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A new approach to stochastic reduced order modeling

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ABSTRACT

This short note presents a new method for stochastic reduced order (SROM) model based on BONUS reweighting scheme. An illustrative case study of IGCC power plant compares the new method with the neural network based reduced order model. The new method shows promising results.

1. Introduction

Reduced order modelling is becoming increasingly popular as a simpler and more economical alternative for analyzing many real-life processes. This is because such processes or systems are so complex that the mathematical models created to represent them are in turn complicated and have many dimensions. Therefore, using such models in numerical simulations and optimization to analyze the process can become an expensive and time-consuming affair because of the multiple iterations involved in running a simulation. Therein lays the benefit of reducing the order of mathematical models by employing approximations. However, this gives rise to the challenge of maintaining the accuracy of system characteristics and response. This can be overcome by being careful in deciding the approximation strategy and in importing data from the original system into the reduced order models (ROM). Thus, if we are able to retain sufficient accuracy, the ROMs obtained can be used to predict the results with substantial precision in considerably lesser amount of time. It is because of this reason that ROM has always been a topic of great interest for researchers.

Bai et al., (2005) have discussed the various ROM techniques used in simulating large scale linear dynamical systems such as electronic circuits and microelectromechanical systems, thus replacing methods such as RCL sub-circuits that have been traditionally applied to model VLSI circuits. Rao et al. (2016) have worked on developing model order reduction using the Kron reduction of weighted Laplacian matrices. They have illustrated the application of this technique in several chemical and biochemical reaction networks governed by general enzyme kinetics. Generally, to analyze such reactions a set of stoichiometric differential equations involving a huge number of metabolites and chemical species have to be solved. In their work, they have reduced the number of metabolites and reactions without any major effect on the dynamics of the original reactions. Amsallem et al. (2012) have ventured into a lesser explored area by developing a non-linear model reduction method replacing CFD models based on the concept of local reduced-order bases. The method is executed in two phases—online and offline. The local base is developed during the offline phase and it is updated in the online phase based on the current state of the system.

In this paper, we present a new approach to reduced order modeling and applied it to analyze the process of power production in an IGCC power plant. The ROM generated by this method can be categorized as stochastic ROMs (SROMs) as it can be used for obtaining stochastic estimates such as expected value, variance of outputs. SROMs are very useful in applications such as sensor and controls. There is very little work done in the area of stochastic ROMs. Warner et al. (2013) present a method for constructing Stochastic Reduced Order Models (SROMs) to efficiently solve random eigenvalue problems encountered in the modal analysis of structural systems with uncertain properties. They have developed an improved algorithm to construct SROMs. The algorithm is able to considerably improve the model accuracy and efficiency. They determined analytical bounds to solve random eigenvalue problems and accounted for uncertainty propagation through the mathematical model. The

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models thus formulated were shown to clearly outperform the classic Monte Carlo simulations in numerical examples. However, this approach requires open equation system and linear models.

Sarkar et al. (2014) use a Stochastic Reduced Order Model (SROM) for uncertainty quantification in systems undergoing corrosion. They demonstrated the application of SROM models for characterizing input uncertainty and propagating the uncertainty to the outputs through the mathematical model. They have developed SROMs for a random vector input X as a set of probable values x and their corresponding probabilities p. The SROM statistics were then calculated and an optimization problem was solved to minimize the error between the SROM statistics and the actual target marginal. When it comes to computationally intensive problems like corroding systems, SROMs are more efficient than the traditional techniques such as spectral nethods, Monte Carlo techniques and stochastic calculus approaches.

Lang et al. (2011) use ROM to replace Fluent CFD models for Gasification and Combined Cycle Combustion Units in IGCC power plant. Accurate CFD models can be developed for key units like Gasification and Combined Cycle Combustion Units. However, developing integrated flowsheets and subsequent optimization is difficult. So they developed two ROMs—Neural Networks & Kriging and integrated them in IGCC process. The performance of the ROMs was evaluated and a 7% increase in power output was obtained by optimizing these models.

The aim of this paper is to compare Stochastic Reduced Order Models for IGCC system created using two different techniques. One of them is Neural Networks which has been fairly applied in building reduced order models. Stochastic simulations are then carried out with this ROM to obtain stochastic ROM. The second and the new approach is based on Better Optimization of Nonlinear Uncertain Systems (BONUS) reweighting approach. We present the case study of an IGCC plant where the rigorous model used for IGCC in this work is taken from the DOE/NETL Case study 8 report (US Department of Energy National Energy Technology Laboratory., 2006). It has been demonstrated in this paper that the latter produces a more accurate SROM more efficiently and thus is useful in optimizing sensors and control for this system.

2. BONUS reweighting approach

The reweighting approach is the basis of the BONUS algorithm proposed by Sahin and Diwekar (2004). BONUS uses reweighting scheme which is the basis of the SROM presented here. Fig. 1 presents the reweighting scheme in perspective. Initially we assume that our inputs are uniformly distributed between minimum and maximum value. We sample these uniformly distributed variables and propagate the sample through our rigorous model. We obtain the output distributions for this initial base distribution based on the rigorous model. Once we have these probability distributions then if the input distributions change then we do not have to sample and propagate these new distributions through the model but use reweighting scheme to obtain the corresponding output distribution. For details, please refer to Diwekar and David (2015). This reweighting approach is beneficial for eliminating the need to recreate a set of new sample points and propagating it through the rigorous model. To obtain SROM for the IGCC system, on the first iteration, a set of N_s sample points uniformly distributed across a d-dimensional sample space are used to perform N_s simulation replications of the IGCC process (i.e., at various operating points) rigorous model. Let $f_0(x_i)$ and $F_0(x_i)$ be the probability density function (pdf) and cumulative distribution function (cdf) associated with the base input distribution for the input variable x_i, i = 1,2,. . ..,S_{in}, respectively. Following the simulation of the IGCC process at iteration k = 1, let $f_0(y_j)$ and $F_0(y_j)$ be the base probability density function (pdf) and cumulative probability density function (cdf) associated with the intermediate and output variable y_j, j = 1,2,. . ..,S_{out}, respectively.

Next, consider when the input distribution is redefined, such as when a sensor is placed at the location of this input variable. The redefined distribution, $f_k(x_i)$, is used to create a set of weights,

$$W_k(x_i) = \frac{f_k(x_i)}{f_0(x_i)} \ldots i = 1, 2, \ldots, S_{in} \tag{1}$$

which gives the likelihood ratio between the redefined and base distributions. Given that the input variables act independently, these weights are used to construct the resulting distribution for the downstream intermediate and output variables by multiplying the associated weights W (x_i) with the base distribution $f_0(y_j)$

$$f_k(y_i) = f_0(y_i)\prod_{i=1}^{S_{in}}(1 + \gamma_{ij}(W_k(x_i) - 1)\ldots j = 1, 2, \ldots S_{out} \tag{2}$$

Where γ_{ij} = 1 if variable y_j is downstream of x_i and γ_{ij} = 0 if variable y_j is not downstream of x_i. The above distribution $f_k(y_j)$ is then normalized using

$$f_k(y_i) = \frac{f_k(y_i)}{\sum_{n=1}^{N_s} f_k(y_n(y_{n+1} - y_{n-1})/2)} \tag{3}$$

Although, the reweighting equations appear to be linear, they are linear in probability space and can easily be used for nonlinear models and is shown applicable to IGCC system below.

This reweighting approach is thus used to construct the resulting change in distributions of corresponding downstream variables by eliminating the need to regenerate a new set of Ns sample points through simulation of the IGCC process. The number of sample points depends on the number of input variables. Here we have used 800 sample points with 8 input variables. There are large number of intermediate and output variables in this flowsheet. The reweighting approach explained above can be used as a SROM for the IGCC process.

3. Methodology

A set of Ns sample points for each of the input parameters was generated using Hammersley Sampling Sequence (HSS) which is a low discrepancy sampling method (Wang et al., 2004) This sampling technique is preferred over the commonly used Monte Carlo simulation because it can provide a more uniform distribution and better coverage of any d-dimensional sample space using lesser number of sample points. The input variables were assumed to follow a uniform distribution and the samples were generated accordingly.

Then, the entire IGCC plant modeled in ASPEN is simulated N_s times, once per input operating condition, to generate a corresponding vector of points for Sout intermediate and output process variables. The input and output data sets thus obtained from our base data which will later form our basis of comparison.

This considerably large amount of data acquired from N_s samples is used to develop a Neural Network (NN), which is our first Reduced Order Model to predict the behavior of the IGCC plant. 70% of the data is used in the training phase whereby both input and output data sets are made available to the NN so that it can follow the trends in the data to "learn" how the IGCC plant functions. Then, the next 15% of the data is used for validation and finally the predictive power of the NN is tested using the last 15% of the data.

The trained Neural Network is now ready to be used on any new, unrelated data set. To test the efficacy of the NN, we generated a new input data set consisting of N_s sample points. However, this time, instead of uniform distribution, we considered normal