Applied Mathematics and Computation 323 (2018) 17–30

Contents lists available at ScienceDirect

Applied Mathematics and Computation

journal homepage: www.elsevier.com/locate/amc

Sparse polynomial chaos expansion based on D-MORPH regression

Kai Cheng, Zhenzhou Lu*

School of Aeronautics, Northwestern Polytechnical University, Xi' an 710072, PR China

ARTICLE INFO

Keywords:
Sparse polynomial chaos expansion
D-MORPH regression
Iterative reweighted scheme
Least angle regression

ABSTRACT

Polynomial chaos expansion (PCE) is widely used by engineers and modelers in various engineering fields for uncertainty analysis. The computational cost of full PCE is unaffordable for the "curse of dimensionality" of the expansion coefficients. In this paper, a new method for developing sparse PCE is proposed based on the diffeomorphic modulation under observable response preserving homotopy (D-MORPH) algorithm. D-MORPH is a regression technique, it can construct the full PCE models with model evaluations much less than the unknown coefficients. This technique determines the unknown coefficients by minimizing the least-squared error and an objective function. For the purpose of developing sparse PCE, an iterative reweighted algorithm is proposed to construct the objective function. As a result, the objective in D-MORPH regression is converted to minimize the ℓ_1 norm of PCE coefficients, and the sparse PCE is established after the proposed algorithm converges to the optimal value. To validate the performance of the developed methodology, several benchmark examples are investigated. The accuracy and efficiency are compared to the well-established least angle regression (LAR) sparse PCE, and results show that the developed method is superior to the LAR-based sparse PCE in terms of efficiency and accuracy.

1. Introduction

Along with the rapid development of computer science and technique, a variety of complex computational models have been developed for simulating and predicting the behavior of systems in nearly all fields of engineering and science. Operations on these models are time consuming and computationally cumbersome, thus a remedy is to substitute these complex models with surrogate models that possess similar statistical properties but a simple functional form [1].

Surrogate model, also known as meta-model, is a technique to generate a mathematical or numerical representation of a complex system based on a small amount of input–output data [2]. Over last few years, many surrogate models have been developed such as response surface method (RSM) [3,4], Kriging [5,6], radial basis function (RBF) [7,8], artificial neural networks (ANN) [9,10], support vector machine (SVM) [11,12], polynomial chaos expansion (PCE) [13–16], among which PCE has gained much attention for uncertainty analysis [17] in engineering applications.

PCE was originally proposed by Wiener with normally distributed random variables using Hermite polynomials [18]. Xiu and Karniadakis [19] extended it to other types of statistical distributions (uniform, beta, gamma,...). The key concept in PCE is to expand the model response onto basis made of multivariate polynomials that are orthogonal with respect to the joint

* Corresponding author.
E-mail address: zhenzhoulu@nwpu.edu.cn (Z. Lu).

https://doi.org/10.1016/j.amc.2017.11.044
0096-3003/

distribution of the input variables. In this setting, characterizing the response probability density function (PDF) is equivalent to evaluating the PCE coefficients, i.e. the coordinates of the random response in this basis [14]. The coefficients of the expansion are evaluated in terms of the response of the original model at a set of points in the input space. Generally, two classes of methods are applied to compute the PCE coefficients non-intrusively, namely projection method and regression method. The former approach estimates each coefficient based on a multi-dimensional numerical integration, and the latter approach computes the coefficients using least square regression. However, the required computational cost increases exponentially with the dimensionality of the input variables, which seriously restricts the engineering applications of PCE.

To address the issue of "curse of dimensionality", several efficient approaches have been proposed in the literature. Raisee [20,21] proposed a POD-based model reduction technique, where the computational expense is reduced by expanding the model output into its principal components [20]. Assuming the PCE representation of the model output is sparse, Blatman [14] firstly proposed a stepwise regression technique to select the significant basis functions sequentially based on cross-validation (CV), and then the least angle regression (LAR) algorithm [15] was exploited to detect the basis function based on the correlation to the model output. In the meanwhile, a well-validated MATLAB software, named UQlab, was developed by Marelli and Sudret [22] based on the LAR sparse PCE algorithm. Another stepwise regression technique was proposed by Abraham et al. [17], where the most important basis functions are selected sequentially based on the efficient tools relevant to probabilistic method. A new approach for building sparse PCE was also proposed by Shao et al. [23] using Bayesian approach based on the Kashyap information criterion for model selection. These methods have been proved to provide a significant computational gain compared to the classic full PCE.

In this paper, the Diffeomorphic Modulation under Observable Response Preserving Homotopy (D-MORPH) regression technique is proposed to build sparse PCE meta-model. D-MORPH is a general approach for model exploration, which was originally established for solving differential equations [24–26]. The goal of D-MORPH regression is to search for the best model that preserves desired features and diminishes undesired properties with an objective function. Inspired by the basis pursuit algorithm in "compressed sensing" technique [27–33], this work converts the objective function of D-MOROH regression to the ℓ_1 norm of PCE coefficients. The idea of ℓ_1-minimization has been widely adopted in "compressed sensing" method for function approximation. Thus sparse PCE meta-model can be obtained by the ℓ_1-minimization approach [34,35]. Compared to the existing work on basis pursuit algorithm, the superiority of D-MORPH regression is twofold: (1) obtaining the sparse solution while preserving fitting accuracy, (2) avoiding determination of the regularization parameter in basis pursuit problem [27–33]. Several benchmark analytical functions are used to validate and assess the performance of the proposed method, and the results are compared with the well-established LAR method in Ref. [15].

The reminder of this paper is organized as follows. In Section 2, we reviews the methodology of classic full PCE. Section 3 provides an overview of D-MORPH algorithm. After the new objective function and the proposed iterative algorithm are proposed, numerical applications are given in Section 4. The conclusion comes in the end.

2. Polynomial chaos approximation

For a model $y = g(\mathbf{x})$ where the input vector $\mathbf{x}$ is composed of n independent random variables $\mathbf{x} = \{x_1, x_2, \ldots, x_n\}$, y is the output response of interest. The classic PCE of second-order random variable may be expanded as follows:

$$y = g(\mathbf{x}) = \sum_{j=0}^{\infty} \beta_j \psi_j(\mathbf{x}) \tag{1}$$

where $\psi_j(\mathbf{x})(j = 0, \ldots, \infty)$ is the basis on the space of second order random variables and $\beta_j(j = 0, \ldots, \infty)$ are the coefficients in the expansion.

PCE in Eq. (1) needs to be truncated for practical applications as follows:

$$y = \sum_{j=1}^{p} \beta_j \psi_j(\mathbf{x}) \tag{2}$$

If the order of the polynomials used is d and there are n input variables $x_i(i = 1, \ldots, n)$, the total number of the expansion terms with order less than or equal to d is given by

$$p = \frac{(d+n)!}{d!n!} \tag{3}$$

Assuming that the input vector $\mathbf{x}$ has independent components x_i with prescribed probability density function (PDF) $f_{X_i}(x_i)$, then the joint PDF of $\mathbf{x}$ can be obtained by

$$f_{\mathbf{X}}(\mathbf{x}) = \prod_{i=1}^{n} f_{X_i}(x_i) \tag{4}$$

For each x_i, one can construct a family of orthogonal univariate polynomials $\{\psi_j^{(i)}, j = 0, 1, 2 \ldots\}$ with respect to their respective PDF satisfying:

$$E\left[\psi_j^{(i)}(x_i)\psi_k^{(i)}(x_i)\right] = \int \psi_j^{(i)}(x_i)\psi_k^{(i)}(x_i) f_{X_i}(x_i) dx_i = c_j^{(i)} \delta_{jk} \tag{5}$$