the Kriging-based dynamic adaptive sampling and the eighth-order PCE.

problem with discontinuities in the responses of output solution. Thus, this paper studies new Kriging-based dynamic adaptive sampling criteria 2–4. In the criterion 4, $\Delta\xi$ is the distance from $\boldsymbol{\xi}$ to the most adjacent sample point, and $D_{\hat{f}}(\boldsymbol{\xi})$ is the extra term to estimate the polynomial errors, which is now formulated as the difference of the Kriging predictors with two different sample sets.

$$\mathrm{Crit1}(\boldsymbol{\xi}) = \hat{s}(\boldsymbol{\xi}) \times \mathrm{PDF}(\boldsymbol{\xi}), \quad \mathrm{Crit2}(\boldsymbol{\xi}) = \left|\frac{\partial \hat{f}(\boldsymbol{\xi})}{\partial \boldsymbol{\xi}}\right| \times \mathrm{PDF}(\boldsymbol{\xi}),$$

$$\mathrm{Crit3}(\boldsymbol{\xi}) = \left|\frac{\partial \hat{f}(\boldsymbol{\xi})}{\partial \boldsymbol{\xi}}\right| \times \hat{s}(\boldsymbol{\xi}) \times \mathrm{PDF}(\boldsymbol{\xi}), \quad \mathrm{Crit4}(\boldsymbol{\xi}) = \left(\left|\frac{\partial \hat{f}(\boldsymbol{\xi})}{\partial \boldsymbol{\xi}}\right| \times \Delta\xi + D_{\hat{f}}(\boldsymbol{\xi})\right) \times \hat{s}(\boldsymbol{\xi}) \times \mathrm{PDF}(\boldsymbol{\xi}).$$

Figure 2 shows the errors in the statistics (mean μ_f and standard deviation σ_f) of one-dimensional non-smooth test functions $f(\xi)$, which are estimated by the dynamic adaptive sampling based on the criteria 1–4 and the eighth-order PCE. Except the criterion 2, the Kriging-model-based dynamic adaptive sampling surpasses the conventional PCE in terms of the speed of error reduction. The proposed criterion 4 achieves the fastest monotonic reduction of the errors. The existing criterion 1 considering only fit uncertainty $\hat{s}(\xi)$ also achieves monotonic reduction but much slower than the criterion 4. The criterion 2 considering only gradient $\frac{\partial \hat{f}(\xi)}{\partial \xi}$ falls into the process termination in the early stage. This is due to the over-detection of discontinuity and the duplication of additional samples around the discontinuity. These results indicate that it is essential to consider the balance between the fit uncertainty and gradient in an estimated response for effective adaptive sampling. The criterion 3 considering both $\frac{\partial \hat{f}(\xi)}{\partial \xi}$ and $\hat{s}(\xi)$ shows similar reduction to the criterion 4 in the early stage, but then degrades the capability of error reduction in the later stage. This is because the criterion 3 does not add samples in smooth response regions with almost zero gradient, and thus cannot reduce the possible polynomial errors. It indicates that the extra error-estimate term ($D_{\hat{f}}(\boldsymbol{\xi})$ in the criterion 4) makes the process of adaptive sampling more effective.

REFERENCES

[1] R. Dwight and Z.-H. Han. Efficient uncertainty quantification using gradient-enhanced Kriging, *11th AIAA NDA Conf.*, AIAA–2009–2276, 2009.