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A NEW MULTIPLE SUB-DOMAIN RS-HDMR METHOD AND ITS APPLICATION TO TROPOSPHERIC ALKANE PHOTOCHEMISTRY MODEL

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Abstract. The high dimensional model representation (HDMR) method was recently proposed as an efficient tool to capture the input-output relationships in high-dimensional systems for many problems in science and engineering. In this paper, we develop a new multiple sub-domain random sampling HDMR method (MSD-RS-HDMR) for general high dimensional input-output systems. The domain splitting technique is applied to divide the whole domain into multiple sub-domains. The RS-HDMR method is used to generate local approximations in sub-domains and a set of weight functions is introduced to obtain approximations near the sub-domain interfaces. Numerical experiments are carried out using the MSD-RS-HDMR method for given high dimensional functions and a real application of the Tropospheric Alkane Photochemistry model. The new method has been demonstrated to be very effective, and numerical results confirm the excellent performance of the method compared to the RS-HDMR and Cut-HMDR methods.

Key words. RS-HDMR, Multiple sub-domains, Weight functions, Random sequence.

1. Introduction

Many problems in science and engineering involve the interaction of a large number of input variables, which leads to complex high dimensional systems. For examples, when describing the condensing complex atmosphere chemistry mechanism in environmental study, the photochemical box-model in [27] is a high dimensional system with 58 input variables; the gas prices in a gas station normally depends on the crude oil market, the gasoline wholesale market, and the prices of nearby gas stations, etc ([29]); and the aerosol thermodynamic equilibrium prediction in the atmosphere involves aerosol components including aerosol water, aqueous sulfate ion, aerosol nitrate, $(NH_4)_2SO_4$, NH_4NO_3, and total sulfate, ammonium, and nitrate, etc, and environmental variables of temperature and relative humidity, which is a multi-phase and multi-component high dimensional system ([4]).

One important objective of high dimensional problems is to explore the relations between input variables and output variables. In a n-dimensional variable space, the computational complexity of a high dimensional problem scales exponentially ([19]). Many methods have been studied to establish the relations in high dimensions such as projection pursuit algorithms ([6, 9, 15]), multi-layer perceptions ([17]) and radial basis functions ([18]). However, these methods are not widely accepted due to their inefficient performance.

The high dimensional model representation (HDMR) method is a new technique of quantitative model assessment and analysis tool to effectively obtain the relationships of inputs and outputs in high dimensional systems ([1, 12, 13, 19, 20],

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etc). The HDMR method is developed to improve the efficiency of the deducing high dimensional behaviors. The method is formed by a particular organization of low dimensional component functions, in which each function is the contribution of one or more input variables to the output variables. Based on the definition of HDMR in [19], its approximations can be constructed in two common ways: the Cut-HDMR and the RS-HDMR ([14, 20]). The HDMR methods have a broad range of applications including fully equivalent operational models ([26]), global uncertainty assessments ([2, 8, 21, 28]), financial and econometrics applications, etc ([5, 22, 23, 27]). However, for many high dimensional systems, due to the complicated input-output relations, the standard HDMR methods, i.e. the Cut-HDMR and the RS-HDMR methods defined in the whole domain, can not achieve sufficient accuracy ([27]). Hence, there have been strong interests in developing efficient HDMR methods for high dimensional systems in large domains. In [13], the Multi-cut-HDMR method is proposed by using multi-cut points but the numerical approximations depend on the locations of the multi-cut points. More recently, Cheng et al. [4] developed the moving cut HDMR method by combining with the multiple local moving cut points to obtain accurate and efficient approximations for high dimensional systems. The method has been successfully applied in the aerosol thermodynamic equilibrium prediction in atmospheric environment ([4]).

In this paper, we develop a new multiple sub-domain random sample HDMR Method (MSD-RS-HDMR), in which the random sample technique is used in sub-domains instead of using the cut point technique. For high dimensional input-output systems in large domains, the domain splitting technique is first applied to divide the large domains into multiple sub-domains and the multiple output variables are then approximated by the random sample HDMR method in sub-domains. The proposed MSD-RS-HDMR method is a combination of the local RS-HDMR approximations built in sub-domains of multiple input variables. Depending on the properties of input-output systems, the sub-domains may be overlapping or non-overlapping. Meanwhile, a set of weight functions is presented to provide approximations near the sub-domain interfaces. The sample points of the high dimensional inputs are generated in a quasi-random sequence by a stochastic algorithm. Numerical experiments are reported using the MSD-RS-HDMR method. First, we consider examples of given multiple dimensional functions, and we focus on the accuracy and efficiency of approximations. Then, the method is applied to a real problem in Tropospheric Alkane Photochemistry model, which describes the species concentration in troposphere ([26, 27]). The computations are based on the reduced model using six input chemical species, i.e. O_3, NO_2, NO, and three lumped alkane species. The proposed MSD-RS-HDMR method improves the accuracy for high dimensional systems compared to the RS-HDMR and Cut-HDMR methods. Numerical tests demonstrate the excellent performance, and it can be regarded as an efficient tool for general high dimensional problems.

The paper is organized as follows. Section 2 gives an introduction of the HDMR method and presents the multiple sub-domain RS-HDMR method. Numerical experiments are reported in Section 3. Application to a real problem in the Tropospheric Alkane Photochemistry model is shown in Section 4. Finally, conclusions are presented in Section 5.

2. The Multiple Sub-domain RS-HDMR Method

In this section, we develop the multiple sub-domain RS-HDMR method for high dimensional systems.