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Polynomial chaos expansion for sensitivity analysis

Thierry Crestaux [a,*], Olivier Le Maître [b], Jean-Marc Martinez [c]

[a] CEA-DM2S, 91 191 Gif sur Yvette, France
[b] LIMSI-CNRS, BP 133, 91 403 Orsay cedex, France
[c] CEA-DM2S, 91000 Saclay, France

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ABSTRACT

In this paper, the computation of Sobol's sensitivity indices from the polynomial chaos expansion of a model output involving uncertain inputs is investigated. It is shown that when the model output is smooth with regards to the inputs, a spectral convergence of the computed sensitivity indices is achieved. However, even for smooth outputs the method is limited to a moderate number of inputs, say 10–20, as it becomes computationally too demanding to reach the convergence domain. Alternative methods (such as sampling strategies) are then more attractive. The method is also challenged when the output is non-smooth even when the number of inputs is limited.

1. Introduction

In mathematical modeling, sensitivity analysis (SA) studies variations in the output of a model (numerical or other) with regards to some inputs. There are two categories of methods for SA: local SA and global SA. Local SA is interested on the local variation of the model with the inputs using gradients methods, while global SA deals with global variations in the output due to the uncertainties on the inputs. Moreover SA is usually said to be qualitative when it classifies the inputs according to their respective impacts on the output variations and quantitatively when it gives a measure of these impacts. Generally a quantitatively SA is also qualitative. SA had been largely studied and many approaches have been proposed. In this article we are interested in global SA using Sobol's indices [1] to determine input variables (or groups of variables) mostly responsible both qualitatively and quantitatively of the uncertainty in the model output [2]. Indeed in uncertainty quantification (UQ) it is important too to determine the uncertain inputs which have the largest impact on the variability of the model output. The Sobol's indices are obtained from the ANOVA decomposition of the output. Several methods had been developed to compute these indices directly through sampling using Monte-Carlo and quasi-Monte-Carlo (QMC) methods or by building a meta-model to approximate the ANOVA decomposition and then compute the indices from the meta-model with less model evaluations. The work presented in this article belong to the meta-modeling approach using polynomial chaos (PC) expansions to approximate the model output.

PC expansions [3] have been used for UQ in a large variety of domains (e.g. in solid mechanics, fluid flows, thermal sciences, etc.). PC expansion is a probabilistic method consisting in the projection of the model output on a basis of orthogonal stochastic polynomials in the random inputs. The stochastic projection provides a compact and convenient representation of the model output variability with regards to the inputs. We show in this paper that the Sobol's sensitivity indices [1] (and even more the ANOVA decomposition or Sobol's decomposition of the model output) can be immediately deduced from the PC expansion of the model output.

We can see this PC approach to compute Sobol's indices as one HDMR (high dimensional model representation) method, indeed HDMR methods consist in approximating the component functions, f_u, of a finite hierarchical correlation function expansion,

$$f(\xi) = \sum_{u \subseteq \{1,2,\ldots,d\}} f_u(\xi_u). \tag{1}$$

We will show that the PC expansion of the model output directly provides one of these functional decompositions. RS-HDMR and cut-HDMR (see [4–6]) are other HDMR approaches. RS-HDMR uses sampling techniques to compute approximations of the component functions of the ANOVA decomposition (which is the same that we compute using PC expansion) while the cut-HDMR uses interpolation through the model values on lines, planes and hyperplanes passing through a cut center point. One essential difference with the PC expansion-based approach of classical HDMR methods is that they limit themselves to the determination

* Corresponding author at: DM2S-SFME, Centre d'Etude de Saclay, F-91 191 Gif sur Yvette, France. Tel.: +33 169 08 9978; fax: +33 169 08 9999.
E-mail addresses: thierry.crestaux@cea.fr, crestaux_thierry@yahoo.fr (T. Crestaux), olm@limsi.fr (O. Le Maître), jean-marc.martinez@cea.fr (J.-M. Martinez).

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of only the low order components of the functional decomposition. This is based on the assumption that for most physical systems only low order correlations of the inputs will have impact on the output. However, the RS-HDMR can use the same orthonormal polynomial basis than the PC expansion. So in a certain way the RS-HDMR with orthonormal polynomials (see [4]) is similar to PC expansion restricted to low order correlations polynomials with the coefficients computed by Monte-Carlo approximation of the projections. Monte-Carlo approximation is less precise for smooth functions than the projection by Smolyak's cubature exposed in this article when the dimension is not too high. Speaking of quadrature techniques for numerical integration, in [5] the authors propose to compute the ANOVA decomposition using quadrature and computing the points on the cut-HDMR expansion. Nevertheless they do not use the Smolyak's cubature.

These meta-modeling methods have been widely used for SA, especially with non-parametric techniques which have shown their efficiency in SA using variables selection approaches for a qualitatively SA (see [7]) or approximation of the ANOVA decomposition for quantitatively SA (see [8]). It has been shown that these meta-modeling methods can be much more efficient than the sampling method for the computation of the Sobol's indices, by relying on a significantly lower number of model evaluations. However, the efficiency of the meta-modeling methods highly depends on the structure and complexity of the considered model, which make their general comparison difficult. Therefore, the efficiency of the proposed PC expansion for SA and determination of the Sobol's indices is here only contrasted with sampling methods (LHS and QMC). Future works will focus on the comparison of the PC approach with alternative meta-modeling methods and also with the Bayesian approach (see [9]). It is also important to note that the PC expansion of the model output can be obtained by means of Galerkin projection schemes when the model is a set of equations (see for instance [3]) with potential computational savings compared to the integration approach used in this work.

The paper is organized as follow. In Section 2, we provide a brief summary of Wiener's homogeneous chaos theory [10] and of the PC representations. We recall the principles of the solution methods used for the determination the PC expansion of a model output. We emphasize on the so-called non-intrusive spectral projection (NISP) and cubature techniques, which we use in the numerical examples. Section 3 reviews Sobol's functional decomposition and define the Sobol sensitivity indices. In Section 4, we provide details on the practical computation of the Sobol's indices via Monte-Carlo sampling strategies, emphasizing on the computational complexity. We then make the connection between the Sobol functional decomposition and the PC expansion of the model output. This connection naturally leads to exact expressions for the Sobol sensitivity indices in terms of the PC expansion coefficients. In Section 5, we present three numerical examples to illustrate the efficiency and the limitations of the computation of Sobol's sensitivity indices from PC expansions. The efficiency of the PC approach is compared and contrasted with the Monte-Carlo and QMC sampling strategies. Finally, in Section 6 we summarize the main findings of this work and weprovide some recommendations for future improvements of the method.

2. PC expansions

2.1. Hermite PC

PC expansions, introduced by Wiener in [10], approximate any well behaved random variable (e.g. a second-order one) by a series of polynomials in centered normalized Gaussian variables. In the following we use the notations of [3]. Let Ω be the space of random events and Θ the space of functions which associate to the elements $\omega \in \Omega$ a value in $\mathbb{R}$. A function $\theta : \omega \in \Omega \mapsto \mathbb{R}$ is a random variable. Let $\{\xi_i\}_{i=1}^{\infty}$ be an infinite but countable set of independent normalized Gaussian random variables. We define:

- $\widehat{\Gamma}_p$ the space of all polynomials of degree less or equal to p in $\{\xi_i(\omega)\}_{i=1}^{\infty}$,
- Γ_p the set of polynomials of $\widehat{\Gamma}_p$ which are orthogonal to $\widehat{\Gamma}_{p-1}$,
- $\widetilde{\Gamma}_p$ the space generated by Γ_p:

$$\widehat{\Gamma}_p = \widehat{\Gamma}_{p-1} \oplus \widetilde{\Gamma}_p, \quad \Theta = \bigoplus_{i=0}^{\infty} \widetilde{\Gamma}_i. \tag{2}$$

The sub-space $\widetilde{\Gamma}_p$ of Θ is called the p-th homogeneous chaos and Γ_p is called PC of order p. In fact, the PC of order p is the set of all polynomials of degree p in all possible combinations of the random variables in $\{\xi_i(\omega)\}_{i=1}^{\infty}$. The PC expansion of a second-order random variable $\theta(\omega)$ is

$$\begin{aligned}\theta(\omega) = a_0\Gamma_0 &+ \sum_{i_1=1}^{\infty} a_{i_1}\Gamma_1(\xi_{i_1}(\omega)) \\ &+ \sum_{i_1=1}^{\infty}\sum_{i_2=1}^{i_1} a_{i_1 i_2}\Gamma_2(\xi_{i_1}(\omega),\xi_{i_2}(\omega)) \\ &+ \sum_{i_1=1}^{\infty}\sum_{i_2=1}^{i_1}\sum_{i_3=1}^{i_2} a_{i_1 i_2 i_3}\Gamma_3(\xi_{i_1}(\omega),\xi_{i_2}(\omega),\xi_{i_3}(\omega)) \\ &+ \sum_{i_1=1}^{\infty}\sum_{i_2=1}^{i_1}\sum_{i_3=1}^{i_2}\sum_{i_4=1}^{i_3} a_{i_1 i_2 i_3 i_4}\Gamma_4(\xi_{i_1}(\omega),\xi_{i_2}(\omega),\xi_{i_3}(\omega),\xi_{i_4}(\omega)) + \cdots\end{aligned} \tag{3}$$

Cameron and Martin have shown in [11] that this expression is convergent in the L_2-sense. To simplify the notations and to ease the formal manipulation of PC expansions, we define an univocal relation between functionals $\Gamma()$ and new functionals $\Psi()$, and rewrite the PC expansion as

$$\theta(\omega) = \sum_{k=0}^{\infty} \theta_k \Psi_k(\boldsymbol{\xi}(\omega)), \quad \boldsymbol{\xi} = \{\xi_1, \xi_2, \ldots\}. \tag{4}$$

We shall adopt in the following the classical convention consisting in taking Ψ_0 as the zero order polynomial: $\Psi_0 = 1$. In Eq. (4), θ_k are deterministic coefficients, namely the PC coefficients of the expansion of the random variable θ, while the Ψ_k are random polynomials, orthogonal in the L_2-space, with regards to the inner product, denoted $\langle , \rangle$, based on the Gaussian measure:

$$\langle \Psi_i, \Psi_j \rangle \equiv \int \Psi_i(\boldsymbol{\xi})\Psi_j(\boldsymbol{\xi})p(\boldsymbol{\xi})\,\mathrm{d}\boldsymbol{\xi} = \delta_{ij}\langle \Psi_i, \Psi_i \rangle,$$

$$p(\boldsymbol{\xi}) = \prod_l \frac{\exp[-\xi_l^2/2]}{\sqrt{2\pi}}. \tag{5}$$

In fact, the Ψ_i are multi-variate Hermite polynomials (the product of univariate Hermite polynomials).

For practical calculations, a finite number d of Gaussian variables are to be used, leading to finite dimensional PC expansions:

$$\theta(\xi_1, \xi_2, \ldots, \xi_d) = \sum_{k=0}^{\infty} \theta_k \Psi_k(\xi_1, \xi_2, \ldots, \xi_d). \tag{6}$$

This is not a limitation, since most physical problems we are focusing on involve a finite number of random inputs (parametric uncertainty). Moreover the expansion is convergent, as we work in a finite dimensional Hilbert space and Hermite polynomials form an Hilbert basis. Also for practical reasons, PC expansions have to be truncated in terms of polynomial degree. Let p denote