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Accelerate global sensitivity analysis using artificial neural network algorithm: Case studies for combustion kinetic model

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ABSTRACT

Global sensitivity and uncertainty analyses have attracted more and more attention in recent combustion kinetic studies. However, the high computational cost hinders their application in complex kinetic models. In order to accelerate the convergence speed, the artificial neural networks (ANN) methodology is applied into two widely used quantitative sensitivity analysis methods in the present work, i.e. the Sobol' sensitivity estimation and the random sampling high dimensional model representations (RS-HDMR). An ANN is constructed and trained using original model samples, which can then be used as a surrogate model to generate numerous samples for a global sensitivity analysis with Sobol' sensitivity estimation or RS-HDMR. It is shown that the ANN greatly reduces computational costs for estimating Sobol' sensitivity indices. The performances of the proposed ANN based HDMR method (ANN-HDMR) have been tested by a widely used analytical function (Sobol' *g*-function) and two practical models in combustion (master equation kinetic model and reaction kinetic model). The results show that the ANN-HDMR only needs a few tenths of original samples in the sensitivity analysis of master equation kinetic model and premixed H_2/O_2 ignition model. The ANN-HDMR is a kind of double-layer surrogate model which couples the advantage of ANN for fast convergence and RS-HDMR for direct sensitivity indices calculation, and thus it exhibits better performance in convergence and stability comparing with the commonly used RS-HDMR.

1. Introduction

Detailed chemical kinetic modeling of pure or mixed fuels combustion enables an in-depth understanding of combustion processes and ultimately makes valuable contributions to worldwide energy production while limiting its environmental impact. Unfortunately, a complete and accurate chemical kinetic model may never exist, because it is impossible to predetermine the completeness of a kinetic model, moreover, the uncertainty of a model is too complicated so that it is very difficult to determine a unique model in the uncertainty space [1]. The development of a chemical kinetic model is thus the process of reducing the uncertainty of model prediction. According to Oberkampf and Roy [2], the sources of a kinetic model's uncertainty include model form error, numerical uncertainty and model input uncertainty. Even if we use appropriate numerical approaches to solve the mathematical equations of a structurally complete model, high uncertainty still exists in the model prediction due to the uncertainties of model input parameters including reaction rate coefficients, thermodynamic and transport parameters. Rigorous studies by experimental measurements or theoretical calculations on each input parameter will undoubtedly reduce the prediction uncertainty. However, for a complex model consisting of hundreds or even thousands of input parameters, it is impractical to accurately determine each parameter due to the prohibitively high computational or experimental costs.

A sensitivity analysis method studies how uncertainty in the output of a model can be apportioned to different sources of uncertainty in the model input [3]. It may take a local or global approach. A local sensitivity analysis explores the response of the model output to a small change of the parameter from its nominal value. Because of its high computational efficiency, the local method has been implemented in widely used chemical kinetic programs such as CHEMKIN [4], KINAL [5], Cantera [6], FlameMaster [7], laminarSMOKE [8] and OpenSMOKE++ [9]. However, if the input parameters have strong nonlinear or coupled effects on the outputs, local methods may produce misleading results. A global sensitivity analysis (GSA) estimates the effect of input parameters across the whole uncertainty space on model predictions. Many methods for GSA are used in chemical kinetic models [10,11]. Sobol' sensitivity estimation [12–14] and RS-HDMR [15–18] are two

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common GSA methods based on analysis of variance (ANOVA) decomposition, which can quantitatively evaluate the independent and coupled effects of input parameters.

Sobol' proposed a method based on Monte Carlo sampling [12] to estimate partial variances and calculate global sensitivity indices, which is able to obtain accurate results but computational expensive. The high computational cost prohibits its application in complex chemical kinetic models, although efforts have been made in past decades to reduce the cost [19,20]. The RS-HDMR is a series of methods to construct low order ANOVA decomposition expression with assuming negligible high order interactive effects [16]. This assumption rests on the fact that one tends to choose the parameters that act the most independently for describing a physical or chemical system [16,17]. Under this assumption, the constructed RS-HDMR expression is actually an effective surrogate model of the original model. Then sensitivity indices can be easily obtained from the RS-HDMR expression. Li et al. [18] have developed several practical approaches to construct RS-HDMR expressions using a minimization process and Monte Carlo integration (named as DMC-HDMR hereafter). To reduce the computational cost and improve the accuracy in RS-HDMR expression, several optimization methods have been proposed, including the control variate methods [21,22], a method proposed by Ziehn and Tomlin which automatically chooses the best order of component functions of RS-HDMR expression [23], and a threshold method [24] used to exclude the unimportant terms. RS-HDMR combined with aforementioned three kinds of methods is named as Optimized-HDMR in this work. The Optimized-HDMR has been implemented in the program GUI_HDMR [25], and this user-friendly program has promoted the application of RS-HDMR in combustion studies. Although the Optimized-HDMR has a better convergence performance comparing with the original RS-HDMR, it may cause instability by, for example, increasing the risk of missing important terms.

As discussed above, the Sobol' sensitivity estimation and the original RS-HDMR require a lot of samples to get convergent results, which requires high computational cost for the analysis of complex combustion kinetic models. A detailed combustion kinetic model aims to describe extensive combustion properties under wide range of combustion conditions, which is the intrinsic reason for its complexity. Fortunately, sensitivity analyses are usually conducted for only a few targets under some specific conditions, thus a drastically simplified surrogate model could be feasible to represent the original combustion chemical model with adequate precision. With such a simplified surrogate model, samples can be quickly generated for a sensitivity analysis using the Sobol' sensitivity estimation or the original RS-HDMR methods. With regard to constructing surrogate models, ANN inspired by biological neural systems is a more popular method compared with RS-HDMR. Because of its powerful potential in exploring a complex model, e.g. massive parallelism, generalization capacity and fault-tolerance ability [26], ANN has been widely used in fields such as pattern recognition [27,28], reliability analysis [29,30], classification [31,32], medical diagnosis [33,34], process control [35,36] and combustion kinetic systems [37–49]. The most popular type of ANN is multilayer perceptron (MLP) feed-forward neural network. A MLP consists of three layers: input, hidden and output layer. Figure 1 illustrates a single hidden layer MLP feed-forward neural network. The back-propagation (BP) algorithm [50] is the most widely used learning algorithm for a MLP neural network. The learning process consists of two parts: feed-forward and backward pass. The outputs of the ANN are calculated in the feed-forward pass process and the output errors are propagated backward to adjust the weights and biases of the ANN.

In this study, the ANN algorithm has been combined with the Sobol' sensitivity estimation (ANN-Sobol') and the original RS-HDMR (ANN-HDMR) respectively to perform the GSA for detailed

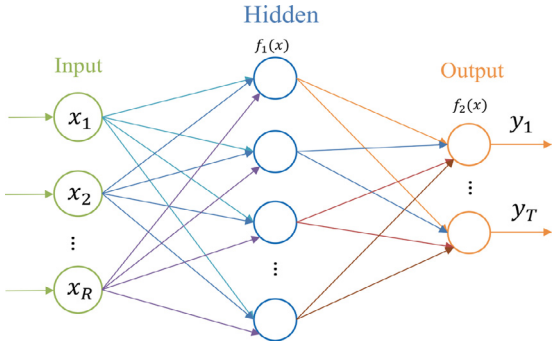

Fig. 1. Example of a single hidden layer MLP feed-forward neural network. $x_1, x_2, \ldots, x_R$ are input parameters, $y_1, \ldots, y_T$ are output targets, R is the number of input parameters, and T is the number of output targets. $f_1(x)$ is the activation function of hidden layer, and $f_2(x)$ is the activation function of output layer.

combustion kinetic models. The objective of this study is to illustrate how the ANN can reduce the computational cost remarkably of the Sobol' sensitivity estimation for kinetic models, and to provide an alternative approach to accelerate the convergence speed of RS-HDMR for GSA by coupling the advantage of ANN for fast convergence and RS-HDMR for direct sensitivity indices calculation, which is different from the Optimized-HDMR methods. Three kinds of cases including the Sobol' *g*-function, a master equation kinetic model, and a premixed H_2/O_2 ignition model were employed to compare the performances of ANN-HDMR against Optimized-HDMR. The difference between these two ANN based GSA methods was demonstrated through the sensitivity analysis of the premixed H_2/O_2 ignition model.

2. Theoretical methods

2.1. ANN based GSA (ANN-GSA) algorithm

The process of ANN-GSA is as follows: (1) Randomly generate a number of input parameters over their uncertainty ranges, and calculate the output targets using the original model. The combination of a set of input parameters and the corresponding output target is called a *sample*. (2) Train the ANN to generate a drastically simplified surrogate model from the original model using the generated samples. (3) Conduct a GSA using the well-trained ANN.

The samples generated by the original model are named as original samples, and those obtained from the well-trained ANN are named as ANN samples hereafter. Two ANN-GSA methods, ANN-Sobol' and ANN-HDMR, were developed in the present work. For ANN-Sobol', the well-trained ANN is used as a surrogate model to generate Monte Carlo samples for estimating sensitivity indices. For ANN-HDMR, the well-trained ANN is taken as the first layer surrogate model and RS-HDMR is used to construct the second layer surrogate model using the samples generated by the first layer. Figure 2 demonstrates the calculation process of ANN-HDMR: the original model is used to generate a number of original samples firstly, then two layer surrogate models are constructed to conduct the GSA.

In this work, a single hidden layer feed-forward MLP ANN was employed in ANN-HDMR and ANN-Sobol', and the back-propagation based on the Marquardt–Levenberg algorithm [51] was used as the learning algorithm. The 'tansig' [$y = 2/(1 + \exp(-2x))-1$] and 'purelin' ($y = x$) functions were used as the activation functions of the hidden and output layers, respectively. In the training process, 80% of the original samples were used for training, 10% were used to validate the generality of the network, and the remaining 10% were used for testing. The number of hidden layer nodes and the maximum iteration number were care-