A Bayesian based algorithm to build up sparse polynomial chaos expansions for global sensitivity analysis

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Global Sensitivity Analysis (GSA) aims at quantifying a mathematical model's output uncertainty due to changes of the input variables over the entire domain. Different methods have been developed in the last few decades to perform GSA [1], such as regression-based methods, variance-based methods, Morris method, sampling methods and so on. Among all these techniques, Sobol' sensitivity indices based on the ANalysis Of VAriance (ANOVA) [2] are of great interest by many researchers. These indices are usually computed by crude Monte Carlo simulation, which is computationally expensive and hardly applicable for complicated industrial models. To circumvent this problem, a metamodel with less expensive evaluations is usually adopted to substitute the original model under consideration for the computation of GSA.

In this context, the polynomial chaos expansion (PCE) using orthogonal polynomial bases has received much interest [3], with which the Sobol' indices can be computed exactly from algebraic operations on the coefficients of PCE. The computation of the PCE coefficients are often conducted in two approaches, the projection approach and the regression approach. The latter reveals efficient when dealing with a moderate number of input variables. However, with a large number of input variables or a high order of PCE, the number of coefficients increases dramatically, which requires a large number of model evaluations accordingly. To reduce the computational cost on direct model evaluations, one needs to decrease the number of coefficients in the PCE. To this aim, several approaches have been developed to construct a sparse PCE, where only basis functions and coefficients that have significant contributions to the variance of the model are retained. The original idea of sparse PCE came from Blatman and Sudret [4, 5], where they developed an iterative forward–backward algorithm to construct sparse PCE based on stepwise regression technique. Later, a least angle regression algorithm to build up sparse PCE was proposed by [6]. Hu and Youn [7] presented a sparse iterative scheme using the projection technique. More recently, Fajraoui et al. [8] developed a simple strategy to construct a sparse PCE using a fixed experimental design.

In this work, a new algorithm based on Bayesian Model Averaging (BMA) is proposed to construct the sparse PCE. The BMA, relying on Bayes' theorem, is a well-known statistical approach to

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perform quantitative comparison of the proposed alternative models. The difficulty of the BMA lies in the evaluation of a quantity named Bayesian model evidence (BME), which involves an integral over the whole parameter space of a model, thus generally has no analytical solution. To approximate BME mathematically, the integral is treated with a Taylor series expansion followed by a Laplace approximation. Based on this approximation, the Kashyap information criterion (KIC) was proposed to evaluate BME for the most likely parameter set instead of the entire parameter space, making the evaluation computationally feasible. In the proposed algorithm, the maximum a posteriori estimate (MAP) is considered as the most likely coefficients for the selected model and used to evaluate KIC. For the sampling technique, the QMC method is adopted due to its space filling and desirable convergence properties. The proposed algorithm is outlined in the following:

(i) An initial experimental design is generated with LPtau samples, followed by the model evaluations at the design points. Then a "full" PCE is constructed at given degree and interaction order.

(ii) The basis functions in "full" PCE are reordered according to the contribution of each term to the variance of the model. This is performed in two steps: first, basis functions are sorted based on the Pearson correlation coefficients between basis functions and model evaluations, then they are reordered again by taking into account the partial correlation coefficients between basis functions and model evaluations.

(iii) The sparse PCE is enriched by adding candidate basis polynomials with decreasing partial variance one by one. One eventually retains those terms that lead to a decrease of KIC to obtain an optimal sparse PCE model with minimized KIC.

The accuracy and efficiency of the proposed algorithm to construct sparse PCE for GSA is assessed by some benchmarking tests. The approach is then applied to perform the GSA on hydraulic models, which highlights the effectiveness and reliability of the proposed algorithm.

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