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Global sensitivity analysis with a hierarchical sparse metamodeling method

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ABSTRACT

To meet the numerical challenges of polynomial chaos expansion for global sensitivity analysis in high stochastic dimensions, this paper proposes a new metamodeling method named hierarchical sparse partial least squares regression-polynomial chaos expansion (HSPLSR-PCE). Firstly, to avoid large data sets, the polynomials are divided into groups according to their nonlinearity degrees and interaction intensities (number of inputs). Then, to circumvent the multicollinearity, latent variables are extracted from each group by using partial least squares regression. Next, the optimal latent variables are automatically selected with the penalized matrix decomposition scheme. Finally, the Sobol sensitivity indices are straightforwardly derived from the expansion coefficients. Results of three examples demonstrate that the proposed method is superior to the traditional counterpart in terms of computational efficiency and accuracy.

1. Introduction

Uncertainties inevitably arise in material and geometrical properties, loads and boundary conditions when modeling structural systems. Sensitivity analysis aims at quantifying and ranking the effect of different uncertainty sources, which provides important information about behaviour of the system. Generally, methods for sensitivity analysis can be classified into two categories,namely local and global methods [1]. The former study the local impact of inputs by providing partial derivatives. By contrast, the latter aim at quantifying the effect of different inputs and their interactions on output uncertainties when the inputs vary in the entire domain. After fast development in the past two decades, global sensitivity analysis can be categorized into regression-based methods [2], variance-based methods [3,4], moment-independent methods [5,6], derivative-based methods [7,8], reliability sensitivity methods [9,10] and so on. State-of-the-art reviews are available in Ref. [11] and Ref. [12]. Of interest in this paper is the variance-based methods since they have been widely applied in various territories.

The theoretical foundation of the variance-based methods is the ANalysis Of VAriance (ANOVA) decomposition [13,14] of a multivariate function. The main and total Sobol indices are used to quantify the importance of different inputs and their interactions, respectively [3,15]. The standard method for computing these coefficients is the Monte Carlo Simulation (MCS) which leads to high computational burden for expensive-to-evaluate models. A remedy to this problem is to build a

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surrogate model (also called metamodel) with similar accuracy but much lower computational complexity. Many metamodeling approaches have been proposed such as polynomial chaos expansion (PCE) [16,17], high dimensional model representation (HDMR) [18–20], Kriging [21], among which PCE has gained much attention for uncertainty quantification of structural systems.

The idea of PCE is to project the random response onto a Hilbert space spanned by polynomials which are orthogonal with respect to some probability measure. This method was originally proposed by Wiener[22] using standard Gaussian random variables and extended by Xiu and Kaniadakis [23] using other types of random variables. Applications of PCE in mechanical systems are classified into two categories, namely intrusive and non-intrusive methods. Intrusive methods compute expansion coefficients with the Galerkin projection-based methods, and were applied for solving initial value problems of stochastic ordinary differential equations. Peng et al. [24] proposed an adaptive PCE scheme for stochastic optimal control of a class of Duffing oscillators by using a displacement-velocity criterion which showed the potential of reducing the dimensionality of the expansion. For large complex structures, the governing equations are usually stochastic partial differential equations with given boundary conditions. Spectral stochastic finite element method [25,26] was originally applied for solving these problems. Some recent works [27,28] were dedicated to reduce memory usage and improve computational efficiency. By coupling stochastic analysis with mechanical analysis, intrusive methods showed capability for solving some classes of uncertainty propagation problems [29]. Non-intrusive methods are based on repeated calls of deterministic computer programs, which is convenient for analyzing large complex systems especially when using a commercial software. The classical approach to represent the random model response is the ordinary least squares regression (OLSR) [30–32]. However, for models with high stochastic dimensions, OLSR will inevitably encounter curse of dimensionality and multicollinearity. It is crucial to reduce the total number of training samples since one single simulation is time-consuming for complex models. Several approaches have been proposed to detect the important terms in the expansion such as stepwise regression [33–35], least angle regression [36], compressive sensing [37–39], support vector regression [40], D-MORPH regression [41] and so on. These methods have been proven to be capable of computing the expansion coefficients with acceptable accuracy under small sample sizes.

This paper is to propose a new non-intrusive PCE method for computing Sobol indices under small sample sizes. Breaking the routine that important polynomials are directly selected from the huge candidate set of finite order polynomials, the proposed method shed new light on PCE by using a divide-and-conquer strategy. Principal directions in each subspace spanned by the polynomials are detected by a partial least squares regression [42,43] -based hierarchical modeling algorithm. The new method can not only achieve significant dimension reduction, but contribute to uncover the latent low-dimensional structure of the model as well.

The remainder of this paper is organized as follows. In Section 2 we provide the basic knowledge of variance-based global sensitivity indices. Section 3 provides an overview of classical full PCE. Section 4 provides a detailed introduction of the proposed method. Numerical examples are given in Section 5.

2. Variance-based global sensitivity analysis

2.1. Sobol decomposition

Consider the physical model in Eq. (1)

$$\boldsymbol{y} = f(\xi) \tag{1}$$

where $\xi = (\xi_1, \ldots, \xi_n)$ is a n-dimensional random vector representing the inputs and $\boldsymbol{y}$ is a random variable representing the response. Under the hypothesis that the components of ξ are independent, the model can be represented with the Sobol decomposition in Eq. (2).

$$f(\xi_1, \ldots, \xi_n) = f_0 + \sum_i f_i(\xi_i) + \sum_{i<j} f_{i,j}(\xi_i, \xi_j) + \cdots + f_{1,2,\cdots,n}(\xi_1, \ldots, \xi_n) \tag{2}$$

Denote the mean value operator as $E[\cdot]$, the components in Eq. (2) are expressed as Eq. (3) to Eq. (6),

$$f_0 = E[f(\xi)] \tag{3}$$

$$f_i(\xi_i) = E[f(\xi)|\xi_i] - f_0 \tag{4}$$

$$f_{i,j}(\xi_i, \xi_j) = E[f(\xi)|\xi_i, \xi_j] - f_i(\xi_i) - f_j(\xi_j) - f_0 \tag{5}$$

...

$$f_{i_1,\ldots,i_l}(\xi_{i_1}, \ldots, \xi_{i_l}) = E[f(\xi)|\xi_{i_1}, \ldots, \xi_{i_l}] - \sum\nolimits_{j_1<\ldots<j_{l-1}\in\{i_1\ldots i_l\}} f_{j_1,\ldots,j_{l-1}}(\xi_{j_1}, \ldots, \xi_{j_{l-1}}) - \cdots - \sum_j f_j(\xi_j) - f_0 \tag{6}$$

and have the properties in Eqs. (7) and (8).

$$E[f_{\boldsymbol{\eta}}(\xi_\eta)] = 0, \;\; \eta \neq \{0\} \tag{7}$$