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Global sensitivity analysis via multi-fidelity polynomial chaos expansion

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ABSTRACT

The presence of uncertainties is inevitable in engineering design and analysis, where failure in understanding their effects might lead to the structural or functional failure of the systems. The role of global sensitivity analysis in this aspect is to quantify and rank the effects of input random variables and their combinations to the variance of the random output. In problems where the use of expensive computer simulations is required, metamodels are widely used to speed up the process of global sensitivity analysis. In this paper, a multi-fidelity framework for global sensitivity analysis using polynomial chaos expansion (PCE) is presented. The goal is to accelerate the computation of Sobol sensitivity indices when the deterministic simulation is expensive and simulations with multiple levels of fidelity are available. This is especially useful in cases where a partial differential equation solver computer code is utilized to solve engineering problems. The multi-fidelity PCE is constructed by combining the low-fidelity and correction PCE. Following this step, the Sobol indices are computed using this combined PCE. The PCE coefficients for both low-fidelity and correction PCE are computed with spectral projection technique and sparse grid integration. In order to demonstrate the capability of the proposed method for sensitivity analysis, several simulations are conducted. On the aerodynamic example, the multi-fidelity approach is able to obtain an accurate value of Sobol indices with 36.66% computational cost compared to the standard single-fidelity PCE for a nearly similar accuracy.

1. Introduction

Computational methods are widely deployed to predict the behavior and to compute the outputs of interest (e.g., stress distribution or force) of physical or engineering systems. In engineering design and analysis, computational partial differential equation (PDE) solvers are routinely employed to aid and enhance such processes. However, due to the existence of uncertainties in the system, deterministic analysis might result in a failure to understand the true probabilistic nature of the system. An example of this is in the field of aerospace engineering, where manufacturing error and environmental uncertainties such as gust, turbulence, and change in design conditions perturb the nominal condition of the aircraft. Understanding the effect of the uncertainties on the system is then a vital task in many engineering and scientific problems. Depending on the nature of the uncertainties, they can be categorized as either aleatory or epistemic uncertainties. While aleatoric uncertainties are irreducible and inherent to the system, epistemic uncertainties are caused by our lack of knowledge of the system being investigated. Aleatoric uncertainties can be conveniently expressed by probability theory using specific measures such as statistical moments.

Sensitivity analysis (SA) in probabilistic modeling plays an important role in understanding the impact of input random variables and their combinations to the model output. By performing SA, the contribution of the input random variables to the model output can be ranked, thus giving the analysts information of which variables are the most and least responsible. This is very useful in uncertainty quantification (UQ), where the dimensionality of the random variable can be high and it is desired to reduce the complexity beforehand. Moreover, sensitivity information can provide important knowledge about the physics of the system being investigated. In engineering analysis, numerical evaluation of PDE is often required in order to obtain necessary information for SA. In the field of fluid and solid mechanics, the model responses are typically evaluated using computational fluid dynamics (CFD) or finite element methods (FEM), respectively.

Based on the range of the domain to be analyzed, SA is commonly classified into two groups [1]:

- *local sensitivity analysis*, which studies the local impact of the input parameters on the model output and typically provides the partial derivatives of the output to the input parameters.
- *global sensitivity analysis*, which studies the uncertainties in the output due to changes of the input parameters over the entire domain.

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Based on how it exploits the model response, SA can be further categorized into [1]:

- *regression-based methods*, which perform linear regression to the relationship between the model input and output. These methods are limited to cases with a linear or almost linear relationship but are inadequate in cases with highly non-linear relationship.
- *variance-based methods*, which decompose the variance of the output into the sum of contributions of each input variables and their combination. In statistic literature, variance based methods are widely known as ANOVA (ANalysis Of VAriance) [2]

In this paper, we have interest in global SA using variance-based methods since our main focus is on UQ, although the methodology itself can be used for other applications such as optimization. More specifically, this paper focuses on Sobol sensitivity analysis method [3].

Monte Carlo simulation (MCS) is the most conventional method to perform SA [3]. The advantage of MCS for SA is that it is straightforward and very simple to be implemented. However, it is infeasible to obtain accurate results using MCS if a demanding computational simulation is used. To cope with this, more advanced techniques have to be employed. SA using cheap analytical replacement of the true function, or a metamodel, is one way to handle this. Metamodeling techniques such as radial basis function [4], Kriging [5–9], probabilistic collocation [10], and polynomial chaos expansion (PCE) [11–14] can be employed for SA purpose.

In the closely related field of structural reliability analysis, metamodeling techniques have been widely employed to accelerate the computation of failure probability [15–20]. Compared to other metamodels, Kriging metamodel is particularly useful for reliability analysis due to the direct availability of error estimation that allows one to deploy active learning strategy [21–23] (i.e., Kriging with adaptive sampling). Active learning works by adding more samples so as to increase the accuracy of the metamodel near the region of interest, that is, the limit state. Besides Kriging, PCE has also been employed for structural reliability analysis purpose [24–27]. Recently, a combination of PCE and Kriging within the framework of universal Kriging and active learning was developed to handle rare event estimation problem [28].

Metamodels in UQ and SA are required to be globally accurate for a precise estimation of sensitivity indices. Although not in the context of global SA, the use of Kriging models with adaptive sampling to progressively refine the global accuracy has been explored by some researchers within the context of UQ [29,30]. Dwight and Han proposed an adaptive sampling technique for UQ by using a criterion based on the product of the Kriging uncertainty and the probability density function of the random inputs [31], which is useful for cases with non-uniform distributions. Another alternative is to construct local surrogate models such as Dutch intrapolation [32] and multivariate interpolation and regression [33,34] in order to provide the error measure. A recent survey of adaptive sampling for Kriging and other surrogate models for various applications can be found in Liu et al. [35]. Other than Kriging, polynomial-based metamodels, especially PCE, are highly useful and competitive to the Kriging model when the quantities of interest are the statistical moments and sensitivity indices.

The advantage of PCE for UQ and SA purpose is that the calculation of Sobol sensitivity indices can be directly performed as the post-processing step [36,37]. This is in contrast to other metamodelling techniques where MCS still needs to be performed on the analytical metamodel to obtain the Sobol indices. The approximation quality of the metamodel can be further enhanced by including gradient information. Some methods that have been reformulated in order to include gradient information are gradient-enhanced Kriging [31,38–41], compressive sensing-based PCE [42], and sparse grid method [43]. However, it is worth noting that obtaining gradient information is a tedious task and is not always possible for many applications. In this paper, we assume that gradient information is not available.

The PCE method is based on homogeneous chaos expansion, which itself is based on the seminal work of Wiener [44]. The earliest version of PCE computes the coefficients by using Galerkin minimization. This intrusive scheme needs modification of the governing equation and the simulation code in order to perform the UQ procedure [14]. The difficulty with the intrusive scheme is that the derivation of the modified governing equation might be very complex and highly time-consuming. In this paper, the method of interest is non-intrusive PCE [12,14], that allows the use of legacy code since it can be treated as black box simulation. Based on how it estimates the PCE coefficients, non-intrusive PCE can be classified into two categories:

1. *Spectral projection*, which estimates the coefficients by exploiting the orthogonality of the polynomial and quadrature [11,12].
2. *Regression*, which estimates the coefficients by using least-square minimization [25,45].

Note that the definition of regression-based PCE is different from the regression-based SA. The definition of the former is that a regression-based technique is used to build the PCE metamodel, while the definition of the latter is the utilization of linear approximation within SA framework.

PCE has been developed and implemented as a tool for SA since the work of Sudret [36]. Further simulations are not necessary because the Sobol indices in PCE are obtained in the post-processing phase [36,37] by exploiting the orthogonality of the polynomial bases. PCE is now a widely used approach in the field of UQ due to its strong mathematical basis [46]. For regression-based PCE, sparse-PCE based on least-angle-regression is an efficient method to obtain the Sobol indices without the need to determine the polynomial bases a priori [47,48]. Another alternative for sparse PCE is using a compressive sensing-based technique [49,50] that employs orthogonal matching pursuit to scan the most influential polynomial bases. While for the spectral-projection based PCE, the sparse grid interpolation technique [51–54] can be employed to reduce the number of collocation points in high-dimensionality for SA purpose [55–59]. Recent advances in this field include the use of PCE for multivariate SA [60]. Our interest in this paper is to obtain Sobol sensitivity indices for global SA purpose by using polynomial chaos expansion (PCE).

In some applications, simulations with multiple levels of fidelity are available. The fidelity here is defined as the measure of how accurate the model approximates the reality. The fidelity level is typically categorized into high- and low-fidelity, where the categorization of the model into high- or low-fidelity depends on the case being investigated. The high-fidelity (HF) simulation is the most accurate but is typically more computationally demanding than the low-fidelity (LF) simulation. On the other hand, the LF simulation is less accurate but many evaluations could be performed since it is cheaper to evaluate. For example, a PDE-solver with a very fine and coarse mesh can be treated as the HF and LF simulation, respectively. An approach that utilizes simulations with multiple levels of accuracy is commonly called multi-fidelity (MF) method. The common technique to apply MF simulations is to use LF simulations to capture the response trend and employ HF simulations to correct the response.

Multi-fidelity simulation is commonly used to aid and accelerate the optimization process. Co-Kriging [61,62] and space-mapping [63,64] are two examples of surrogate-based methods that rely on MF simulations; mainly for optimization purposes. Multi-fidelity techniques for UQ purpose recently appeared in literature. Among the first is the multi-level Monte Carlo (MLMC) method which was firstly developed in the context of solving stochastic PDEs problem [65,66] and was further developed to handle general black-box problems [67]. The MF Kriging method is also applicable for UQ purpose [68]. Recently, a non-intrusive MF-PCE based technique to solve UQ problems was developed. The method works by combining the LF and correction PCE into a single MF-PCE [69]. The coefficients of the LF and correction PCE can be obtained by employing spectral projection [69] or regression-based