Transactions of the Korean Nuclear Society Spring Meeting
Jeju, Korea, May 17-18, 2012

Multi-Surrogate Modeling for Computational Cost Reduction

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1. Introduction

To utilize high-fidelity simulation for computationally intensive engineering applications such as sensitivity analysis and uncertainty quantification, the surrogate modeling techniques have become an indispensible tool and have been widely used. However, for reactor physics problems that can be characterized as very large number of input parameters (i.e. reaction cross sections), the required computational cost to build a surrogate model itself would be impractical with the sole conventional surrogate modeling techniques. We have been exploring the efficient way of reducing the computational cost in surrogate modeling and contributed the surrogate approach incorporated with reduced order modeling techniques [1].

Basic approach summarized in Ref. [1] is to transform the input parameters into low dimension by hybridizing two prominent methods - variational methods and sampling methods. As a preprocessing for the surrogate modeling, the influential subspace of the input parameters with respect to response change is extracted by range finding algorithm and the input parameters are projected onto that subspace. Because the number of subspace basis vectors are much smaller than the number of input parameters, reduced order form of the surrogate model can be constructed, which means that the number of unknowns to be determined in the surrogate modeling is reduced and, opposed to the curse of dimensionality, one can save significant computational cost to generate the training sample set.

This study is the extension of the previous method for further cost reduction. In Ref. [1], the input parameter transformation and the surrogate modeling are conducted independently. By doing that, one can estimate the error due to input parameter transformation and the surrogate modeling, separately and theoretically one can eliminate the error due to input parameter transformation within the machine precision. However, in practice, the input parameter variations, which may be considered significant in view of the input parameter transformation, may not be influential on the actual response change. By properly filtering those components, we expect that more reduction would be achieved. The basic idea and the preliminary test results are presented.

2. Multi-Surrogate Modeling

We have observed that: 1) reactor physics calculations are mildly nonlinear problems, i.e. large portion of the response changes can be captured by the linear approximation; 2) as the response variation increases, the nonlinear effect also increases; 3) computational cost explodes due to nonlinear terms. These motivate that the multi-surrogate approach in which the response change is considered as a sum of the linear component and the nonlinear component and those are estimated separately. According to the first observation, the discrepancy of linear approximation, i.e. nonlinear component, would be small compared to total response change. If the surrogate is built only for the discrepancy, we can filter out insignificant components of input parameter variations more easily. Moreover, because those are directly related to nonlinear terms, opposed to curse of dimensionality, the computational cost could be saved super-linearly.

The advantage of the multi-surrogate approach can be illustrated by an example. Consider that a response change is the sum of 90% linear component and 10% nonlinear component, i.e. higher order terms. Note that though there is 10% error in the estimation of the nonlinear component, the error in the total response estimation would be only 1%. This implies that the higher order terms can be reduced further depending on the nonlinearity and required level of accuracy. The linear component can be efficiently and accurately captured by the first order Taylor expansion based on adjoint sensitivity analysis [2]. Then, only the discrepancy between the original model and the first order estimation is fitted, i.e. the surrogate modeling with reduced input parameters. The proposed multi-surrogate modeling is illustrated in Fig. 1.

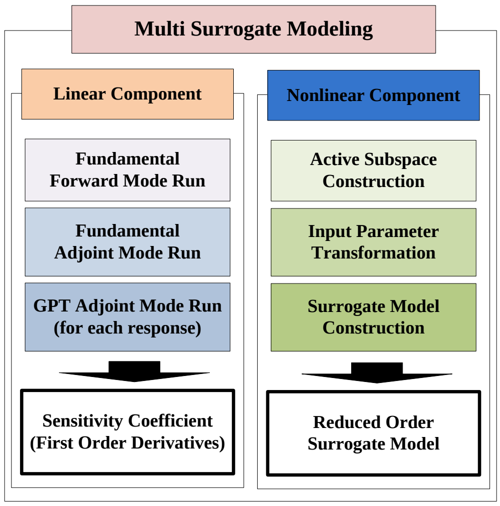

Fig. 1. Schematics of Multi-Surrogate Construction

3. Numerical Tests

The SCALE6.1 [3] is used as a simulation code (SAMS for first order sensitivity information calculation and NEWT as a transport solver). Fig. 2 depicts the model analyzed [4]. The fission cross sections of four nuclides (i.e. U-234, U-235, U-236 and U-238) in 44 energy group in 9 fuel mixtures are perturbed by $\pm$ 30% from uniform distribution, i.e. the dimension of input parameters is $\mathbb{R}^{1584}$. The responses are chosen to the mixture fluxes in the fuel mixture 1, i.e. the dimension of input parameters is $\mathbb{R}^{44}$.

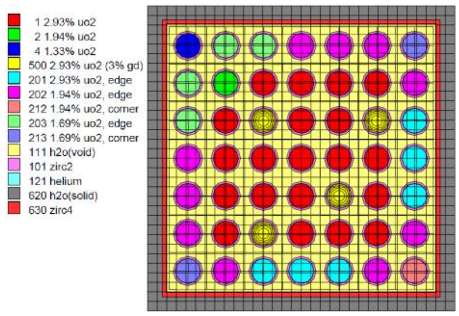

Fig. 2. 7×7 BWR Benchmark Assembly Model

As described in the previous section, the linear component is estimated by the adjoint sensitivity analysis. The discrepancies between the actual response changes and the adjoint based first order estimation are corrected by the second order polynomial regression analysis with reduced order modeling, i.e.:

$$\begin{aligned}
&\Delta R_m\left(\Delta\vec{\Sigma}\right)=\Delta R_{m,linear}\left(\Delta\vec{\Sigma}\right)+\Delta R_{m,nonlinear}\left(\Delta\vec{\Sigma}\right)\\
&R_{m,linear}\left(\Delta\vec{\Sigma}\right)=\left(\left.\frac{\partial R_m}{\partial\vec{\Sigma}}\right|_{\vec{\Sigma}_0}\right)^T\Delta\vec{\Sigma}\\
&R_{m,nonlinear}\left(\Delta\vec{\Sigma}\right)=\vec{\beta}_{m,1}^T\mathbf{Q}^T\Delta\vec{\Sigma}+\left\{\vec{\beta}_{m,2}^T\mathbf{Q}^T\Delta\vec{\Sigma}\right\}^2
\end{aligned}\tag{1}$$

where $\Delta\vec{\Sigma}$ is the vector of input parameter variations, $\vec{\beta}_{m,1},\vec{\beta}_{m,2}\in\mathbb{R}^r$ are the coefficient vectors and $\mathbf{Q}\in\mathbb{R}^{1584\times r}$ is the matrix of which columns are basis of the influential input parameter subspace with respect to response change. Two different number of basis vectors are tested; $r=30$ and $r=50$. As training sets, the 1000 and 3000 sample sets generated by Latin-Hypercube sampling (LHS) are used for $r=30$ and $r=50$, respectively. To check the estimation accuracy according to the magnitude of the input parameter perturbation, the base perturbation is generated by $\pm$ 1% from uniform distribution and increases by multiplying integer values up to 30.

To estimate the required number of basis vectors, the singular value spectrum of the pseudo-response sensitivity vectors are investigated. One can consider that the singular value as importance of the corresponding basis vector. Fig. 3 shows that 30 and 50 basis vectors capture only 75% and 82% of the subspace spanned by input parameter variations. The surrogate model with those basis vectors showed very poor estimation accuracy. However, with multi-surrogate modeling, the response change can be predicted accurately as shown in Fig. 4.

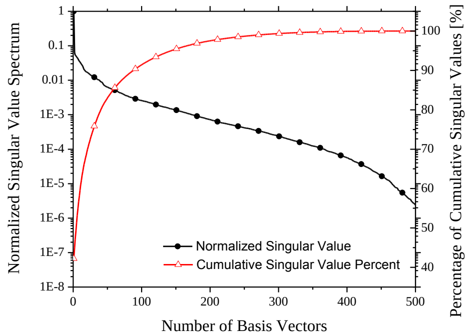

Fig. 3. Singular Value Spectrum of Pseudo Response Sensitivity Vectors

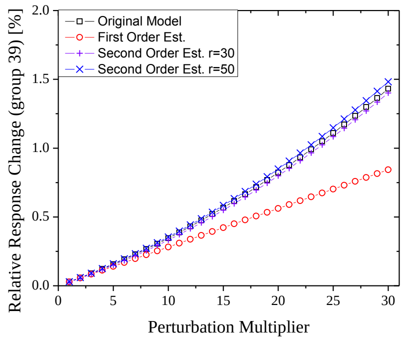

Fig. 4. Comparison of Estimation Accuracy

4. Conclusion

The multi-surrogate approach can be useful for quasi-nonlinear problems for surrogate modeling. By utilizing adjoint sensitivity analysis for linear response change estimation, the required additional simulations would be increased linearly while the required simulation to capture the nonlinear effect can be reduced super-linearly; thus, overall computational cost can be saved.

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