Polynomial Chaos Expansion for Sensitivity Analysis

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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 to 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.

Key words: Sensitivity analysis, Sobol's decomposition, Polynomial Chaos, Uncertainty Quantification

1 Introduction

In mathematical modelling, 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 sensitivity analysis and global sensitivity analysis. Local sensitivity analysis is interested on the local variation of the model with the inputs using gradients methods, while global sensitivity analysis deals with global variations in the output due to the uncertainties on the

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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 sensitivity analysis 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 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 expansions to approximate the model output.

Polynomial Chaos (PC) expansions [3] have been used for UQ in a large variety of domains (*e.g.* in solid mechanics, fluid flows, thermal sciences,...). PC expansions 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,

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

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],[5] and [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 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 don't use the Smolyak's cubature.

These meta-modeling methods have been widely used for SA, especially with nonparametric 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 Quasi-Monte-Carlo sampling strategies. Finally, in

Section 6 we summarize the main findings of this work and we provide some recommendations for future improvements of the method.

2 Polynomial Chaos Expansions

2.1 Hermite Polynomial Chaos

Polynomial Chaos 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 $\theta : \omega \in \Omega \longmapsto \mathbb{R}$ 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 Polynomial Chaos of order p. In fact, the Polynomial Chaos 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 Polynomial Chaos expansion of a second order random variable $\theta(\omega)$ is

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

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:

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

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:

$$\langle \Psi_i, \Psi_j \rangle \equiv \int \Psi_i(\boldsymbol{\xi}) \Psi_j(\boldsymbol{\xi}) p(\boldsymbol{\xi}) d\boldsymbol{\xi} = \delta_{ij} \langle \Psi_i, \Psi_i \rangle , \quad p(\boldsymbol{\xi}) = \prod_l \frac{\exp[-\xi_l^2/2]}{\sqrt{2\pi}}. \tag{5}$$

In fact, the Ψ_i are multivariate 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 Polynomial Chaos expansions:

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

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 the order of the PC expansion. The finite dimensional and finite order PC expansion of a random variable θ is finally

$$\theta(\boldsymbol{\xi}) \approx \sum_{k=0}^{P} \theta_k \Psi_k(\boldsymbol{\xi}), \quad \boldsymbol{\xi} = \{\xi_1, \ldots, \xi_d\}, \tag{7}$$

where the basis dimension is related to d and p by

$$P + 1 = \frac{(p+d)!}{p!\ d!}. \tag{8}$$

2.2 Generalized Polynomial Chaos

In [12], Xiu and Karniadakis used the Askey scheme to generalize Wiener's Polynomial Chaos expansion to common non-Gaussian measures. This generalization can be useful to improve the expansion convergence for non-Gaussian

random variables. Table 1 reports the correspondence between the random variable distribution and orthogonal polynomial family. The polynomials are orthogonal in the Hilbert space corresponding to the support and the density function of the random variable; they form an Hilbert basis of the respective space.

Type	Random variable distribution	Orthogonal polynomial family	Support
Continuous	Gaussian	Hermite	$(-\infty, \infty)$
	Gamma	Laguerre	$[0, \infty)$
	Beta	Jacobi	$[a, b]$
	Uniform	Legendre	$[a, b]$
Discrete	Poisson	Charlier	$\{0, 1, 2, ...\}$
	Binomial	Krawtchouk	$\{0, 1, 2, ..., N\}$

Table 1
Relation (Askey-scheme) between the random variable distribution and orthogonal polynomial family [12].

Denoting $\{\phi_k\}_{k=0}^{\infty}$ the one-dimensional orthogonal polynomials from the Askey-scheme, and assuming the random variables to be independent, the muti-dimensional Generalized Polynomial Chaos (GPC) basis $\{\Psi_i\}$ is constructed by tensor products of the corresponding one dimensional polynomials,

$$\Psi_i(\xi_1, \xi_2, ..., \xi_d) = \prod_{k=1}^{d} \phi_{\alpha_k^i}(\xi_k), \quad |\alpha^i| \equiv \sum_{k=1}^{d} \alpha_k^i \leq p, \quad i = 0, \ldots, P. \tag{9}$$

2.3 Determination of PC-coefficients

We are interested in the uncertainty quantification and analysis for some output quantity y, which depends on some random input $\boldsymbol{D}(\omega)$. We assume that the uncertain input is parameterized using a finite set of d independent random variables $\boldsymbol{\xi} = \{\xi_1, \ldots, \xi_d\}$ with known densities $p(\boldsymbol{\xi})$, *i.e.* $\boldsymbol{D}(\omega) \equiv \boldsymbol{D}(\boldsymbol{\xi}(\omega))$. Clearly, the output y being a functional of the random input it is also random and we can write

$$y(\boldsymbol{D}(\boldsymbol{\xi})) = y(\boldsymbol{\xi}). \tag{10}$$

Let $\{\Psi_i\}$ be an Hilbert basis of $L_2(\boldsymbol{\xi}, p(\boldsymbol{\xi}))$ the space of second order random variables spanned by $\boldsymbol{\xi}$. Assuming that $y \in L_2(\boldsymbol{\xi}, p(\boldsymbol{\xi}))$, it has a convergent PC expansion that we write as

$$y(\boldsymbol{\xi}) = \sum_k \beta_k \Psi_k(\boldsymbol{\xi}). \tag{11}$$

Since the PC-coefficients fully determine a second-order random variable, the knowledge of the β_k in the expansion of the output y allows for a complete characterization of the uncertainty. It also makes explicit the functional dependences with regards to the input, a property that will be fully exploited later for the determination of the Sobol sensitivity indices.

To improve the convergence of the PC expansion, in situations where the output y presents non-smooth or discontinuous depedences with regards to the uncertain inputs, piecewise continuous polynomials expansions were recently proposed (*e.g.* using multi-wavelets and multi-resolution schemes [13,14,15] and multi-element methods [16]).

We thus need efficient procedures for the determination of the PC coefficients of the output y. In the following, we assume that y is the result of a numerical simulation, *i.e.* the output of a numerical code involving a mathematical model. Classically, two classes of methods are distinguished for the determination of the PC coefficients: the intrusive and non-intrusive methods.

In the intrusive method, a weak solution of the mathematical model involving the random input is sought by means of a Galerkin projection of the model equations on the PC basis [3]. This procedure, shortly described in Section 2.3.1, requires modifications of the numerical code and is therefore intrusive. On the contrary, non-intrusive methods require realizations of the deterministic code only, for different values of the input. Two such non-intrusive methods are described below: the least square approximation in Section 2.3.2, and the non-intrusive spectral projection (NISP [17]) in Section 2.3.3. The NISP procedure being used in the examples of Section 5, more details are provided.

2.3.1 Galerkin projection

Let us consider the mathematical model $\mathcal{M}$ relating the random output y to the input $\boldsymbol{D}$. We write in a formal way

$$\mathcal{M}(y(\boldsymbol{\xi}); \boldsymbol{D}(\boldsymbol{\xi})) = 0. \tag{12}$$

Substituting to y its PC expansion Eq. (11), truncated at order p, the model equation is generally not satisfied anymore but yields a residual. Imposing the residual to be orthogonal to the expansion basis, it comes

$$\left\langle \mathcal{M}\left(\sum_{i=0}^{P} \beta_i \Psi_i(\boldsymbol{\xi}); \boldsymbol{D}(\boldsymbol{\xi})\right), \Psi_k \right\rangle = 0, \quad \forall k = 0, \ldots, P. \tag{13}$$

It is seen that the Galerkin procedure leads to the resolution of a set of $P+1$ coupled problems. It usually requires an adaptation of the numerical code.

Furthermore, if the mathematical model involves complex non-linearities, the Galerkin procedure can be a challenging task and difficult to implement. To overcome these difficulties, non-intrusive methods described below are useful.

2.3.2 Least square approximation

The PC coefficients can be estimated by solving a least square problem. Let us denote $\{\boldsymbol{\xi}^{(i)}\}$ a sample set of the random parameters, and $\mathbf{y} = \{y^{(i)}\}$ the corresponding set of simulation output, such that

$$\mathcal{M}\left(y^{(i)}; \boldsymbol{D}\left(\boldsymbol{\xi}^{(i)}\right)\right) = 0, \quad \forall i. \tag{14}$$

Since the determination of the output sample set uses the deterministic code only, the method is non-intrusive. Denoting $\beta = (\beta_0 \dots \beta_P)^T$ the vector of sought PC coefficients in the truncated expansion of the output y, an approximation $\hat{\beta}$ of β can be obtained by solving the least square problem

$$\hat{\beta} = \arg\min_{\beta} \sum_{i=1}^{n} \left(y^{(i)} - \sum_{k=0}^{P} \beta_k \Psi_k(\boldsymbol{\xi}^{(i)}) \right)^2, \tag{15}$$

where $n > P + 1$ is the sample set size. Denoting

$$Z = \begin{pmatrix} \Psi_0(\boldsymbol{\xi}^{(1)}) & \Psi_1(\boldsymbol{\xi}^{(1)}) & \dots & \Psi_P(\boldsymbol{\xi}^{(1)}) \\ \Psi_0(\boldsymbol{\xi}^{(2)}) & \Psi_1(\boldsymbol{\xi}^{(2)}) & \dots & \Psi_P(\boldsymbol{\xi}^{(2)}) \\ \vdots & \vdots & \ddots & \vdots \\ \Psi_0(\boldsymbol{\xi}^{(n)}) & \Psi_1(\boldsymbol{\xi}^{(n)}) & \dots & \Psi_P(\boldsymbol{\xi}^{(n)}) \end{pmatrix}, \tag{16}$$

the well known solution of the least square problem is

$$\hat{\beta} = (Z^T Z)^{-1} Z^T \mathbf{y}, \tag{17}$$

where $Z^T Z$ is the Fisher matrix. It is to be noted that Least Square does not exploit the orthogonality of the polynomials. The sample sets can be constructed by simple random sampling (SRS), Latin hypercube sampling (LHS), maximin LHS, ... However, there is yet only empirical results on the way to construct the sample sets, and to choose its size. To prevent overfitting, methods from regression and statistical learning can be used.In [18] the authors consider three methods to choose the degree of the polynomial approximation in order to prevent overfitting: *Adjusted* R^2*, Early Stopping* and *Wilcoxon Rank Sum Test*. These methods can be used in the PC expansion context to prevent overfitting.

2.3.3 Non-intrusive spectral projection

On the contrary of the least square approximation, the non-intrusive spectral projection (NISP) exploits the orthogonality of the PC basis. Taking the inner product of the output PC expansion with Ψ_k and making use of the orthogonality of the basis, it comes

$$\beta_k = \frac{\langle y(\boldsymbol{\xi}), \Psi_k(\boldsymbol{\xi})\rangle}{\langle \Psi_k, \Psi_k\rangle}, \quad \forall k. \tag{18}$$

Recalling the definition of the inner product,

$$\langle f(\boldsymbol{\xi}), g(\boldsymbol{\xi})\rangle = \int_{\Omega^d} f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) p(\boldsymbol{\xi}) d\boldsymbol{\xi}, \tag{19}$$

where we have denoted Ω^d the support of $\boldsymbol{\xi}$ and $p(\boldsymbol{\xi})$ its joined density, it is seen that the determination of the PC coefficients of the output reduces to the evaluation of $(P+1)$ d-dimensional integrals:

$$I_k \equiv \int_{\Omega^d} y(\boldsymbol{\xi}) \Psi_k(\boldsymbol{\xi}) p(\boldsymbol{\xi}) d\boldsymbol{\xi}. \tag{20}$$

In fact, I_k is the correlation between the output and the k-th PC. Note that thanks to the polynomial character of the Ψ_k, the exact evaluation of $\langle \Psi_k, \Psi_k\rangle$ is immediate.

Numerical multi-dimensional integration or quadrature is a classical problem and many methods have been proposed for this purpose. The numerical integration methods can be recasted in the following generic form,

$$I_k \approx \sum_{i=1}^{n} y(\boldsymbol{\xi}^{(i)}) \Psi_k(\boldsymbol{\xi}^{(i)}) w^{(i)}, \tag{21}$$

where $\boldsymbol{\xi}^{(i)}$, $w^{(i)}$ are the integration points and weights respectively while n is the number integration points. In our applications, the numerical cost of the integration scales essentially with n, since it is dominated by the evaluation (or model resolution) of the output y for given $\boldsymbol{\xi}^{(i)}$ using Eq. (14). The integration methods have specific strengths and weaknesses, to be taken into account when selecting one of them. Let us recall the main properties of the most common integration methods available:

- Monte-Carlo sampling is robust and converges for any L^2-function with a convergence rate independent of the dimension d; however the asymptotic rate is in $1/\sqrt{n}$ only.
- Quasi Monte-Carlo sampling is less robust than Monte-Carlo sampling as it involves some assumptions on the smoothness of the integrand. However, when these assumptions are satisfied a convergence rate in $\log(n)^d/n$ is achieved.

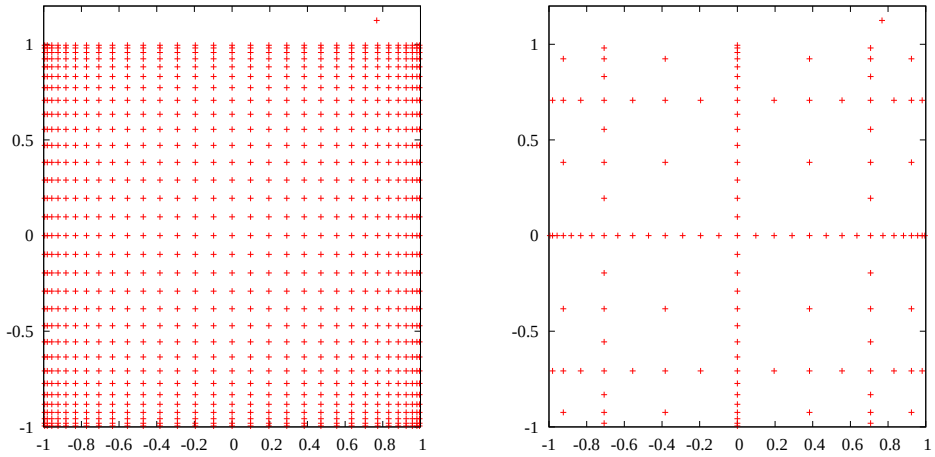

Figure 1. Quadrature points for the 2-D fully tensored formula (left plot) and 2-D Smolyak's partially tensored formula (right plot). Note that the two formulas have the same degree of exactness for polynomial integrand.

- Full tensorization of 1-d quadrature formula exhibits fast convergence rate for smooth integrand, but have a numerical cost scaling with d exponentially: $n = (n_1)^d$, with n_1 the number of quadrature points in the 1-D formula, see the left plot of Figure 1.
- Composite methods, based on an adaptive partition of the integration domain, are robust with regards to the smoothness of the integrand, achieve fast convergence rates, but have a numerical cost that scales exponentially with d.
- Cubature formulas based on Smolyak's coarse tensorization (see [19,20]) have fast convergence rate for smooth integrand and their numerical cost increases less quickly than fully tensored formula (see the right plot in Figure 1).

In our applications, the output is expected to be relatively smooth while the PC are C^∞. As a result, the integrand in I_k are expected to be smooth. In this context, the integration formulas based on the Smolyak's partial tensorization are thought to yield a good trade-off between accuracy and numerical cost, for input involving a moderate number of random parameters, say for $d < 15$, while for higher dimensional problems Monte-Carlo methods are expected to perform better. However, it is underlined that one usually has no *a priori* knowledge on the smoothness of the output, so one has to be cautious when selecting a integration method. In the example section, the Smolyak's method will used to perform the NISP of the output, so we found necessary to provide more details on the construction of the method.

Smolyak's cubature

Smolyak's cubature formulas are based on partial tensorization of one-dimensional quadrature formulas (see [19,20]). Let us consider for $l = 0, 1, \ldots$ a sequence of 1-D integration formulas involving a number of points n_l increasing with l. We call l the level of the formula. The 1-D quadrature formula of level l, with points and weights $\xi^{(i,l)}$ and $w^{(i,l)}$ respectively, writes:

$$\int_\Omega f(\xi)p(\xi)d\xi \simeq Q_l^1 f \equiv \sum_{i=1}^{n_l} w^{(i,l)} f\left(\xi^{(i,l)}\right). \tag{22}$$

Setting $Q_0^1 f = 0$, the difference quadrature formula is defined as

$$\Delta_{k\geq 1}^1 f \equiv \left(Q_k^1 - Q_{k-1}^1\right) f. \tag{23}$$

Using a multi-index $\boldsymbol{k} = (k_1, \ldots, k_d)$, the d-dimensional difference formula is the tensor product of 1-D difference quadrature:

$$\Delta_{\boldsymbol{k}} f = (\Delta_{k_1}^1 \otimes \cdots \otimes \Delta_{k_d}^1) f. \tag{24}$$

Then, the d-dimensional Smolyak's cubature formula of level l is constructed by the sum of tensor products of difference quadratures, over a set of multi-indices $\boldsymbol{k}$,

$$\int_{\Omega^d} f(\boldsymbol{\xi})p(\boldsymbol{\xi})d\boldsymbol{\xi} \simeq Q_l^d f = \sum_{|\boldsymbol{k}|\leq l+d-1} \Delta_{\boldsymbol{k}} f, \quad \text{with } l \in \mathbb{N},\ \boldsymbol{k} \in \mathbb{N}^d. \tag{25}$$

In practice, imbedded one-dimensional quadrature formulas are used to minimize the number of integrand evaluations. The Smolyak's cubature has a convergence rate which depends on the smoothness of the integrand. Specifically, for 1-D quadrature where $n_l = O(2^l)$, the theoretical convergence rate is in $O(2^{-rl} l^{(d-1)(r+1)})$ for integrand $f \in \mathcal{W}_d^r$, where

$$\mathcal{W}_d^r := \left\{ g : \Omega^d \longrightarrow \mathbb{R}, \quad \left\| \frac{\partial^{|\mathbf{s}|} g}{\partial \xi_1^{s_1} \ldots \partial \xi_d^{s_d}} \right\|_\infty < \infty,\ s_i \leq r \right\}, \tag{26}$$

is the class of functions with bounded mixed derivatives of order r. In the application section we shall use the software[1] of K. Petras to compute the points and the weights of the Smolyak's cubature for integration over a d-dimensional unit cube.

Projection error

Similarly to over-fitting in least square approximation, numerical integration errors infer errors on the computed PC expansion coefficients that may become

[1] http://www-public.tu-bs.de:8080/ petras/software.html

significant if the expansion degree is selected too high. In fact, the polynomial degree of the sought PC expansion is an hyper-parameter that need be appropriately set. Indeed, for a fixed cubature formula it is usually observed that the projection error increases with the polynomial degree of the PC expansion, and it exists an optimal polynomial degree d yielding the lowest projection error. This degree d is unknown in general and the projection error can not be computed. However, the cubature formula exactly integrates polynomials with known degree equal or less then d_1. A classical rule of thumb is then to select an expansion degree $\leq d_1/2$.

3 Global Sensitivity Analysis

We consider the classical variance-based method of the Sobol sensitivity indices for sensitivity analysis [1]. We start by recalling the main features of the Sobol functional decomposition (or ANOVA decomposition), and then we define Sobol's sensitivity indices.

3.1 The Sobol functional decomposition

For simplicity, let us consider vectors of the random input $\boldsymbol{\xi}$ composed of d independent identically distributed random variables ξ_i, with Ω_d as range and $p(\boldsymbol{\xi})$ as probability density function (pdf). We denote the d-dimensional range by

$$\Omega^d = \underbrace{\Omega \times \cdots \times \Omega}_{d \text{ times}}. \tag{27}$$

Since the ξ_i are independent, $p(\boldsymbol{\xi}) = \prod_i p(\xi_i)$. The stochastic output y depends on the random input: $y = f(\boldsymbol{\xi})$. We assume $\boldsymbol{\xi} \in \Omega^d \longmapsto f(\boldsymbol{\xi}) \in L^2(\Omega^d, p(\boldsymbol{\xi}))$.

The Sobol functional decomposition for every function $f \in L^2(\Omega^d, p(\boldsymbol{\xi}))$ is

$$f(\boldsymbol{\xi}) = \sum_{u \subseteq \{1,2,\ldots,d\}} f_u(\boldsymbol{\xi}_u), \tag{28}$$

where u is a set of integers, $\boldsymbol{\xi}_u = (\xi_{u_1}, \ldots, \xi_{u_s})$ with $s = \text{card}(u) = |u|$ and $f_\emptyset = f_0$. Each of the 2^d elements f_u of the decomposition, except f_0, verifies for any ξ_i

$$\int_\Omega f_u(\boldsymbol{\xi}_u) p(\xi_i) d\xi_i = 0, \quad \forall u \ni i. \tag{29}$$

This result implies the orthogonality of the functions f_u, *i.e.*

$$\int_{\Omega^d} f_u(\boldsymbol{\xi}_u) f_v(\boldsymbol{\xi}_v) p(\boldsymbol{\xi}) d\boldsymbol{\xi} = 0, \quad \forall u \neq v. \tag{30}$$

Furthermore, the Sobol decomposition is unique. The Sobol functions can be computed using the relation

$$f_u(\boldsymbol{\xi}_u) = \int_{\Omega^{d-|u|}} f(\boldsymbol{\xi}) p(\boldsymbol{\xi}_{\sim u}) d\boldsymbol{\xi}_{\sim u} - \sum_{\substack{v \subset u \\ v \neq u}} f_v(\boldsymbol{\xi}_v), \tag{31}$$

where $\boldsymbol{\xi}_{\sim u}$ is the vector $\boldsymbol{\xi}$ without the elements of u. For example

$$\boldsymbol{\xi}_{\sim\{i\}} = (\xi_1, \ldots, \xi_{i-1}, \xi_{i+1}, \ldots, \xi_d). \tag{32}$$

3.2 The Sobol sensitivity indices

We start by defining the variance of the output $y = f(\boldsymbol{\xi})$, denoted D and the variances D_u, often called conditional variances in the litterature, of the functions f_u of the Sobol decomposition:

$$D = \int_{\Omega^d} f^2(\boldsymbol{\xi}) p(\boldsymbol{\xi}) d\boldsymbol{\xi} - f_0^2, \tag{33}$$

$$D_u = \int_{\Omega^{|u|}} f_u^2(\boldsymbol{\xi}_u) p(\boldsymbol{\xi}_u) d\boldsymbol{\xi}_u. \tag{34}$$

D_u can be expressed as a combination of conditional variances:

$$D_u = V(E[y|\boldsymbol{\xi}_u]) - \sum_{\substack{v \subset u \\ v \neq u \\ v \neq \emptyset}} D_v, \tag{35}$$

where E and V denote the probabilistic expectation and variance operators. Thanks to the orthogonality of the decomposition, the sum of the variances D_u is the variance of y, *i.e.*

$$D = \sum_{\substack{u \subseteq \{1,2,\ldots,d\} \\ u \neq \emptyset}} D_u. \tag{36}$$

The Sobol sensitivity indices are defined by,

$$S_u \equiv \frac{D_u}{D}, \tag{37}$$

so that

$$\sum_{\substack{u \subseteq \{1,2,\ldots,d\} \\ u \neq \emptyset}} S_u = 1. \tag{38}$$

S_u is called an s-order sensitivity index if $|u| = s$. Each of the Sobol sensitivity indices, S_u, measures the sensitivity of the variance of y due to the interaction between the variables $\boldsymbol{\xi}_u$, without taking into account the effect of the variables

in $\boldsymbol{\xi}_v$ for $v \subset u$ and $v \neq u$. For example the second order sensitivity index $S_{\{i,j\}}$, expresses the sensitivity of the variance of y with regards to ξ_i **and** ξ_j, without taking into account the effect of each variables separately (which are in turns measured by S_i and S_j).

There are 2^d-1 Sobol's sensitivity indices. This number becomes quickly large when d increases. To ease the interpretation and analysis when d increases, Homma and Saltelli [2] have introduced the total indices, noted S_{T_i}, which express the total sensitivity of the variance of y due to a variable ξ_i, *i.e.* its sensitivity with ξ_i alone and all its interactions with the others variables:

$$S_{T_i} \equiv \sum_{u \ni i} S_u. \tag{39}$$

For example for $d = 3$, we have,

$$S_{T_1} = S_{\{1\}} + S_{\{1,2\}} + S_{\{1,3\}} + S_{\{1,2,3\}}. \tag{40}$$

We can also express the total indices using the probabilistic form:

$$S_{T_i} = \frac{E[V(y|\boldsymbol{\xi}_{\sim\{i\}})]}{V(y)}. \tag{41}$$

A useful property, to be used in the next section for the computation of the total indices, is

$$1 = \frac{V(E[y|\boldsymbol{\xi}_{\sim\{i\}}])}{V(y)} + \underbrace{\frac{E[V(y|\boldsymbol{\xi}_{\sim\{i\}})]}{V(y)}}_{S_{T_i}}. \tag{42}$$

4 Computation of Sobol's indices

4.1 Computation of the indices by a Monte-Carlo sampling

Let us consider a sample set of n realizations of the input variables $\{\boldsymbol{\xi}^{(i)}\}_{i=1}^n$. The sample estimates of the average, $E[y] = f_0$, and the variance, $D = (E[y^2] - E[y]^2)$, are

$$\hat{f}_0 = \frac{1}{n}\sum_{i=1}^{n} f\left(\boldsymbol{\xi}^{(i)}\right), \tag{43}$$

$$\hat{D} = \frac{1}{n}\sum_{i=1}^{n} f^2\left(\boldsymbol{\xi}^{(i)}\right) - \hat{D}_{\emptyset}, \tag{44}$$

where $\hat{D}_\emptyset \equiv \hat{f}_0^{\,2}$. To compute D_u from Eq. (35), we have to estimate the conditional variance $V(E[y|\boldsymbol{\xi}_u])$. The sample estimate of the conditional variance is

$$\begin{aligned} V(E[y|\boldsymbol{\xi}_u]) &= E[E[y|\boldsymbol{\xi}_u]^2] - E[E[y|\boldsymbol{\xi}_u]]^2 = E[E[y|\boldsymbol{\xi}_u]^2] - E[y]^2 \\ &\approx \frac{1}{n}\sum_{i=1}^{n}\left(\frac{1}{n}\sum_{j=1}^{n} f(\boldsymbol{\xi}_{\sim u}^{(j)}, \boldsymbol{\xi}_u^{(i)})\right)^2 - f_0^2. \end{aligned} \tag{45}$$

The computational cost of this estimate is in $\mathcal{O}(n^2)$, and is too expensive to be used in practice. Sobol [1] proposed a less expensive method to approximate the indices by Monte-Carlo sampling. This method computes the terms $E[E[y|\boldsymbol{\xi}_u]^2]$ as a unique integral. This is achieved by making use of two independent sample sets $\{\boldsymbol{\xi}^{(i)}\}_{i=1}^n$ and $\{\boldsymbol{\eta}^{(i)}\}_{i=1}^n$. Using these two sample sets, the conditional variance can be recasted in

$$\begin{aligned} E[E[y|\boldsymbol{\xi}_u]^2] &= E[E[y|\boldsymbol{\xi}_u]\, E[y|\boldsymbol{\xi}_u]] \\ &= \int\left(\int f(\boldsymbol{\xi}_{\sim u}, \boldsymbol{\xi}_u) p(\boldsymbol{\xi}_{\sim u}) d\boldsymbol{\xi}_{\sim u}\right)\left(\int f(\boldsymbol{\xi}_{\sim u}, \boldsymbol{\xi}_u) p(\boldsymbol{\xi}_{\sim u}) d\boldsymbol{\xi}_{\sim u}\right) p(\boldsymbol{\xi}_u) d\boldsymbol{\xi}_u \\ &= \int\int\int f(\boldsymbol{\xi}) f(\boldsymbol{\eta}_{\sim u}, \boldsymbol{\xi}_u) p(\boldsymbol{\xi}) p(\boldsymbol{\eta}_{\sim u}) d\boldsymbol{\xi} d\boldsymbol{\eta}_{\sim u}. \end{aligned} \tag{46}$$

Using this formula, and after some manipulations, the sample estimate of D_u becomes:

$$\hat{D}_u = \frac{1}{n}\sum_{i=1} f\left(\boldsymbol{\xi}^{(i)}\right) f\left(\boldsymbol{\zeta}_u^{(i)}\right) - \sum_{\substack{v\subset u \\ v\neq u}} \hat{D}_v, \tag{47}$$

where

$$(\zeta_j)_u^{(i)} = \begin{cases} \xi_j^{(i)} & \text{if } j \in u, \\ \eta_j^{(i)} & \text{otherwise.} \end{cases}$$

For example, if $u = \{j\}$ we have

$$\hat{D}_{\{j\}} = \frac{1}{n}\sum_{i=1} f\left(\xi_1^{(i)}, \ldots, \xi_d^{(i)}\right) f\left(\eta_1^{(i)}, \ldots, \eta_{j-1}^{(i)}, \xi_j^{(i)}, \eta_{j+1}^{(i)}, \ldots, \eta_d^{(i)}\right) - \hat{D}_\emptyset.$$

Finally the estimate of the Sobol sensitivity indices are given by Eq. (37):

$$\hat{S}_u = \frac{\hat{D}_u}{\hat{D}}. \tag{48}$$

It is seen that the numerical cost (*i.e.* the total number of function evaluations) for the estimation of $E[E[y|\boldsymbol{\xi}_u]^2]$ is in $\mathcal{O}(2n)$. Therefore, using the same sample sets to compute all the indices, the method requires a total of $n\times(\text{card}(\{v \subset u, v \neq \emptyset\}) + 1)$ function evaluations to estimate $\hat{S}_u$. As a result,

the evaluation of all the $(2^d - 1)$ sensitivity indices requires $\mathcal{O}(n2^d)$ evaluations of f. This complexity can be greatly reduced if one is interested in the total indices only. In fact, expressing the total indices from the conditional variances (see Eq. (42)),

$$S_{T_i} = 1 - \frac{V(E[y|\boldsymbol{\xi}_{\sim\{i\}}])}{V(y)}, \tag{49}$$

and using

$$\begin{aligned} V(E[y|\boldsymbol{\xi}_{\sim\{i\}}]) &= E[E[y|\boldsymbol{\xi}_{\sim\{i\}}]^2] - E[E[y|\boldsymbol{\xi}_{\sim\{i\}}]]^2 = E[E[y|\boldsymbol{\xi}_{\sim\{i\}}]^2] - f_0^2 \\ &= \int\int\int f(\boldsymbol{\xi}) f(\boldsymbol{\xi}_{\sim\{i\}}, \boldsymbol{\eta}_{\{i\}}) p(\boldsymbol{\xi}) p(\boldsymbol{\eta}_{\{i\}}) d\boldsymbol{\xi} d\boldsymbol{\eta}_{\{i\}} - f_0^2, \end{aligned} \tag{50}$$

one obtains the sample estimates of the total indices

$$S_{T_i} = 1 - \frac{1}{\hat{D}} \left(\frac{1}{n} \sum_{l=1} f\left(\boldsymbol{\xi}^{(l)}\right) f\left(\boldsymbol{\zeta}_{\{i\}}^{(l)}\right) - \hat{D}_{\emptyset} \right), \tag{51}$$

where

$$(\zeta_j)_{\{i\}}^{(l)} = \begin{cases} \eta_j^{(l)} & \text{if } j = i, \\ \xi_j^{(l)} & \text{otherwise.} \end{cases}$$

Using Eq. (51), the computational cost for the computation of the d total indices is reduced to $\mathcal{O}(n(d+1))$. In the application section, we shall use LHS techniques [21] to construct the sample sets $\{\boldsymbol{\xi}^{(i)}\}_{i=1}^n$ and $\{\boldsymbol{\eta}^{(i)}\}_{i=1}^n$.

4.2 Computation of the indices by a Quasi Monte-Carlo method

One may also use Quasi Monte-Carlo (QMC) sequences (see [22]) to generate the sample sets $\{\boldsymbol{\xi}^{(i)}\}_{i=1}^n$ and $\{\boldsymbol{\eta}^{(i)}\}_{i=1}^n$ to be used in Eqs. (47,51). In the example Section 5, we used QMC sequences based on Sobol's sequences (see GSL - GNU Scientific library [2]). We are well aware that the sample sets have to be independent to estimate the conditional variances involved in Eqs. (47,51). In practice, we generate a unique sample set, of size n, but with $2d$ dimensions as in [2]. The first d dimensions are affected to $\{\boldsymbol{\xi}^{(i)}\}$, while the remaining d dimensions are affected to $\{\boldsymbol{\eta}^{(i)}\}$. Numerical tests (see below) have shown a significant improvement of the convergence of the sensitivity index estimate using the sample sets generated from QMC sequences, compared to the LHS sampling. Still, further explanations and analysis are required to understand and fully justify the use of QMC sequences with Eqs. (47,51).

[2] http://www.gnu.org/software/gsl/

For $f \in L^2(\Omega^d, p(\boldsymbol{\xi}))$, we denote g its PC expansion truncated at order p:

$$f(\boldsymbol{\xi}) \approx g(\boldsymbol{\xi}) = \sum_{k=0}^{P} \beta_k \Psi_k(\boldsymbol{\xi}), \quad P+1 = \frac{(p+d)!}{p!d!}. \tag{52}$$

The elements f_u of the Sobol decomposition of f are approximated by the elements g_u of the decomposition of g:

$$f_u \approx g_u, \quad \forall u. \tag{53}$$

It is also clear that the PC-expansion truncated at order p of an element f_u of the Sobol decomposition of f is equal to the element g_u of the Sobol decomposition of g, the PC-expansion truncated at order p of f. Then, the interest of using an intermediate projection of f on a PC basis, in view of the determination of the sensitivity indices, comes from the fact that the computation of the Sobol decomposition of a PC expansion is simple and immediate. Indeed, the expression of an element g_u of the Sobol decomposition of the PC-expansion g, is simply expressed by

$$g_u(\boldsymbol{\xi}_u) = \sum_{k \in K_u} \beta_k \Psi_k(\boldsymbol{\xi}_u), \tag{54}$$

where the set of indices K_u is given by

$$K_u = \left\{ k \in \{1, \dots, P\} | \Psi_k(\boldsymbol{\xi}) = \prod_{i=1}^{|u|} \phi_{\alpha_i^k}(\xi_{u_i}), \alpha_i^k > 0 \right\}. \tag{55}$$

It is stressed that the indices sets K_u depend only on the PC basis and not on the function f. Moreover, thanks to the orthogonality of the PC basis, we have a simple expression for the variance and conditional variances:

$$\hat{D} \approx \sum_{k=1}^{P} \beta_k^2 \left\langle \Psi_k, \Psi_k \right\rangle, \quad \hat{D}_u \approx \sum_{k \in K_u} \beta_k^2 \left\langle \Psi_k, \Psi_k \right\rangle. \tag{56}$$

Finally, the Sobol indices of f are approximated by

$$S_u \approx \hat{S}_u = \frac{\sum_{k \in K_u} \beta_k^2 \left\langle \Psi_k, \Psi_k \right\rangle}{\sum_{k=0}^{P} \beta_k^2 \left\langle \Psi_k, \Psi_k \right\rangle}, \tag{57}$$

and Eq. (39) is used to compute the total indices. The previous expressions show that the determination of the Sobol decomposition and sensitivity indices is immediate as soon as the PC expansion of f is known. Thus, the method will be efficient provided that the computation of the PC coefficients is accurate and not too expensive. In the context of non-intrusive methods (see

Section 2.3), the computational cost of the PC expansion essentially scales with the number of function evaluations (or model resolutions) needed to estimate correctly the PC coefficients. This number of evaluations is in turns essentially related to the smoothness of the output with regards to the uncertain input which controls the expansion order and convergence rate of the solution method (*e.g.* of the cubature formula). Consequently, the projection of the output on a PC basis is expected to significantly reduce the computational cost of the Sobol sensitivity indices, compared to alternative methods such as MC and QMC, for smooth output. This claim is verified in the examples of the next section.

5 Examples

We illustrate the use of PC expansions for the determination of the Sobol sensitivity indices on three classical test functions, namely the Ishigami function, a polynomial function and the so-called g-function. These test functions are selected to analyze the effectiveness of the proposed method on smooth and non-smooth functions with variable number of uncertain input dimensions.

For the three test functions, the uncertain inputs have uniform distributions, but we expect the analysis to be independent of the statistical distribution of the uncertain inputs. In all the tests, the PC expansions use multi-variate Legendre polynomials (the family of polynomials orthogonal for the uniform measure). The PC coefficients are computed by means of NISP as described in Section 2.3, using coarse cubature formulas based on Smolyak scheme [19] and imbedded Féjer's one-dimensional formulas [23].

The error on the computed sensitivity indices S_u from the PC expansion of the output (*i.e.* using Eq. (57)) is compared with the estimates obtained using Monte-Carlo (LHS) and Quasi Monte-Carlo methods as described in Section 4.1 (*i.e.* using Eq. (47)). Specifically, we compare the three methods (PC, MC and QMC) for three error criteria: the sum of the L_1-error on the $2^d - 1$ indices (noted e), the sum of the L_1-error on the d first order indices, (noted e_i) and the sum of the L_1-error on the d total indices (noted e_T):

$$e \equiv \sum_{\substack{u \subseteq \{1,2,\ldots,d\} \\ u \neq \emptyset}} |S_u - \hat{S}_u|, \tag{58}$$

$$e_i \equiv \sum_{i \in \{1,2,\ldots,d\}} |S_{\{i\}} - \hat{S}_{\{i\}}|, \tag{59}$$

$$e_T \equiv \sum_{i \in \{1,2,\ldots,d\}} |S_{T_i} - \hat{S}_{T_i}|. \tag{60}$$

Note that on the contrary of PC method, the MC and QMC methods estimate the total indices S_{T_i} from Eq. (51) and not Eq. (39). Also, the estimates being random for the MC method, the errors are averaged over 100 independent realizations of the LHS sample sets.

5.1 Ishigami function

The first tests use the Ishigami function [24]:

$$f(\xi) = \sin(\xi_1) + a\ \sin^2(\xi_2) + b\ \xi_3^4 \sin(\xi_1), \tag{61}$$

where $\xi_i \sim \mathcal{U}([-\pi, \pi])$ for $i = 1, 2, 3$. This function is smooth, non-linear and non-monotonous. The exact variance and the conditional variances are

$$\begin{aligned} D &= \frac{a^2}{8} + \frac{b\pi^4}{5} + \frac{b^2\pi^8}{18} + \frac{1}{2}, \\ D_{\{1\}} &= \frac{b\pi^4}{5} + \frac{b^2\pi^8}{50} + \frac{1}{2}, \quad D_{\{2\}} = \frac{a^2}{8}, \quad D_{\{3\}} = 0, \\ D_{\{1,2\}} &= 0, \quad D_{\{1,3\}} = \frac{b^2\pi^8}{18} - \frac{b^2\pi^8}{50}, \quad D_{\{2,3\}} = 0, \quad D_{\{1,2,3\}} = 0. \end{aligned}$$

We set $a = 7$ and $b = 0.1$.

To compute the PC expansion of f, we need first to select an expansion order p for the NISP. The expansion order has to be selected in relation with the level of the cubature formula. For the Féjer one-dimensional formula selected in this work, the Smolyak formula of level l is exact for polynomial integrand of degree $\leq 2l$. If f was polynomial of degree p, setting $l = p$ would yield exact PC coefficients up to order p. However, the Ishigami function is not polynomial and numerical tests are needed to properly select p given l. We show in Figure 2 the errors e for different values of l and fixed $p \leq l$ (left plot). It is seen that the errors do not decrease much when we increase the level l for fixed order $p \leq l$. In fact, when we increase the level l of the formula with p held fixed, the approximation error on the integrals (so on the expansion coefficients of f) becomes negligible: the error e on the sensitivity indices is then dominated by the truncature error of the PC expansion. Consequently, $p = l$ appears to be a relevant rule for the selection of the expansion order given l. This is confirmed by the right plot in Figure 2, which depicts the resulting errors on the sensitivity indices for different relations between p and l. This plot demonstrates that the same convergence rates are obtained for the different rules (provided that $p \leq l$), but that the rule $p = l$ is the least expensive one in terms of number of function evaluations (which increases with l).

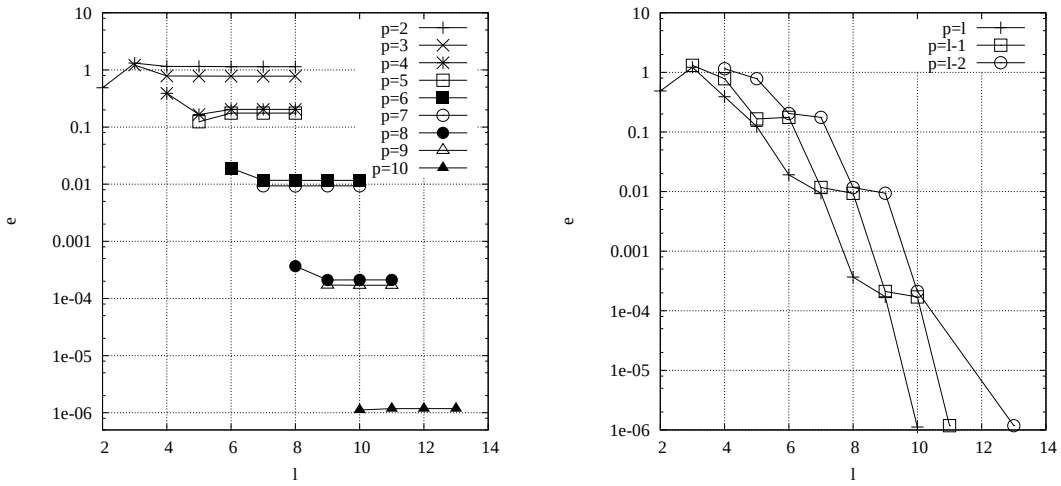

Figure 2. The left plot shows the errors e on the sensitivity indices computed from the PC-expansion using different orders of truncature (p) and levels (l) for the cubature formula as indicated. The right plot shows the errors e on the sensitivity indices computed from the PC-expansion using different rules for the selection of the expansion order p at given level l of the cubature formula.

Next, the errors on the sensitivity indices, computed using the rule $p = l$ in the NISP, are compared with the errors for the MC and QMC methods. The comparison is provided in terms of the three errors criteria (e, e_T and e_i) in Figures (3-5) respectively. The errors are reported as functions of the number of function evaluations to allow for a direct assessment of the respective methods efficiencies. It is first observed that the convergence rates of the methods are essentially the same for the three error criteria. However, the convergence rates of the three methods are different. Specifically, for the PC method a convergence rate in $\frac{1}{n^6}$ is reported, while it is only $\frac{1}{n}$ for QMC and $\frac{1}{\sqrt{n}}$ for MC (averaged over 100 LHS samples).

The higher convergence rate of the errors on the sensitivity indices with the number of function evaluations reported for the PC method is explained by the smoothness of the Ishigami function: this smoothness ensures a fast convergence of both the polynomial approximation and cubature formula. This fast convergence of the PC method is in fact expected for any smooth function: for smooth functions and low to medium dimensional problems, the PC method is expected to exhibit a spectral-like asymptotic convergence rate.

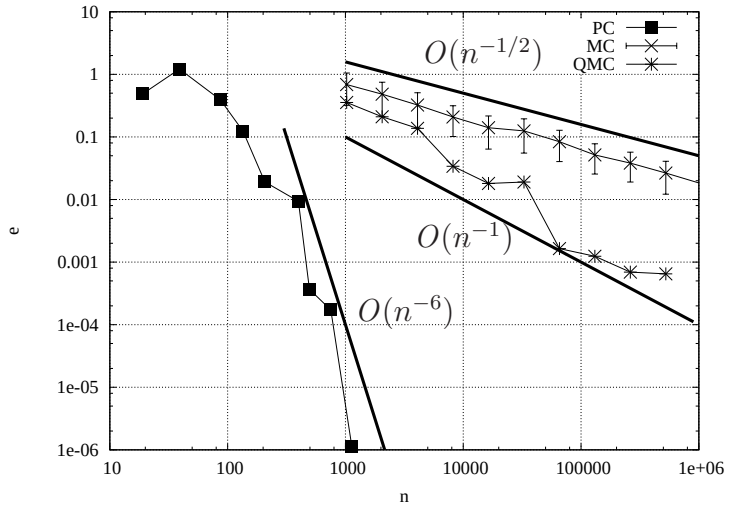

Figure 3. Errors e on sensitivity indices computed from PC expansions, Quasi Monte-Carlo sequences and Monte-Carlo simulations (averaged over 100 LHS sample sets) as a function of the number of function evaluations.

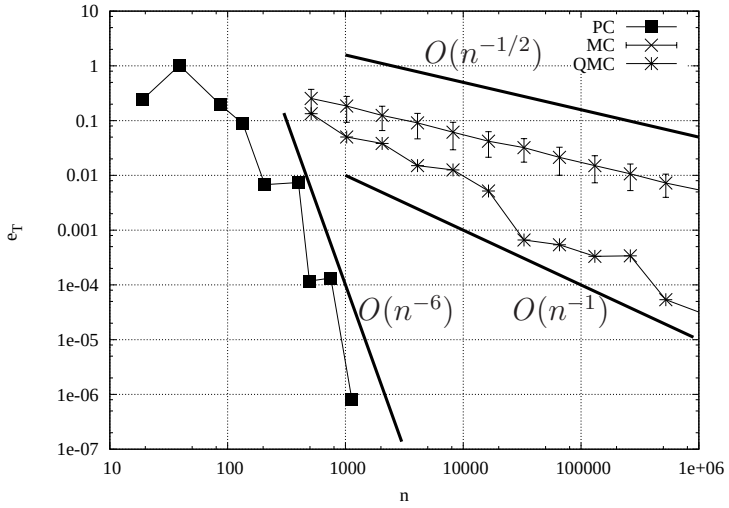

Figure 4. Errors e_T on total sensitivity indices computed from PC expansions, Quasi Monte-Carlo sequences and Monte-Carlo simulations (averaged over 100 LHS sample sets) as a function of the number of function evaluations.

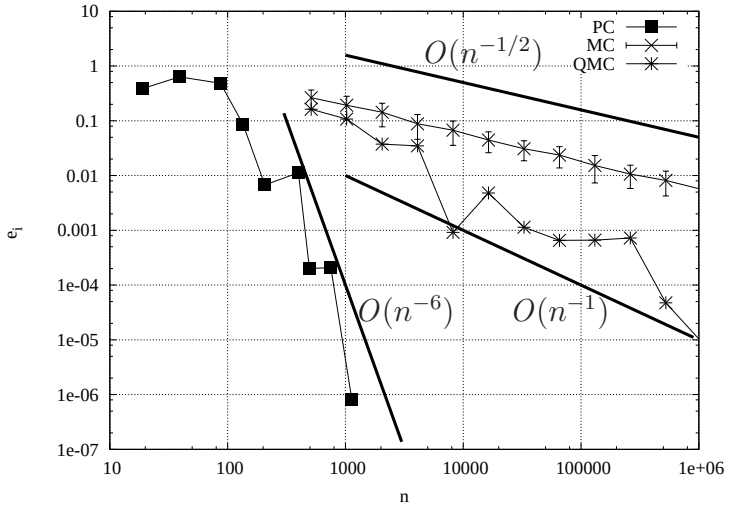

Figure 5. Errors e_i on first order sensitivity indices computed from PC expansions, Quasi Monte-Carlo sequences and Monte-Carlo simulations (averaged over 100 LHS sample sets) as a function of the number of function evaluations.

The fast convergence of the sensitivity indices for the PC method on the Ishigami function may have been attributed to the low dimensionality of the test function ($d = 3$). To support the claim of spectral asymptotic convergence rates of the PC method for any smooth function, we consider the following polynomial function,

$$f(\boldsymbol{\xi}) = \prod_{i=1}^{d} \frac{2\xi_i + 1}{2}, \tag{62}$$

with $\xi_i \sim \mathcal{U}([0,1])$ for $i = 1, \ldots, d$. The exact Sobol's sensitivity indices and total indices of f have for expressions:

$$S_u = \frac{2^{-|u|}}{(\frac{13}{12})^d - 1}, \quad S_{T_i} = 1 - \frac{(\frac{13}{12})^{d-1} - 1}{(\frac{13}{12})^d - 1}. \tag{63}$$

The polynomial function f has a degree equal to d such that its exact PC projection would require a cubature formula with level $l = d$. For large d, this results in a prohibitively large number of cubature points, so the projection can be only approximated. Furthermore, if we select an expansion order $p < d$, it is clear from Eq. (57) that

$$\hat{S}_u = 0, \quad \forall |u| > p. \tag{64}$$

Numerical limitations impose $l < d$ for large d, and for the consistancy of the integration method we have to select $p \leq l$, so we can not expect to compute sensitivity indices of order $> l$. Consequently, the effects of the PC truncature and approximated projection on the computed sensitivity indices have to be investigated. To do so, we set $d = 12$. Figure 6 presents the convergence with the number of function evaluations of the errors e_T on the total sensitivity indices for PC (with the rule $p = l$), QMC and MC methods. We recall that for the PC method, the total sensitivity indices are computed from Eq. (39) and therefore incorporate the errors on all the sensitivity indices (including those neglected by the PC truncature); on the contrary, QMC and MC methods use the favorable direct estimation based on Eq. (51). Figure 6 shows that even-though the cubature formulas used do not allow for an exact determination of the PC coefficients (we have $l < d$ in all cases), the S_{T_i} computed with the PC method are much more accurate than for MC and QMC methods. Furthermore, the spectral convergence of the PC expansion can be seen from the improvement of the convergence rate of the PC method when the number of evaluation points increases (or equivalently when $l = p$ is increased). On the contrary, the convergence rates of MC and QMC methods are found to remain constant.

To gain further evidence on the spectral convergence of the PC expansion and

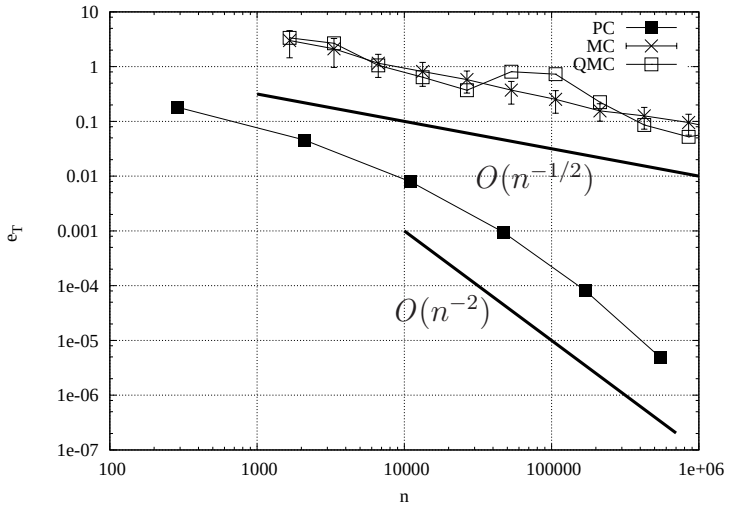

Figure 6. Errors e_T on total sensitivity indices computed from PC expansions, Quasi Monte-Carlo sequences and Monte-Carlo simulations (averaged over 100 LHS sample sets) as a function of the number of function evaluations.

total sensitivity estimates, we have plotted in Figure 7 the errors e_T for the PC method only, as a function of the number n of function evaluations and different dimensionality d of the polynomial function (it is recalled that for this test function, the PC method gives the exact sensitivity indices for $l = d$). It is seen that for all the d tested, the convergence rates increase with the number of function evaluations. However, the convergence rates and error magnitudes at a given number of function evaluations (*i.e.* for a fixed computational cost) deteriorate as d increases. This trend indicates that there is a dimensionality d_{max} above which MC and QMC methods are expected to perform better than the PC method: for $d > d_{max}$ a prohibitive number of function evaluations is necessary to reach the spectral convergence domain of the PC method.

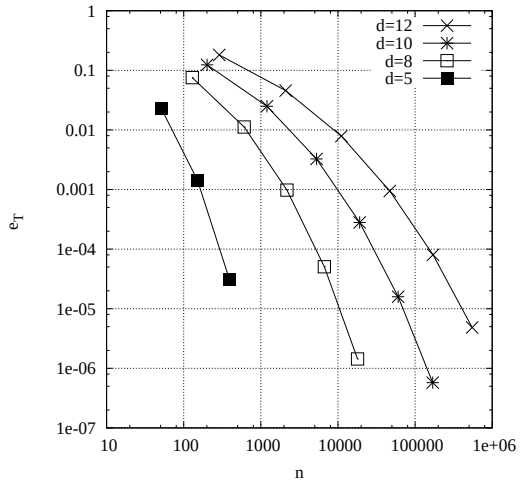

Figure 7. Errors e_T on total sensitivity indices computed by PC expansions for different numbers of dimension d, as a function of the number of function evaluations.

The third test function is the so-called g-function [25]:

$$f(\xi) = \prod_{i=1}^{d} \frac{|4\xi_i - 2| + a_i}{1 + a_i}, \tag{65}$$

where $\xi_i \sim \mathcal{U}([0,1])$ for $i = 1, \ldots, d$. This function is non-smooth and non-monotonous. The exact variance and the conditional variances are

$$D = \prod_{i=1}^{d}(D_{\{i\}} + 1), \quad D_{\{i\}} = \frac{1}{3(1+a_i)^2}, \quad D_u = \prod_{i=1}^{|u|} D_{\{u_i\}}. \tag{66}$$

We set $a_i = (i-1)/2$ and $d = 5$. This function is a challenging test for the PC expansion, due to the presence of the absolute value which first prevents the spectral convergence of the PC expansion, and second compromises the convergence of the cubature formula ($f \notin \mathcal{W}_5^2$). As a consequence, the selection of PC truncature p, for given level l of the cubature formula, is less straightforward than for the previous smooth functions. This is illustrated in the left plot of Figure 8, where plotted are the evolutions of the errors e for fixed PC order p and increasing cubature level l. This plot shows that, on the contrary of the observations for the smooth functions (see Figure 2), the errors do not level-off when l increases, denoting that the integration errors are at least of the same order as the truncature errors. This is not a surprise considering the error estimate given in the end of Section 2.3.3. Also, the right plot of Figure 8, where plotted are the evolutions of the errors e with the level l and different rules for choosing the expansion order p, clearly indicates that there is no rule that performs better than the others. Consequently, we make in the following the conservative choice of using the rule $p = l - 4$.

Figures (9-11) compare the PC, MC and QMC methods for the different error criteria on the sensitivity indices. These results show that the convergence rates of the different errors are essentially the same for PC and QMC methods. On the contrary of the results for the smooth functions, the convergence rates for the PC method do not improve when the number of function evaluations increases. This trend is explained jointly by the loss of spectral convergence for the PC expansion, and by the inadequacy of Féjer's quadrature formula to approximate integrals of non-smooth functions. It is however interesting to note that the PC method remains competitive compared to MC and QMC methods.

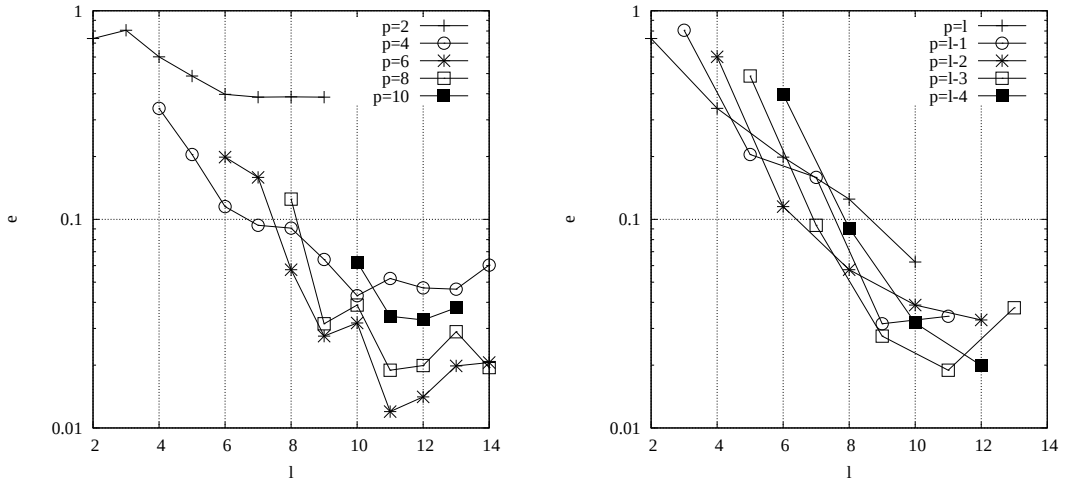

Figure 8. Errors e on the sensitivity indices computed from PC-expansions truncated at fixed orders p as a function of the level l of the cubature formula (left plot). Errors e on the sensitivity indices computed from PC-expansions with different the level l of the cubature formula and different rules of truncature order as indicated (right plot).

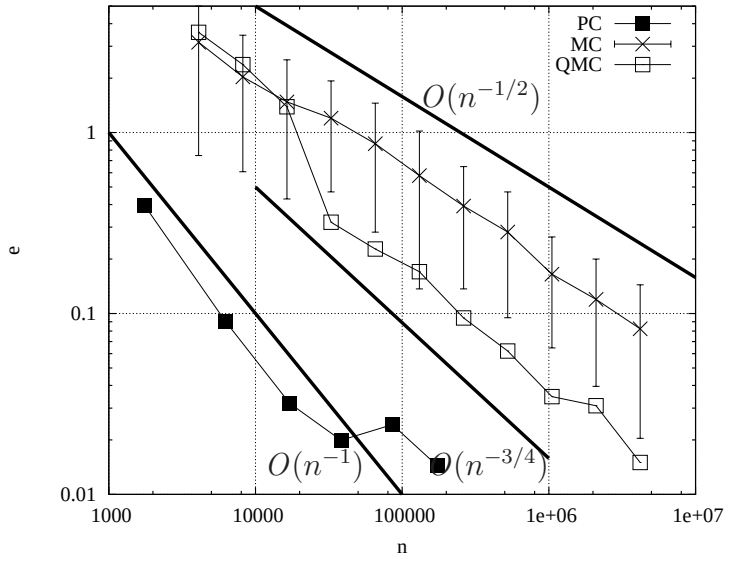

Figure 9. Errors e on sensitivity indices computed from PC expansions, Quasi Monte-Carlo sequences and Monte-Carlo simulations (averaged over 100 LHS sample sets) as a function of the number of function evaluations.

6 Conclusions

In this paper, we have presented a method for the computation of the Sobol sensitivity indices of a function (or model output) involving independent random input, with known probability distributions. The method uses the polynomial chaos expansion of the function to directly compute the conditional

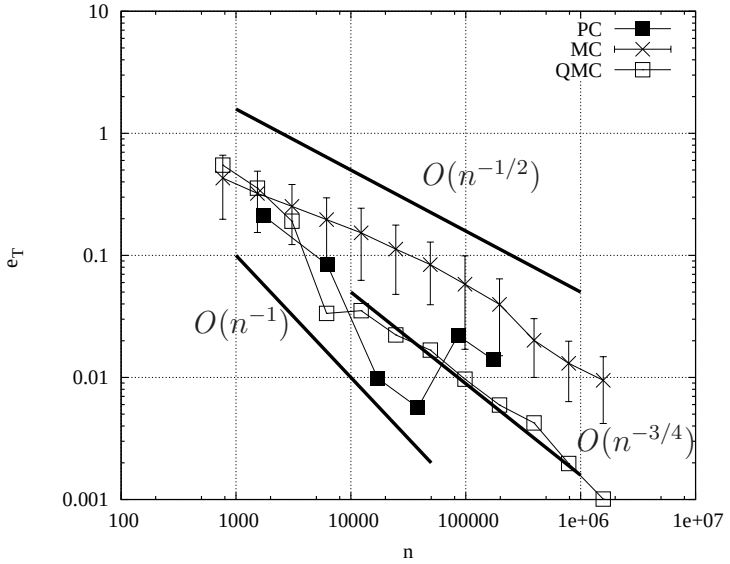

Figure 10. Errors e_T on total sensitivity indices computed from PC expansions, Quasi Monte-Carlo sequences and Monte-Carlo simulations (averaged over 100 LHS sample sets) as a function of the number of function evaluations.

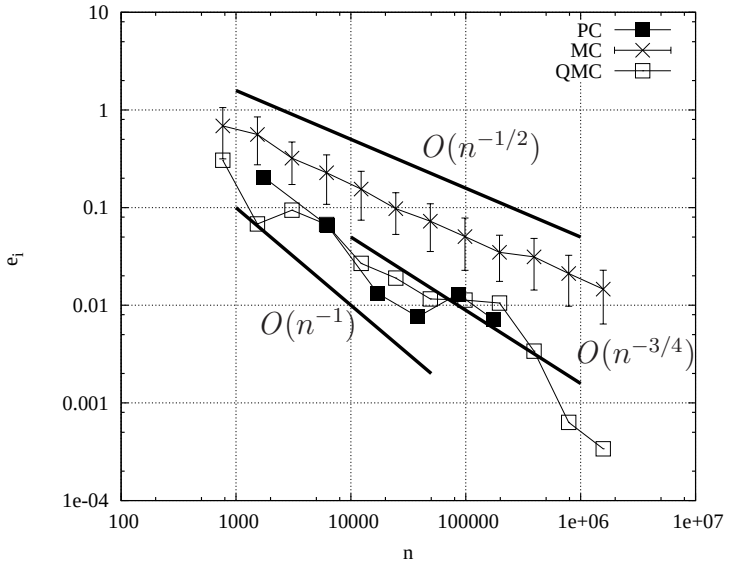

Figure 11. Errors e_i on first order sensitivity indices computed from PC expansions, Quasi Monte-Carlo sequences and Monte-Carlo simulations (averaged over 100 LHS sample sets) as a function of the number of function evaluations.

variances and Sobol's sensitivity indices. The interest of this approach lies in two essential points:

- the simple and immediate computation of the sensitivity indices from the PC-expansion,
- the different methods available for the determination of the PC-expansion (Galerkin projection, Non-Intrusive Spectral Projection and least square

approximation).

The application of the PC method is entirely conditioned on the availability of the PC expansion and its accuracy. For smooth functions, where the PC basis allows for spectral convergence of the PC expansions, the method is expected to exhibit spectral-like convergence rates and therefore to outperform the alternative methods (Monte-Carlo, Quasi Monte-Carlo). This expectations are verified for the two smooth functions tested, which PC expansions were computed by means of Non-Intrusive Spectral Projections involving sparse cubature formulas. This procedure allowed for a direct comparison of the methods efficiencies, by comparing the respective errors on the sensitivity indices as a function of the number of function evaluations.

The examples provided also demonstrate that the proposed method suffers from the usual limitations of the PC expansions. The first limitation has for origin the exponential growth of the basis dimension with the number of independent uncertain inputs. From the computational point of view, the growth of the basis dimension results in a numerical cost that quickly becomes prohibitive (for instance the evolution with d of the number of function evaluations in the non-intrusive techniques or "curse of dimensionality"). The second limitation is due to the loss of the spectral convergence of the PC expansion for non-smooth functions, as illustrated by the last example of Section 5. However, recent works and on-going researches on PC approximations (*e.g.* multiresolution analysis [13,14] and adaptive cubature techniques [26,27]) allow for some optimism, even-though Monte-Carlo methods will certainly remain the only viable alternative for large dimensional problems (say for $d > 20$). Finally, we would like to mention that PC expansions may be a suitable way to perform sensitivity analysis in situations where the input parameters are not independent [28].

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