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B. Sudret and C. V. Mai

Chair of Risk, Safety and Uncertainty Quantification
Stefano-Franscini-Platz 5
CH-8093 Zürich

Risk, Safety & Uncertainty Quantification

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Computing derivative-based global sensitivity measures using polynomial chaos expansions

B. Sudret[1] and C.V. Mai[1]

[1] *Chair of Risk, Safety and Uncertainty Quantification, Department of Civil Engineering, ETH Zurich, Stefano-Franscini-Platz 5, 8093 Zurich, Switzerland*

Abstract

In the field of computer experiments sensitivity analysis aims at quantifying the relative importance of each input parameter (or combinations thereof) of a computational model with respect to the model output uncertainty. Variance decomposition methods leading to the well-known Sobol' indices are recognized as accurate techniques, at a rather high computational cost though. The use of polynomial chaos expansions (PCE) to compute Sobol' indices has allowed to alleviate the computational burden though. However, when dealing with large dimensional input vectors, it is good practice to first use screening methods in order to discard unimportant variables. The *derivative-based global sensitivity measures* (DGSM) have been developed recently in this respect. In this paper we show how polynomial chaos expansions may be used to compute analytically DGSMs as a mere post-processing. This requires the analytical derivation of derivatives of the orthonormal polynomials which enter PC expansions. Closed-form expressions for Hermite, Legendre and Laguerre polynomial expansions are given. The efficiency of the approach is illustrated on two well-known benchmark problems in sensitivity analysis.

Keywords: global sensitivity analysis – derivative-based global sensitivity measures (DGSM) – Sobol' indices – polynomial chaos expansions – derivatives of orthogonal polynomials – Morris method

1 Introduction

Nowadays, the increasing computing power allows one to use numerical models to simulate or predict the behavior of physical systems in various fields, *e.g.* mechanical engineering (Reuter and Liebscher, 2008), civil engineering (Hasofer, 2009), chemistry (Campolongo et al., 2007), etc. The considered systems usually lead to highly complex models with numerous input factors (possibly tens to hundreds (Patelli and Pradlwarter, 2010; Sudret and Mai, 2013)) that are required to represent all the parameters driving the system's behaviour, *e.g.* boundary and initial conditions, material properties, external excitations, etc. In practice these input factors are often not perfectly known, since they are obtained from possibly noisy measurements, or simply by expert judgment. In order to take into account the uncertainty, probabilistic approaches have been developed in the last two decades, in which the model input parameters are represented by random variables. Then the input uncertainties are propagated through the computational model and the distribution, moments or probability of exceeding prescribed thresholds may be computed (Sudret, 2007; de Rocquigny, 2012).

In this context, sensitivity analysis (SA) examines the sensitivity of the model output with respect to the input parameters, *i.e.* how the output variability is affected by the uncertain input factors (Saltelli et al., 2000, 2004, 2008). The use of SA is common in various fields: engineering (Hasofer, 2009; Pappenberger et al., 2008; Reuter and Liebscher, 2008; Kala, 2011), chemistry Campolongo et al. (2007), nuclear safety Fassò (2013), economy Borgonovo and Peccati (2006), biology Marino et al. (2008), and medicine Abraham et al. (2007), among others. One can traditionally classify SA into *local* and *global* sensitivity analyses. The former aims at assessing the output sensitivity to small input perturbations around a selected *reference value*, *e.g.* the mean value of the input random vector, or the so-called *design point* in reliability analysis (Ditlevsen and Madsen, 1996). The latter aims at assessing the overall or average influence of input parameters onto the output. Local SA has the disadvantage of being related to a fixed nominal point in the input space, and the interaction between the inputs is not accounted for Kucherenko

et al. (2009). In contrast, global SA techniques take into account the input interactions and are not based on the choice of a reference point but account for the whole input space, usually at a larger computational cost though.

The most common sensitivity analysis methods found in the literature are the method of Morris Morris (1991), FAST Cukier et al. (1973, 1978); Mara (2009) and variance decomposition methods originally investigated in Sobol' (1993); Sobol (2001); Sobol' and Kucherenko (2005); Archer et al. (1997); Saltelli (2002); Saltelli et al. (2010). Usually standard Monte Carlo simulation (MCS) or quasi Monte Carlo (QMC) techniques are employed for estimating the sensitivity indices in all these approaches. This requires a large number of model evaluations though, which becomes unaffordable when complex systems are investigated. To overcome this problem, metamodels (also called *surrogate models* or emulators) are usually used in order to carry out the Monte Carlo simulation Sathyanarayanamurthy and Chinnam (2009); Zhang and Pandey (2014). In particular, polynomial chaos expansions (PCE) have been recognized as a versatile tool for building surrogate models and for conducting reliability and sensitivity analyses, as originally shown in Sudret (2006, 2008); Blatman and Sudret (2010a). Using PCE, variance-based sensitivity analysis becomes a mere post-processing of the polynomial coefficients once they have been computed.

More recently, a new gradient-based technique has been proposed for screening unimportant factors. The so-called *derivative-based global sensitivity measures* (DGSM) are shown to be upper bounds of the total Sobol' indices while being less computationally demanding Sobol' and Kucherenko (2009, 2010); Kucherenko et al. (2009); Lamboni et al. (2013). Although the computational cost of this technique is reduced compared to the variance-based technique Kucherenko et al. (2009), its practical computation still relies on sampling techniques, *e.g.* the Monte Carlo simulation.

In this paper we investigate the potential of polynomial chaos expansions for computing derivative-based sensitivity indices and allow for an efficient screening procedure. The paper is organized as follows: the classical derivation of Sobol' indices and their link to derivative-based sensitivity indices is summarized in Section 2. The machinery of polynomial chaos expansions and

the link with sensitivity analysis is developed in Section 3. The computation of the DGSM based on PC expansions is then presented in Section 4, in which an original method for computing the derivatives of orthogonal polynomials is presented. Finally two numerical tests are carried out in Section 5.

2 Derivative-based global sensitivity measures

2.1 Variance-based sensitivity measures

Global sensitivity analysis (SA) aims at quantifying the impact of input parameters onto the output quantities of interest. One input factor is considered insignificant (unessential) when it has little or no effect on the output variability. In practice, screening out the insignificant factors allows one to reduce the dimension of the problem, *e.g.* by fixing the unessential parameters.

Variance-based SA relies upon the decomposition of the output variance into contributions of different components, *i.e.* marginal effects and interactions of input factors. Consider a numerical model $Y = \mathcal{M}(\boldsymbol{X})$ where the input vector $\boldsymbol{X}$ contains M independent input variables $\boldsymbol{X} = \{X_1, \ldots, X_M\}$ with uniform distribution over the unit-hypercube $\mathcal{H}^M$ and Y is the scalar output. The *Sobol' decomposition* reads Sobol' (1993):

$$\begin{aligned} Y = \mathcal{M}(\boldsymbol{X}) =& \mathcal{M}_0 + \sum_{i=1}^{M} \mathcal{M}_i(X_i) + \sum_{1 \le i < j \le M} \mathcal{M}_{i,j}(X_i, X_j) + \ldots \\ &+ \mathcal{M}_{1,\ldots,M}(X_1, \ldots, X_M) \end{aligned} \tag{1}$$

in which $\mathcal{M}_0 = \mathbb{E}\left[\mathcal{M}(\boldsymbol{X})\right]$ is a constant term and each summand $\mathcal{M}_{i_1,\ldots,i_s}(X_{i_1}, \ldots, X_{i_s})$ is a function of the variables $\{X_{i_1}, \ldots, X_{i_s}\}, s \le M$. For the sake of conciseness we introduce the following notation for the subset of indices:

$$\mathbf{u} \stackrel{\text{def}}{=} \{i_1, \ldots, i_s\} \tag{2}$$

and denote by $\boldsymbol{X}_{\mathbf{u}}$ the subvector of $\boldsymbol{X}$ that consists of the variables indexed by $\mathbf{u}$. Using this set notation, Eq. (1) rewrites:

$$Y \stackrel{\text{def}}{=} \mathcal{M}_0 + \sum_{\substack{\mathbf{u} \subset \{1,\ldots,M\} \\ \mathbf{u} \neq \mathbf{0}}} \mathcal{M}_{\mathbf{u}}(\boldsymbol{X}_{\mathbf{u}}), \tag{3}$$

in which $\mathcal{M}_{\mathbf{u}}(\boldsymbol{X}_{\mathbf{u}})$ is the summand including the subset of parameters $\boldsymbol{X}_{\mathbf{u}}$. According to Sobol' (1993), a unique decomposition requires the orthogonality of the summands, *i.e.*:

$$\mathbb{E}\left[\mathcal{M}_{\mathbf{u}}(\boldsymbol{X}_{\mathbf{u}})\,\mathcal{M}_{\mathbf{v}}(\boldsymbol{X}_{\mathbf{v}})\right] = \int_{\mathcal{H}^M} \mathcal{M}_{\mathbf{u}}(\boldsymbol{x}_{\mathbf{u}})\,\mathcal{M}_{\mathbf{v}}(\boldsymbol{x}_{\mathbf{v}})\,\mathrm{d}\boldsymbol{x} = 0 \quad , \quad \mathbf{u} \neq \mathbf{v} \tag{4}$$

In particular each summand shall be of zero mean value. Accordingly the variance of the response $Y = \mathcal{M}(\boldsymbol{X})$ reads:

$$D \overset{\text{def}}{=} \mathrm{Var}\left[Y\right] = \sum_{\substack{\mathbf{u}\subset\{1,\ldots,M\} \\ \mathbf{u}\neq\mathbf{0}}} \mathrm{Var}\left[\mathcal{M}_{\mathbf{u}}(\boldsymbol{X}_{\mathbf{u}})\right]. \tag{5}$$

In this expansion $\mathrm{Var}\left[\mathcal{M}_{\mathbf{u}}(\boldsymbol{X}_{\mathbf{u}})\right]$ is the contribution of summand $\mathcal{M}_{\mathbf{u}}(\boldsymbol{X}_{\mathbf{u}})$ to the output variance.

The *Sobol' sensitivity index* $S_{\mathbf{u}}$ for the subset of variables $\boldsymbol{X}_{\mathbf{u}}$ is defined as follows Sobol (2001):

$$S_{\mathbf{u}} \overset{\text{def}}{=} \frac{D_{\mathbf{u}}}{D} = \frac{\mathrm{Var}\left[\mathcal{M}_{\mathbf{u}}(\boldsymbol{X}_{\mathbf{u}})\right]}{D} \tag{6}$$

The *total sensitivity index* for subset $\boldsymbol{X}_{\mathbf{u}}$ is given by Sobol (2001):

$$S^T_{\mathbf{u}} \overset{\text{def}}{=} \frac{D^T_{\mathbf{u}}}{D} = \sum_{\mathbf{v}\supset\mathbf{u}} \frac{\mathrm{Var}\left[\mathcal{M}_{\mathbf{v}}(\boldsymbol{X}_{\mathbf{v}})\right]}{D} \tag{7}$$

where the sum is extended over all sets $\mathbf{v} = \{j_1, \ldots, j_t\}$ which contains $\mathbf{u}$. It represents the total amount of uncertainty apportioned to the subset of variables $\boldsymbol{X}_{\mathbf{u}}$. For instance, for a single variable X_i, $i = 1, \ldots, M$ the *first order* Sobol' sensitivity index reads:

$$S_i = \frac{\mathrm{Var}\left[\mathcal{M}_i(X_i)\right]}{D}, \tag{8}$$

and the total Sobol' sensitivity index reads:

$$S^T_i = \sum_{\mathbf{v}\ni i} \frac{\mathrm{Var}\left[\mathcal{M}_{\mathbf{v}}(\boldsymbol{X}_{\mathbf{v}})\right]}{D}. \tag{9}$$

S_i and S^T_i respectively represent the sole and total effect of the factor X_i on the system's output variability. The smaller S^T_i is, the less important the factor X_i is. In the case when $S^T_i \ll 1$, say $S^T_i \approx 1 - 5\%$, X_i is considered as unimportant (unessential or insignificant) and may be replaced in the analysis by a deterministic value.

In the literature one can find different approaches for computing the total Sobol' indices, such as the Monte Carlo simulation (MCS) and the spectral approach. Sobol' (1993); Sobol (2001) proposed direct estimation of the sensitivity indices for subsets of variables using only the model evaluations at specially selected points. The approach relies on computing analytically the integral representations of $D_{\mathbf{u}}$ and $D_{\mathbf{u}}^T$ respectively defined in Eq. (6) and Eq. (7).

Let us denote by $\overline{\mathbf{u}}$ the set that is complementary to $\mathbf{u}$, *i.e.* $\boldsymbol{X} = (\boldsymbol{X}_{\mathbf{u}}, \boldsymbol{X}_{\overline{\mathbf{u}}})$. Let $\boldsymbol{X}$ and $\boldsymbol{X}'$ be vectors of independent uniform variables defined on the unit hypercube $\mathcal{H}^M$ and define $\boldsymbol{X}' = (\boldsymbol{X}_{\mathbf{u}}^{'}, \boldsymbol{X}_{\overline{\mathbf{u}}}^{'})$. The partial variance $D_{\mathbf{u}}$ is represented as follows Sobol' and Kucherenko (2005):

$$D_{\mathbf{u}} = \iint \mathcal{M}(\boldsymbol{x})\mathcal{M}(\boldsymbol{x}_{\mathbf{u}}, \boldsymbol{x}_{\overline{\mathbf{u}}}^{'})\,\mathrm{d}\boldsymbol{x}\;\mathrm{d}\boldsymbol{x}_{\overline{\mathbf{u}}}^{'} - {\mathcal{M}_0}^2 \tag{10}$$

The total variance $D_{\mathbf{u}}^T$ is given by Sobol' and Kucherenko (2005):

$$D_{\mathbf{u}}^T = \frac{1}{2}\iint \left[\mathcal{M}(\boldsymbol{x}) - \mathcal{M}(\boldsymbol{x}_{\mathbf{u}}^{'}, \boldsymbol{x}_{\overline{\mathbf{u}}})\right]^2 \mathrm{d}\boldsymbol{x}\;\mathrm{d}\boldsymbol{x}_{\overline{\mathbf{u}}} \tag{11}$$

A Monte Carlo algorithm is used to estimate the above integrals. For each sample point, one generates two M-dimensional samples $\boldsymbol{x} = (\boldsymbol{x}_{\mathbf{u}}, \boldsymbol{x}_{\overline{\mathbf{u}}})$ and $\boldsymbol{x}^{'} = ({\boldsymbol{x}_{\mathbf{u}}}^{'}, {\boldsymbol{x}_{\overline{\mathbf{u}}}}^{'})$. The function is evaluated at three points $(\boldsymbol{x}_{\mathbf{u}}, \boldsymbol{x}_{\overline{\mathbf{u}}})$, $(\boldsymbol{x}_{\mathbf{u}}^{'}, \boldsymbol{x}_{\overline{\mathbf{u}}})$ and $(\boldsymbol{x}_{\mathbf{u}}, \boldsymbol{x}_{\overline{\mathbf{u}}}^{'})$. Using N independent sample points, one computes the quantities of interest D, $D_{\mathbf{u}}$ and $D_{\mathbf{u}}^T$ by means of the following crude Monte Carlo estimators:

$$\mathcal{M}_0 = \frac{1}{N}\sum_{i=1}^{N} \mathcal{M}\left(\boldsymbol{x}^{(i)}\right) \tag{12}$$

$$D + {\mathcal{M}_0}^2 = \frac{1}{N}\sum_{i=1}^{N} \left[\mathcal{M}\left(\boldsymbol{x}^{(i)}\right)\right]^2 \tag{13}$$

$$D_{\mathbf{u}} + {\mathcal{M}_0}^2 = \frac{1}{N}\sum_{i=1}^{N} \mathcal{M}\left(\boldsymbol{x}^{(i)}\right)\mathcal{M}\left(\boldsymbol{x}_{\mathbf{u}}^{(i)}, \boldsymbol{x}_{\overline{\mathbf{u}}}^{(i)'}\right) \tag{14}$$

$$D_{\mathbf{u}}^T = \frac{1}{N}\sum_{i=1}^{N} \frac{1}{2}\left[\mathcal{M}\left(\boldsymbol{x}^{(i)}\right) - \mathcal{M}\left(\boldsymbol{x}_{\mathbf{u}}^{(i)'}, \boldsymbol{x}_{\overline{\mathbf{u}}}^{(i)}\right)\right]^2 \tag{15}$$

The computation of the sensitivity indices by MCS may exhibit reduced accuracy when the mean value $\mathcal{M}_0$ is large. In addition, the computational cost is prohibitive: in order to compute the sensitivity indices for M parameters, MCS requires $(M+2) \times N$ model runs, in which N is the number of sample

points typically chosen equal to $10^3 - 10^4$ to reach an acceptable accuracy. Saltelli (2002) suggested a procedure that is more efficient for computing the first and total sensitivity indices. Sobol' et al. (2007) modified the MCS procedure in order to reduce the lack of accuracy. Some other estimators for the sensitivity indices by MCS may be found in Monod et al. (2006); Janon et al. (2013).

2.2 Derivative-based sensitivity indices

The total Sobol' indices may be used for screening purposes. Indeeed a negligible total Sobol' index S_i^T means that variable X_i does not contribute to the output variance, neither directly nor in interaction with orther variables. In order to avoid the computational burden associated with estimating all total Sobol' indices, a new technique based on derivatives has been recently proposed by Kucherenko et al. (2009).

Derivative-based sensitivity analysis originates from the *Morris method* introduced in Morris (1991). The idea is to measure the average of the *elementary effects* over the input space. Considering variable X_i one first samples an experimental design (ED) in the input space $\mathcal{X} = \left\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(N)}\right\}$ and then varies this sample in the i^{th} direction. The elementary effect (EE) is defined as:

$$EE_i^{(j)} = \frac{\mathcal{M}(\boldsymbol{x}_r^{(j)}) - \mathcal{M}(\boldsymbol{x}^{(j)})}{\Delta} \tag{16}$$

in which $\boldsymbol{x}^{(j)} = \left\{x_1^{(j)}, \ldots, x_i^{(j)}, \ldots, x_M^{(j)}\right\}$ is the j^{th} sample point and $\boldsymbol{x}_r^{(j)} = \left\{x_1^{(j)}, \ldots, x_i^{(j)} + \Delta, \ldots, x_M^{(j)}\right\}$ is the perturbed sample point in the i-th direction. The Morris importance measure (Morris factor) is defined as the average of the EE_i's:

$$\mu_i = \frac{1}{N}\sum_{j=1}^{N} EE_i^{(j)} \tag{17}$$

By definition, the variance σ_i^2 of the EEs is calculated from:

$$\sigma_i^2 = \frac{1}{N-1}\sum_{j=1}^{N}(EE_i^{(j)} - \mu_i)^2 \tag{18}$$

The resulting mean $\mu_i$and standard deviation σ_i are usually plotted in a two-dimensional graph, see Figure 1.

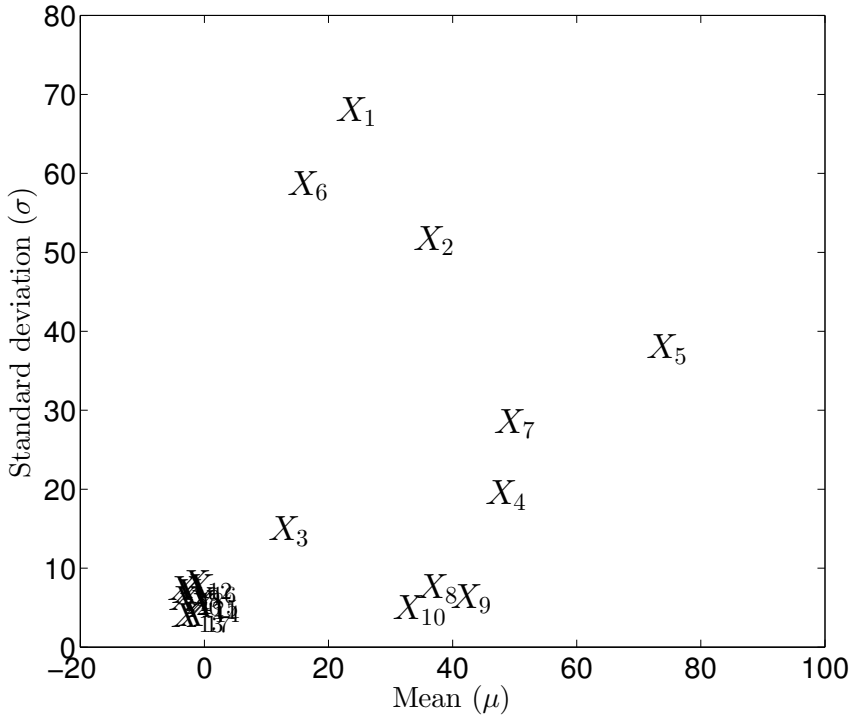


Figure 1: Morris method: representation of the mean and standard deviation of the elementary effects

The interpretation of this graph reads as follows: when μ_i and σ_i are jointly small (lower left corner of the plot), the parameter X_i is considered as unimportant. When μ_i is large and σ_i is small (lower right corner) then X_i is considered as an important parameter, from which the model output quasi-linearly depends (a zero standard deviation indicates a fully linear relationship). Finally, when σ_i is also large (upper part of the plot), parameter X_i is considered as important, and the output depends on this very parameter in a nonlinear way and/or it interacts with other parameters.

Kucherenko *et al.* (Kucherenko et al., 2009) generalized the quantities in Eqs.(17)-(18) as follows:

$$\mu_i \stackrel{\text{def}}{=} \mathbb{E}\left[\frac{\partial \mathcal{M}}{\partial x_i}(\boldsymbol{X})\right] = \int_{\mathcal{H}^M} \frac{\partial \mathcal{M}}{\partial x_i}(\boldsymbol{x})\mathrm{d}\boldsymbol{x} \tag{19}$$

$$\sigma_i^2 = \int\limits_{\mathcal{H}^M} \left[\frac{\partial \mathcal{M}}{\partial x_i}(\boldsymbol{x})\right]^2 \mathrm{d}\boldsymbol{x} - \mu_i^2 \tag{20}$$

provided that $\dfrac{\partial \mathcal{M}}{\partial x_i}$ is square-integrable. The interpretation of these measures is similar as for the original Morris method.

Because the elementary effects may be positive or negative, they can cancel each other, which might lead to a misinterpretation of the importance of X_i. To avoid this, Campolongo et al. (2007) modified the Morris factor as follows:

$$\mu_i^* = \mathbb{E}\left[\left|\frac{\partial \mathcal{M}}{\partial x_i}(\boldsymbol{X})\right|\right] \tag{21}$$

Recently, Sobol' and Kucherenko (2009) introduced a new sensitivity measure (SM) which is the mean-squared derivative of the model with respect to X_i:

$$\nu_i = \mathbb{E}\left[\left(\frac{\partial \mathcal{M}}{\partial x_i}(\boldsymbol{X})\right)^2\right] \tag{22}$$

Sobol' and Kucherenko (2009) and Lamboni et al. (2013) have established a link between the ν_i in Eq. (22) and the total Sobol' indices in Eq. (9). In case X_i is a uniform random variable over [0, 1], one gets:

$$S_i^T \leq S_i^{DGSM} \stackrel{\text{def}}{=} \frac{\nu_i}{\pi^2 D} \tag{23}$$

where S_i^{DGSM} is the upper-bound to the total sensitivity index S_i^T and D is the model output variance. In case of a uniform variable $X_i \sim [a_i, b_i]$ this upper bound scales to:

$$S_i^T \leq S_i^{DGSM} = \frac{(b_i - a_i)^2}{\pi^2}\frac{\nu_i}{D} \tag{24}$$

Finally the above results can be extended to other types of distributions. If $X_i \sim \mathcal{N}(a_i, b_i)$ is a Gaussian random variable with mean and variance a_i and b_i^2 respectively, one gets:

$$S_i^T \leq S_i^{DGSM} = {b_i}^2\frac{\nu_i}{D} \tag{25}$$

In the general case, Lamboni et al. (2013) define the upper bound of the total Sobol' index of X_i as:

$$S_i^{DGSM} = 4{C_i}^2\frac{\nu_i}{D} \tag{26}$$

in which $C_i = \sup_{x\in\mathbb{R}} \dfrac{\min\left[F_{X_i}(x), 1 - F_{X_i}(x)\right]}{f_{X_i}(x)}$ is the Cheeger constant, F_{X_i} is the cumulative distribution function of X_i and f_{X_i} is the probability density function of X_i.

3 Polynomial chaos expansions

Let us consider a numerical model $Y = \mathcal{M}(\boldsymbol{X})$ where the input vector $\boldsymbol{X}$ is composed of M *independent* random variables $\boldsymbol{X} = \{X_i,\, i = 1, \ldots, M\}$ and Y is the output quantity of interest. Assuming that Y has a finite variance, it can be represented as follows Ghanem and Spanos (2003); Soize and Ghanem (2004):

$$Y = \mathcal{M}(\boldsymbol{X}) = \sum_{j=0}^{\infty} y_j \phi_j(\boldsymbol{X}) \tag{27}$$

in which $\{\phi_j(\boldsymbol{X}), j = 0, \ldots, \infty\}$ form a basis on the space of second order random variables and y_j's are the coordinates of Y onto this basis. In case the basis terms are multivariate orthonormal polynomials of the input variables $\boldsymbol{X}$, Eq. (27) is called polynomial chaos expansion.

Assuming that the input vector $\boldsymbol{X}$ has independent components X_i with prescribed probability distribution functions f_{X_i}, one obtains the joint probability density function:

$$f_{\boldsymbol{X}}(\boldsymbol{x}) = \prod_{i=1}^{M} f_{X_i}(x_i) \tag{28}$$

For each X_i, one can construct a family of orthogonal univariate polynomials $\left\{P_k^{(i)}, k \in \mathbb{N}\right\}$ with respect to the probability measure $\mathbb{P}_{X_i}(\mathrm{d}x_i) = f_{X_i}(x_i)\mathrm{d}x_i$ satifying:

$$\langle P_j^{(i)}, P_k^{(i)} \rangle \overset{\text{def}}{=} \mathbb{E}\left[P_j^{(i)}(X_i) P_k^{(i)}(X_i)\right] = \int P_j^{(i)}(x_i) P_k^{(i)}(x_i) f_{X_i}(x_i)\mathrm{d}x_i = c_j^{(i)} \delta_{jk} \tag{29}$$

where $\langle \cdot, \cdot \rangle$ is the inner product defined on the space associated with the probability measure $\mathbb{P}_{X_i}(\mathrm{d}x_i)$, δ_{jk} is the Kronecker symbol with $\delta_{jk} = 1$ if $j = k$, otherwise $\delta_{jk} = 0$ and $c_j^{(i)}$ is a constant. The univariate polynomial $P_j^{(i)}$ belongs to a specific class according to the distribution of X_i. For instance, if X_i is standard uniform (resp. Gaussian) random variable, $\left\{P_j^{(i)}\right\}_{j \geq 0}$ are orthogonal Legendre (resp. Hermite) polynomials. Then the orthonormal univariate polynomials are obtained by normalization:

$$\Psi_j^{(i)} = P_j^{(i)} / \sqrt{c_j^{(i)}} \tag{30}$$

Introducing the multi-indices $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_M)$, a multivariate polynomial

can be defined by tensor product as:

$$\Psi_{\boldsymbol{\alpha}}(\boldsymbol{x}) \stackrel{\text{def}}{=} \prod_{i=1}^{M} \Psi_{\alpha_i}^{(i)}(x_i) \tag{31}$$

Soize and Ghanem (2004) prove that the set of all multivariate polynomials $\Psi_{\boldsymbol{\alpha}}$ in the input random vector $\boldsymbol{X}$ forms a basis of the Hilbert space of second order random variables:

$$Y = \sum_{\boldsymbol{\alpha} \in \mathbb{N}^M} a_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(\boldsymbol{X}) \tag{32}$$

where $a_{\boldsymbol{\alpha}}$'s are the deterministic coefficients of the representation.

In practice, the input random variables are usually not standardized, therefore it is necessary to transform the input vector into a set of standard variables. We define the isoprobabilistic transform $\boldsymbol{Z} = \mathcal{T}^{-1}(\boldsymbol{X})$ which is a unique mapping from the original random space of X_i's onto a standard space of M basic independent random variables Z_i's. As an example Z_i may be a standard normal random variable or a uniform variable over $[-1, 1]$.

In engineering applications, only a finite number of terms can be computed in Eq.(32). Accordingly, the truncated polynomial chaos expansion of Y can be represented as follows Sudret (2007):

$$Y = \mathcal{M}(\boldsymbol{X}) = \mathcal{M}\left(\mathcal{T}(\boldsymbol{Z})\right) = \sum_{\boldsymbol{\alpha} \in \mathcal{A}} a_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(\boldsymbol{Z}) \tag{33}$$

in which $\mathcal{A}$ is the set of multi-indices $\boldsymbol{\alpha}$'s retained by the truncation scheme.

The application of PCE consists in choosing a suitable polynomial basis and then computing the appropriate coefficients $a_{\boldsymbol{\alpha}}$'s. To this end, there exist several techniques including spectral projection Le Maître et al. (2002); Matthies and Keese (2005), stochastic collocation method Xiu (2009) or least square analysis (also called regression, see (Berveiller et al., 2004, 2006)). A review of these so-called non-intrusive techniques is given in (Blatman, 2009). Recently, the least-square approach has been extended to obtain *sparse* expansions (Blatman and Sudret, 2010b, 2011). This technique has been applied to global sensitivity analysis in Blatman and Sudret (2010a). The main results are now summarized.

First note that the orthonormality of the polynomial basis leads to the following properties:

$$\mathbb{E}\left[\Psi_{\boldsymbol{\alpha}}(\boldsymbol{Z})\right] = 0 \qquad \text{and} \qquad \mathbb{E}\left[\Psi_{\boldsymbol{\alpha}}(\boldsymbol{Z})\, \Psi_{\boldsymbol{\beta}}(\boldsymbol{Z})\right] = \delta_{\boldsymbol{\alpha}\boldsymbol{\beta}} \tag{34}$$

As a consequence the mean value of the model output y is $\mathbb{E}[Y] = a_0$ whereas the variance is the sum of the square of the other coefficients:

$$D = \mathrm{Var}[Y] = \mathrm{Var}\left[\sum_{\boldsymbol{\alpha}\in\mathcal{A}} a_{\boldsymbol{\alpha}}\Psi_{\boldsymbol{\alpha}}(\boldsymbol{Z})\right] = \sum_{\substack{\boldsymbol{\alpha}\in\mathcal{A}\\ \boldsymbol{\alpha}\neq\mathbf{0}}} {a_{\boldsymbol{\alpha}}}^2 \mathrm{Var}[\Psi_{\boldsymbol{\alpha}}(\boldsymbol{Z})] = \sum_{\substack{\boldsymbol{\alpha}\in\mathcal{A}\\ \boldsymbol{\alpha}\neq\mathbf{0}}} {a_{\boldsymbol{\alpha}}}^2 \quad (35)$$

Making use of the unique orthonormality properties of the basis, Sudret (2006, 2008) proposed an original post-processing of the PCE for performing global sensitivity analysis. For any subset variables $\mathbf{u} = \{i_1, \ldots, i_s\} \subset \{1, \ldots, M\}$, one defines the set of multivariate polynomials $\Psi_{\boldsymbol{\alpha}}$ which depends only on $\mathbf{u}$:

$$\mathcal{A}_{\mathbf{u}} = \{\boldsymbol{\alpha} \in \mathcal{A} : \alpha_k \neq 0 \,\text{if and only if}\, k \in \mathbf{u}\} \quad (36)$$

The $\mathcal{A}_{\mathbf{u}}$'s form a partition of $\mathcal{A}$, thus the Sobol' decomposition of the truncated PCE in Eq. (33) may be written as follows:

$$Y = a_0 + \sum_{\substack{\mathbf{u}\subset\{1,\ldots,M\}\\ \mathbf{u}\neq\emptyset}} \mathcal{M}_{\mathbf{u}}(\boldsymbol{Z}_{\mathbf{u}}) \quad (37)$$

where:

$$\mathcal{M}_{\mathbf{u}}(\boldsymbol{Z}_{\mathbf{u}}) \overset{\text{def}}{=} \sum_{\boldsymbol{\alpha}\in\mathcal{A}_{\mathbf{u}}} a_{\boldsymbol{\alpha}}\Psi_{\boldsymbol{\alpha}}(\boldsymbol{Z}) \quad (38)$$

In other words the Sobol' decomposition is directly read from the PC expansion. Consequently, due to the orthonormality of PC basis, the partial variance $D_{\mathbf{u}}$ reads:

$$D_{\mathbf{u}} = \mathrm{Var}[\mathcal{M}_{\mathbf{u}}(\boldsymbol{Z}_{\mathbf{u}})] = \sum_{\boldsymbol{\alpha}\in\mathcal{A}_{\mathbf{u}}} a_{\boldsymbol{\alpha}}^2 \quad (39)$$

As a consequence the Sobol' indices at any order may be computed by a mere combination of the squares of the coefficients. As an illustration, the first order PC-based Sobol' indices read:

$$S_i = \sum_{\boldsymbol{\alpha}\in\mathcal{A}_i} a_{\boldsymbol{\alpha}}^2/D, \quad \mathcal{A}_i = \{\boldsymbol{\alpha} \in \mathcal{A} : \alpha_i > 0,\, \alpha_{j\neq i} = 0\} \quad (40)$$

whereas the total PC-based Sobol' indices are:

$$S_i^T = \sum_{\boldsymbol{\alpha}\in\mathcal{A}_i^T} a_{\boldsymbol{\alpha}}^2/D, \quad \mathcal{A}_i^T = \{\boldsymbol{\alpha} \in \mathcal{A} : \alpha_i > 0\} \quad (41)$$

4 Derivative of polynomial chaos expansions

In this paper, we consider the combination of polynomial chaos expansions with derivative-based global sensitivity analysis. On the one hand, PCE are already known to provide accurate metamodels at reasonable cost. On the other hand, the derivative-based sensitivity measure (DGSM) is effective for screening unimportant input factors. The combination of PCE and DGSM appears as a promising approach for effective low-cost SA. In fact, once the PCE metamodel is built, the DGSM can be computed as a mere post-processing of the metamodel which simply consists of polynomial functions.

As seen in Section 2, a DGSM is related to the expectation of the square of the model derivative, which was denoted by ν_i. We will express the model derivative in a way such that the expectation operator can be easily computed, more precisely by projecting the components of the gradient $\nabla\mathcal{M}$ onto a PC expansion.

4.1 Hermite polynomial chaos expansions

In this section we consider a numerical model $Y = \mathcal{M}(\boldsymbol{X})$ where Y is the scalar output and $\boldsymbol{X} = \{X_i, \ldots, X_M\}$ is the input vector composed of M *independent Gaussian* variables $X_i \sim \mathcal{N}(\mu_i, \sigma_i)$. The isoprobabilistic transform reads:

$$\boldsymbol{X} = \mathcal{T}(\boldsymbol{Z}): \qquad X_i = \mu_i + \sigma_i Z_i \tag{42}$$

where $Z_i \sim \mathcal{N}(0,1)$ are standard normal random variables. The truncated PCE of Y reads:

$$Y = \mathcal{M}(\boldsymbol{X}) = \mathcal{M}(\mathcal{T}(\boldsymbol{Z})) = \sum_{\boldsymbol{\alpha}\in\mathcal{A}} a_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(\boldsymbol{Z}) \tag{43}$$

in which $\boldsymbol{\alpha} = \{\alpha_1, \ldots, \alpha_M\}$ is a multi-index, $\mathcal{A}$ is the set of indices $\boldsymbol{\alpha}$ in the truncated expansion, $\Psi_{\boldsymbol{\alpha}}(\boldsymbol{z}) = \prod_{i=1}^{M} \tilde{He}_{\alpha_i}(z_i)$ is the multivariate polynomial basis obtained as the tensor product of univariate orthonormal Hermite polynomials $\tilde{He}_{\alpha_i}(z_i)$ (see A) and $a_{\boldsymbol{\alpha}}$ is the deterministic coefficient associated with $\Psi_{\boldsymbol{\alpha}}(\boldsymbol{z})$.

Since $\mathcal{T}$ is a one-to-one mapping with $\dfrac{\partial z_i}{\partial x_i} = \dfrac{1}{\sigma_i}$, the derivative-based sensitivity index reads:

$$\nu_i = \mathbb{E}\left[\left(\frac{\partial \mathcal{M}}{\partial x_i}(\boldsymbol{X})\right)^2\right] = \mathbb{E}\left[\left(\frac{\partial \mathcal{M}\circ\mathcal{T}}{\partial z_i}\frac{\partial z_i}{\partial x_i}\right)^2\right] = \frac{1}{{\sigma_i}^2}\mathbb{E}\left[\left(\frac{\partial \mathcal{M}\circ\mathcal{T}}{\partial z_i}(\boldsymbol{Z})\right)^2\right] \tag{44}$$

The DGSM of X_i, in other words the corresponding upper bound to the total Sobol' index S_i^T, is computed according to Eq. (25):

$$S_i^{DGSM} = \sigma_i^2\frac{\nu_i}{D} = \frac{1}{D}\mathbb{E}\left[\left(\frac{\partial \mathcal{M}\circ\mathcal{T}}{\partial z_i}(\boldsymbol{Z})\right)^2\right] = \frac{1}{D}\mathbb{E}\left[\left(\frac{\partial}{\partial z_i}\sum_{\boldsymbol{\alpha}\in\mathcal{A}} a_{\boldsymbol{\alpha}}\Psi_{\boldsymbol{\alpha}}(\boldsymbol{Z})\right)^2\right] \tag{45}$$

in which $D = \mathrm{Var}[Y] = \sum_{\boldsymbol{\alpha}\in\mathcal{A},\,\boldsymbol{\alpha}\neq\boldsymbol{0}} a_{\boldsymbol{\alpha}}^2$. This requires computing the partial derivatives of polynomial functions of the form $\mathcal{M}_{\mathcal{A}}(\boldsymbol{z}) = \sum_{\boldsymbol{\alpha}\in\mathcal{A}} a_{\boldsymbol{\alpha}}\Psi_{\boldsymbol{\alpha}}(\boldsymbol{z})$. One can prove that the derivatives $\tilde{He}_n^{'}(z) = \dfrac{\mathrm{d}\tilde{He}_n}{\mathrm{d}z}(z)$ read (see A):

$$\tilde{He}_n^{'}(z) = \sqrt{n}\,\tilde{He}_{n-1}(z) \tag{46}$$

Therefore the derivative of the multivariate orthonormal Hermite polynomial $\Psi_{\boldsymbol{\alpha}}(\boldsymbol{z}) = \prod_{i=1}^{M}\tilde{He}_{\alpha_i}(z_i)$ with respect to z_i reads:

$$\frac{\partial\Psi_{\boldsymbol{\alpha}}}{\partial z_i}(\boldsymbol{z}) = \prod_{\substack{j=1\\ j\neq i}}^{M}\tilde{He}_{\alpha_j}(z_j)\,\sqrt{\alpha_i}\tilde{He}_{\alpha_i-1}(z_i) \tag{47}$$

provided that $\alpha_i > 0$, and $\dfrac{\partial\Psi_{\boldsymbol{\alpha}}}{\partial z_i}(\boldsymbol{z}) = 0$ otherwise. Then the derivative of a Hermite PCE with respect to z_i is given the following expression:

$$\frac{\partial\mathcal{M}_{\mathcal{A}}}{\partial z_i}(\boldsymbol{z}) = \sum_{\boldsymbol{\alpha}\in\mathcal{A}^{(i)}}\sqrt{\alpha_i}\,a_{\boldsymbol{\alpha}}\Psi_{\boldsymbol{\alpha}_i'} \tag{48}$$

in which $\mathcal{A}^{(i)} = \{\boldsymbol{\alpha}\in\mathcal{A}, \alpha_i > 0\}$ is the set of multi-indices $\boldsymbol{\alpha}$ having a non-zero i^{th} component and $\boldsymbol{\alpha}_i^{'} = \{\alpha_1, \ldots, \alpha_i - 1, \ldots, \alpha_M\}$ is the index vector derived from $\boldsymbol{\alpha}$ by subtracting 1 from α_i. The expectation of the squared derivative in Eq. (45) is reformulated as:

$$\mathbb{E}\left[\left(\frac{\partial\mathcal{M}_{\mathcal{A}}}{\partial z_i}(\boldsymbol{Z})\right)^2\right] = \mathbb{E}\left[\sum_{\boldsymbol{\alpha}\in\mathcal{A}^{(i)}}\sum_{\boldsymbol{\beta}\in\mathcal{A}^{(i)}}\sqrt{\alpha_i\,\beta_i}\,a_{\boldsymbol{\alpha}}a_{\boldsymbol{\beta}}\,\Psi_{\boldsymbol{\alpha}_i{}'}\Psi_{\boldsymbol{\beta}_i'}\right] \tag{49}$$

Due to the linearity of the expectation operator, the above equation requires computing $\mathbb{E}\left[\Psi_{\boldsymbol{\alpha}_i{}'}\Psi_{\boldsymbol{\beta}_i'}\right]$. Note that the orthonormality of the polynomial basis

leads to $\mathbb{E}\left[\Psi_{\boldsymbol{\alpha}_i{}'}\Psi_{\boldsymbol{\beta}_i'}\right] = \delta_{\boldsymbol{\alpha}\boldsymbol{\beta}}$ where $\delta_{\boldsymbol{\alpha}\boldsymbol{\beta}}$ is the Kronecker symbol. Thus one has:

$$\mathbb{E}\left[\left(\frac{\partial \mathcal{M}_{\mathcal{A}}}{\partial z_i}(\boldsymbol{Z})\right)^2\right] = \sum_{\boldsymbol{\alpha}\in\mathcal{A}^{(i)}} \alpha_i\, a_{\boldsymbol{\alpha}}^2 \tag{50}$$

As a consequence, in case of a Hermite PCE the DGSM can be given the following *analytical expression*:

$$\hat{S}_i^{DGSM} = \frac{1}{D}\sum_{\boldsymbol{\alpha}\in\mathcal{A}^{(i)}} \alpha_i\, a_{\boldsymbol{\alpha}}^2 = \frac{\sum\limits_{\boldsymbol{\alpha}\in\mathcal{A}^{(i)}} \alpha_i\, a_{\boldsymbol{\alpha}}^2}{\sum\limits_{\boldsymbol{\alpha}\in\mathcal{A},\,\boldsymbol{\alpha}\neq\boldsymbol{0}} a_{\boldsymbol{\alpha}}^2} \tag{51}$$

Note that the total Sobol' indices S_i^T can be obtained directly from the PCE by $\hat{S}_i^T = \sum\limits_{\boldsymbol{\alpha}\in\mathcal{A}^{(i)}} a_{\boldsymbol{\alpha}}^2 / \sum\limits_{\boldsymbol{\alpha}\in\mathcal{A},\,\boldsymbol{\alpha}\neq\boldsymbol{0}} a_{\boldsymbol{\alpha}}^2$ as shown in Eq. (41). With integer indices $\alpha_i > 0$, it is clear that the inequality $S_i^T \leq S_i^{DGSM}$ is always true by construction.

4.2 Legendre polynomial chaos expansions

Consider now a computational model $Y = \mathcal{M}(\boldsymbol{X})$ where the input vector $\boldsymbol{X}$ contains M independent uniform random variables $X_i \sim \mathcal{U}[a_i, b_i]$. We first use an isoprobabilistic transform to convert the input factors into normalized variables $\boldsymbol{Z} = \{Z_i, \ldots, Z_M\}$:

$$\boldsymbol{X} = \mathcal{T}(\boldsymbol{Z}): \qquad X_i = \frac{b_i + a_i}{2} + \frac{b_i - a_i}{2} Z_i \tag{52}$$

where $Z_i \sim \mathcal{U}[-1, 1]$ are uniform random variables. The Legendre PCE has the form of the expansion in Eq. (43), except that $\Psi_{\boldsymbol{\alpha}}(\boldsymbol{z}) = \prod\limits_{i=1}^{M} \tilde{Le}_{\alpha_i}(z_i)$ is now the multivariate polynomial basis made of univariate orthonormal Legendre polynomials $\tilde{Le}_{\alpha_i}(z_i)$ (see B). Again, since $\mathcal{T}$ is a one-to-one linear mapping with $\dfrac{\partial z_i}{\partial x_i} = \dfrac{2}{b_i - a_i}$ the derivative-based sensitivity index reads:

$$\nu_i = \mathbb{E}\left[\left(\frac{\partial \mathcal{M}}{\partial x_i}(\boldsymbol{X})\right)^2\right] = \frac{4}{(b_i - a_i)^2}\,\mathbb{E}\left[\left(\frac{\partial \mathcal{M}\circ\mathcal{T}}{\partial z_i}(\boldsymbol{Z})\right)^2\right] \tag{53}$$

Similarly to Eq. (45), the upper bound DGSM to the total Sobol' index S_i^T is computed from Eq. (24) as:

$$\begin{aligned} S_i^{DGSM} &= \frac{(b_i - a_i)^2}{\pi^2}\frac{\nu_i}{D} = \frac{4}{\pi^2 D}\,\mathbb{E}\left[\left(\frac{\partial \mathcal{M}\circ\mathcal{T}}{\partial z_i}(\boldsymbol{Z})\right)^2\right] \\ &= \frac{4}{\pi^2 D}\,\mathbb{E}\left[\left(\frac{\partial}{\partial z_i}\sum_{\boldsymbol{\alpha}\in\mathcal{A}} a_{\boldsymbol{\alpha}}\,\Psi_{\boldsymbol{\alpha}}(\boldsymbol{Z})\right)^2\right] \end{aligned} \tag{54}$$

Thus the derivative of univariate and multivariate Legendre polynomials are required. Denoting by $\tilde{Le}_i^{'}(z) \stackrel{\text{def}}{=} \dfrac{\mathrm{d}\tilde{Le}(z)}{\mathrm{d}z}$, one shows in B that:

$$\left\{\tilde{Le}_1^{'}(z), \ldots, \tilde{Le}_n^{'}(z)\right\}^{\mathsf{T}} = \boldsymbol{C}^{\mathcal{L}e} \cdot \{\tilde{Le}_0(z), \ldots, \tilde{Le}_{n-1}(z)\}^{\mathsf{T}} \tag{55}$$

in which $\boldsymbol{C}^{\mathcal{L}e}$ is a constant matrix whose i^{th} row contains the coordinates of the derivative of $\tilde{Le}_i(z)$ onto a basis made of lower-degree polynomials $\left\{\tilde{Le}_j(z),\, j = 0, \ldots, i-1\right\}$. In other words, $\tilde{Le}_i^{'}(z) = \sum_{j=1}^{i} C_{ij}^{\mathcal{L}e} \tilde{Le}_{j-1}(z)$. Using this notation, the derivative of the multivariate orthonormal Legendre polynomials $\Psi_{\boldsymbol{\alpha}}(\boldsymbol{z}) = \prod_{i=1}^{M} \tilde{Le}_{\alpha_i}(z_i)$ with respect to z_i reads:

$$\frac{\partial \Psi_{\boldsymbol{\alpha}}}{\partial z_i}(\boldsymbol{z}) = \prod_{\substack{j=1 \\ j \neq i}}^{M} \tilde{Le}_{\alpha_j}(z_j) \left(\sum_{l=1}^{\alpha_i} C_{\alpha_i l}^{\mathcal{L}e} \tilde{Le}_{l-1}(z_i) \right) \tag{56}$$

For a given $\boldsymbol{\alpha} = \{\alpha_1, \ldots, \alpha_M\}$ let us define by $\boldsymbol{\alpha}_i^r$ the index vector having the i^{th} component equal to r:

$$\boldsymbol{\alpha}_i^r = \left\{ \alpha_1, \ldots, \overbrace{r}^{i^{th} position}, \ldots, \alpha_M \right\} \tag{57}$$

Using this notation Eq. (56) rewrites as follows:

$$\frac{\partial \Psi_{\boldsymbol{\alpha}}}{\partial z_i}(\boldsymbol{z}) = \sum_{l=1}^{\alpha_i} C_{\alpha_i l}^{\mathcal{L}e} \Psi_{\boldsymbol{\alpha}_i^{l-1}} \tag{58}$$

Denote by $\mathcal{A}^{(i)}$ the set of $\boldsymbol{\alpha}$ having a non-zero index α_i, *i.e.* $\mathcal{A}^{(i)} = \{\boldsymbol{\alpha} \in \mathcal{A}, \alpha_i > 0\}$. The derivative of a Legendre PCE with respect to z_i then reads:

$$\frac{\partial \mathcal{M}_{\mathcal{A}}}{\partial z_i}(\boldsymbol{z}) = \sum_{\boldsymbol{\alpha} \in \mathcal{A}^{(i)}} a_{\boldsymbol{\alpha}} \frac{\partial \Psi_{\boldsymbol{\alpha}}}{\partial z_i}(\boldsymbol{z}) = \sum_{\boldsymbol{\alpha} \in \mathcal{A}^{(i)}} \sum_{l=1}^{\alpha_i} a_{\boldsymbol{\alpha}}\, C_{\alpha_i l}^{\mathcal{L}}\, \Psi_{\boldsymbol{\alpha}_i^{l-1}}(\boldsymbol{z}) \tag{59}$$

Denote by $\mathcal{B}^{(i)}$ the set of multi-indices $\boldsymbol{\beta}$ representing the ensemble of multivariate polynomials generated by differentiating the linear combination of polynomials $\left\{\Psi_{\boldsymbol{\alpha}}(\boldsymbol{z}),\, \boldsymbol{\alpha} \in \mathcal{A}^{(i)}\right\}$. $\mathcal{B}^{(i)}$ is obtained as:

$$\mathcal{B}^{(i)} = \left\{ \boldsymbol{\beta} = \boldsymbol{\alpha} + (k - \alpha_i) \cdot \boldsymbol{e}_i,\, \boldsymbol{\alpha} \in \mathcal{A}^{(i)},\, k = 0, \ldots, \alpha_i - 1 \right\} \tag{60}$$

where:

$$\boldsymbol{e}_i = (0, \ldots, 0, \overbrace{1}^{i^{th}\text{pos.}}, 0 \ldots, 0) \tag{61}$$

The derivative of Legendre PCE rewrites:

$$\frac{\partial \mathcal{M}_{\mathcal{A}}}{\partial z_i}(\boldsymbol{z}) = \sum_{\boldsymbol{\beta} \in \mathcal{B}^{(i)}} b_{\boldsymbol{\beta}}\, \Psi_{\boldsymbol{\beta}}(\boldsymbol{z}) \tag{62}$$

in which the coefficient $b_{\boldsymbol{\beta}}$ is obtained from Eq.(59). Since the polynomials $\Psi_{\boldsymbol{\beta}}$ are also orthonormal, one obtains:

$$\mathbb{E}\left[\left(\frac{\partial \mathcal{M}_{\mathcal{A}}}{\partial z_i}(\boldsymbol{Z})\right)^2\right] = \sum_{\boldsymbol{\beta} \in \mathcal{B}^{(i)}} b_{\boldsymbol{\beta}}^2 \tag{63}$$

Finally, the DGSMs read:

$$\hat{S}_i^{DGSM} = \frac{4}{\pi^2} \frac{\sum\limits_{\boldsymbol{\beta} \in \mathcal{B}^{(i)}} b_{\boldsymbol{\beta}}^2}{\sum\limits_{\boldsymbol{\alpha} \in \mathcal{A},\, \boldsymbol{\alpha} \neq \mathbf{0}} a_{\boldsymbol{\alpha}}^2} \tag{64}$$

4.3 General case

Consider now the general case where the input vector $\boldsymbol{X}$ contains M independent random variables with different prescribed probability distribution functions, *i.e.* Gaussian, uniform or others. Such a problem can be addressed using generalized polynomial chaos expansions Xiu and Karniadakis (2002). As the above derivations for Hermite and Legendre polynomials are valid componentwise, they remain identical when dealing with generalized expansions. Only the proper matrix yielding the derivative of the univariate polynomials in the same univariate orthonormal basis is needed, see Appendix A for Hermite polynomials and Appendix B for Legendre polynomials. The derivation for Laguerre polynomials is also given in Appendix C for the sake of completeness.

5 Application examples

5.1 Morris function

We first consider the Morris function that is widely used in the literature for sensitivity analysis Morris (1991); Lamboni et al. (2013). This function reads:

$$y = \beta_o + \sum_{i=1}^{20} \beta_i\, \omega_i + \sum_{i<j}^{20} \beta_{ij}\, \omega_i\, \omega_j + \sum_{i<j<l}^{20} \beta_{ijl}\, \omega_i\, \omega_j\, \omega_l + \beta_{1234}\, \omega_1\, \omega_2\, \omega_3\, \omega_4 \tag{65}$$

in which:

- $\omega_i = 2\,(X_i - 1/2)$ except for $i = 3, 5, 7$ where $\omega_i = 2\left(1.2\dfrac{X_i}{X_i + 1} - \dfrac{1}{2}\right)$,
- the input vector $\boldsymbol{X} = \{X_1, \ldots, X_{20}\}$ contains 20 uniform random variables $\{X_i \sim \mathcal{U}[0, 1],\, i = 1, \ldots, 20\}$,
- $\beta_i = 20$ for $i = 1, 2, \ldots, 10$,
- $\beta_{ij} = -15$ for $i, j = 1, 2, \ldots, 6,\, i < j$,
- $\beta_{ijl} = -10$ for $i, j, l = 1, 2, \ldots, 5,\, i < j < l$,
- $\beta_{1234} = 5$,
- the remaining first and second order coefficients are defined by $\beta_i = (-1)^i$, $\beta_0 = 0$ and $\beta_{ij} = (-1)^{i+j}$,
- and the remaining third order coefficients are set to 0.

First, a PCE is built using the Least Angle Regression technique based on a Latin Hypercube experimental design of size $N = 500$. Then the PCE is post-processed to obtain the total Sobol' indices and the upper-bound derivative-based sensitivity measures (DGSMs) using Eq. (41) and Eq. (64), respectively. The procedure is replicated 100 times in order to provide the 95% confidence interval of the resulting sensitivity indices.

As a reference, the total Sobol' indices are computed by Monte Carlo simulation as described in Section 2.1 using the `sensitivity` package in `R` Pujol et al. (2013). One samples two experimental designs of size $N = 5,000$ denoted respectively by A and B then computes the corresponding output vectors Y_A and Y_B. To estimate the total sensitivity index S_i^T with respect to random variable X_i, one replaces the entire i^{th} column in sample A (which contains the samples of X_i) by the i^{th} column in sample B to obtain a new experimental design denoted by C_i. Then the output Y_{C_i} is computed from the input C_i. The variance-based S_i^T is obtained by means of Y_A, Y_B and Y_{C_i} using the `sobol2007` function Pujol et al. (2013); Saltelli et al. (2010). The total number of model evaluations required by the MCS approach is $5,000 \times (2 + 20) = 110,000$. After 100 replications we also obtain the 95% confidence interval on the sensitivity indices.

The DGSMs are also computed by Monte Carlo simulation for comparison, using a finite difference scheme to evaluate the gradient for each realization.

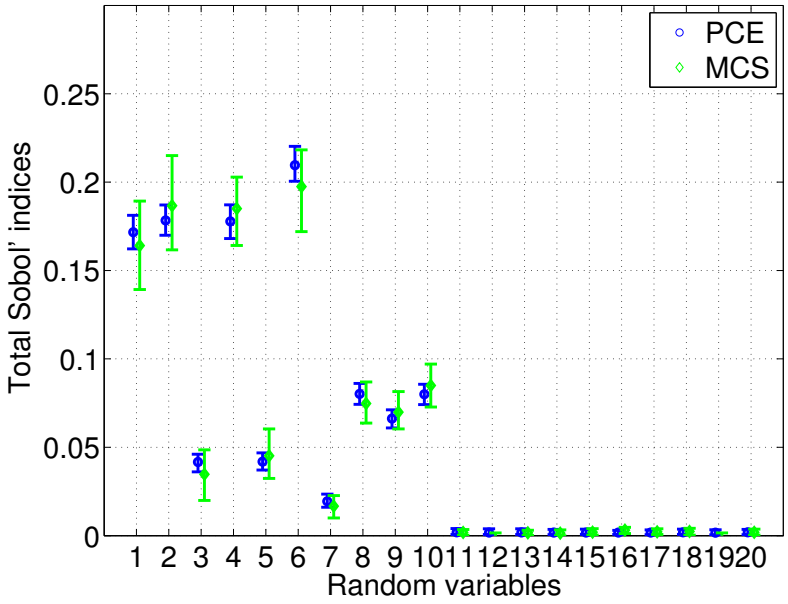


Figure 2: Morris function: PCE-based *vs.* MCS-based total Sobol' indices

500 realizations are used, leading to a total number of $500 \times (20 + 1) = 11{,}000$ model evaluations. Again the approach is replicated 100 times to get confidence intervals.

Figure 2 shows the total Sobol' sensitivity indices computed by MCS and from the PC expansion as well as their 95% confidence intervals. The median results (circle and diamonds) are close to each other, and show that input parameters $X_{11}, \ldots, X_{20}$ are unimportant factors, while X_1, X_2, X_4 and X_6 are important ones. It is observed that the confidence intervals are much smaller for the PCE-based indices than for the MCS-based indices, at a cost which is two order of magnitude smaller though (500 runs instead of 110,000).

Figure 3 shows the DGSMs computed by MCS and from the PC expansion as well as their 95% confidence intervals. Again the results obtained by the two approaches compare very well to each other and it is observed that the confidence intervals are smaller when using PC expansions. By comparing Figures 2 and 3, one can check that the obtained total Sobol' indices are always smaller than the DGSMs, as expected. Moreover, the less significant the parameter, the closer the DGSMs gets to the total Sobol' index.

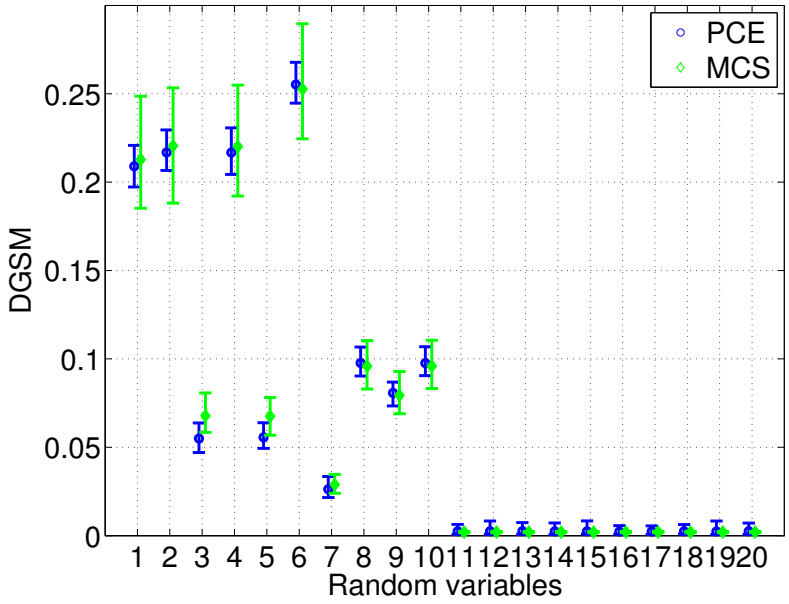


Figure 3: Morris function: PCE-based *vs.* MCS-based derivative-based global sensitivity measures (DGSM)

5.2 Oakley & O'Hagan function

The second numerical example is the Oakley & O'Hagan function Sobol' and Kucherenko (2009); Oakley and O'Hagan (2004) which reads:

$$f(\boldsymbol{X}) = \boldsymbol{a}_1^T \boldsymbol{X} + \boldsymbol{a}_2^T \cos(\boldsymbol{X}) + \boldsymbol{a}_3^T \sin(\boldsymbol{X}) + \boldsymbol{X}^T \boldsymbol{M} \boldsymbol{X} \tag{66}$$

in which the input vector $\boldsymbol{X} = \{X_1, \ldots, X_{15}\}$ consists of 15 independent standard normal random variables $\{X_i \sim \mathcal{N}(0,1),\, i = 1, \ldots, 15\}$. The 15×1 vectors $\boldsymbol{a}_j$, $j = 1, 2, 3$ and the 15×15 matrix $\boldsymbol{M}$ are provided at `www.sheffield.ac.uk/st1jeo`.

Given the complexity of the function, the PCE-based approach is run with a Latin Hypercube experimental design of size $N = 600$. The size of a single sample set for the MCS approach is $N = 10,000$ resulting in $10,000 \times (2+15) = 170,000$ model runs. The procedure is similar as in Section 5.1.

Figures 4 and 5 show the total Sobol' indices and the DGSMs computed both from a PC expansion and by Monte Carlo simulation. The conclusions are similar to the ones already drawn from the first example: the median values of the PCE-based DGSMs are almost identical to the MCS-based estimators while the confidence intervals are much smaller. Here the computational

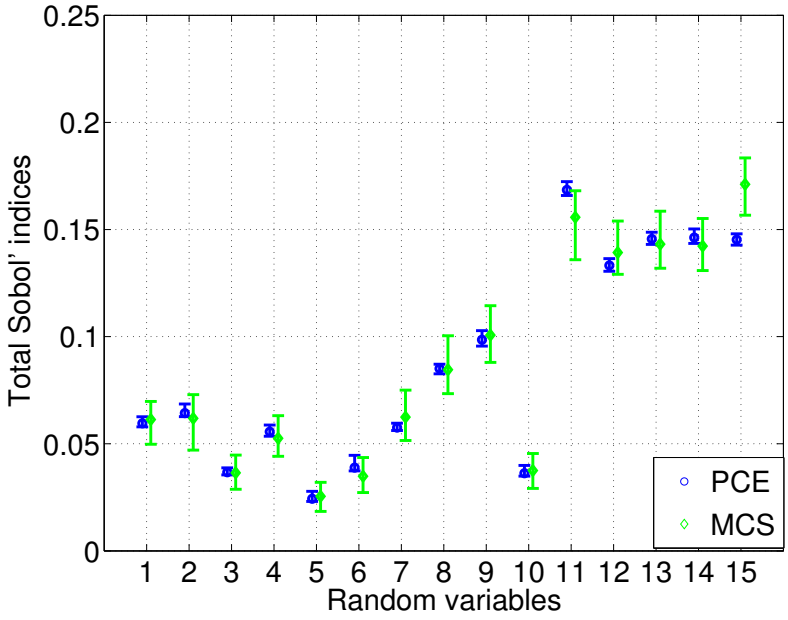


Figure 4: Oakley & O'Hagan function: PCE-based *vs.* MCS-based total Sobol' indices

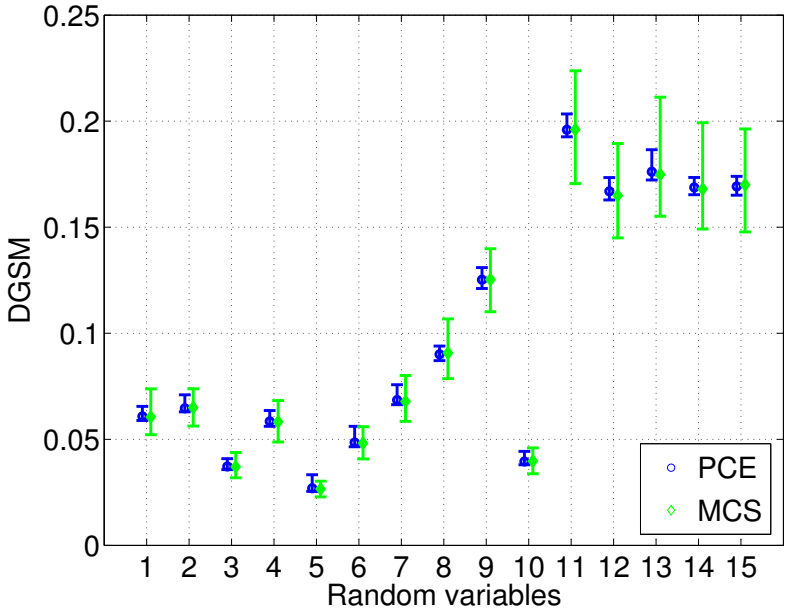
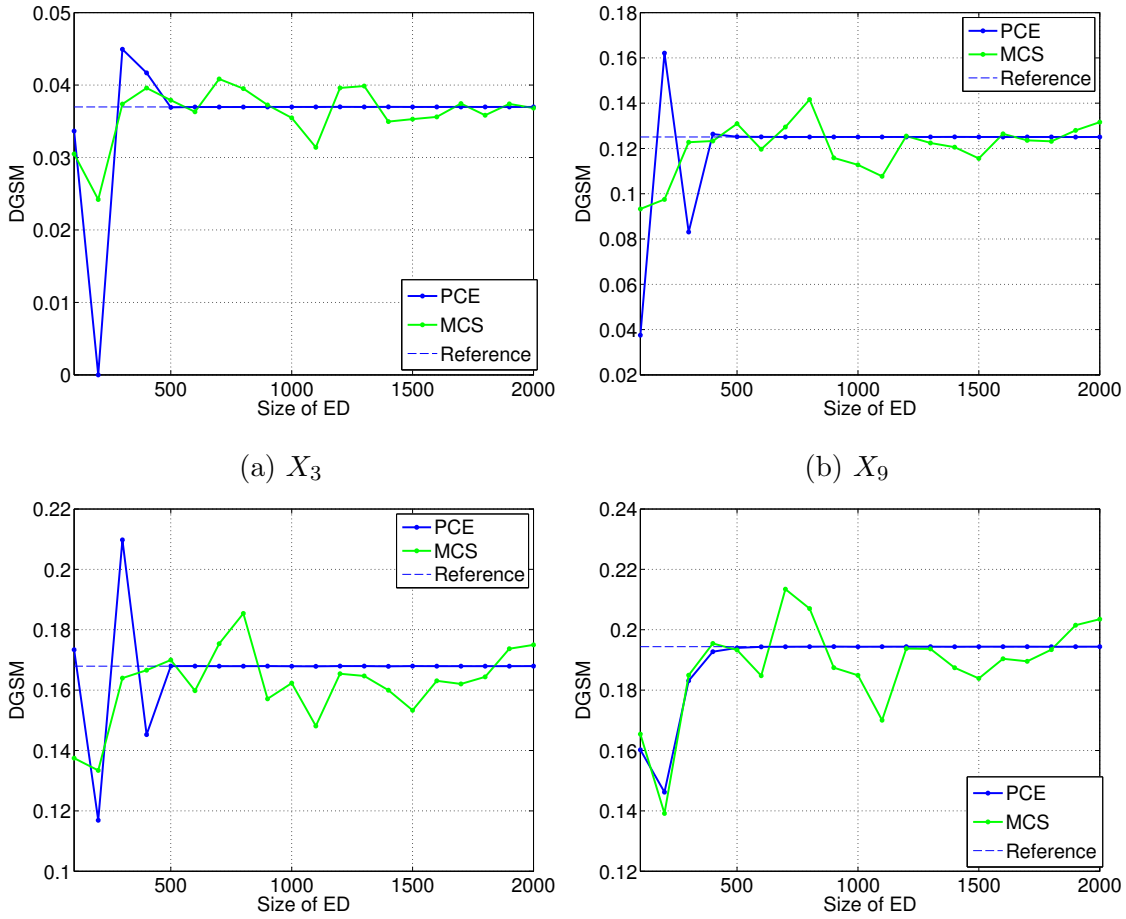


Figure 5: Oakley & O'Hagan function: PCE-based *vs.* MCS-based derivative-based global sensitivity measures (DGSM)

cost is 600 runs for PCE against $500 \times (15+1) = 8,000$ for the DGSMs. From the values one can conclude that $X_{11}, \ldots, X_{15}$ are important parameters, whereas the other have medium to little importance.

5.3 Oakley & O'Hagan function: convergence

In order to better assess the accuracy of the polynomial chaos expansions as a tool for computing the DGSMs, we carry out a parametric study on the number of samples used in the analysis. Precisely, a Latin hypercube sample of size N is used as the experimental design for establishing the PC expansion, and as the set of points where the gradient is computed for the MCS-based approach (thus $2\,N$ points are used for computing a single $DGSM$).



(a) X_3 (b) X_9

(c) X_{15} (d) X_{11}

Figure 6: Oakley & O'Hagan function: convergence of the PCE-based (resp. MCS-based) DGSMs as a function of the number of runs (NB: abscissa is the size of the experimental design for PCE, whereas the actual number of runs for MCS is twice larger, for *each* DGSM)

The convergence plots are shown for variables X_3, X_9, X_{15} and X_{11} which range from unimportant to most important. In each case the reference solution

is attained using 500 runs or less using PC expansions whereas the convergence is not attained even for $2 \times 2,000$ runs using MCS. Again it is emphasized that a *single experimental design* (*e.g.* of size 500) is used for computing all 15 DGSMs, whereas Monte Carlo simulation requires $(15 + 1)$ times this number as a whole, which makes PC expansions even more appealing in large dimensions.

6 Conclusions

In practical problems, the system of interest usually contains numerous random input factors which might lead to large uncertainty in the model output. Therefore, it is important to quantify the important factors according to their contributions to the output uncertainty so as to fix unimportant factors to deterministic values and simplify the model. However, the commonly used sampling-based approaches for global sensitivity analysis may be computationally prohibitive in large dimensions.

In this paper, we combined the polynomial chaos expansions (PCE) metamodelling with a derivative-based sensitivity analysis technique. Polynomial chaos expansions are effective surrogate models for global sensitivity analysis. The very nature of the orthogonal expansions reduces the computation of (total) Sobol' indices to a mere post-processing of the PC coefficients. Similarly, DGSMs can be computed by a straightforward post-processing, *i.e.* without requiring additional model runs. One only needs to differentiate the multivariate polynomials, which in the end reduces to differentiating univariate polynomial functions. Expressions were given for the classical Hermite, Legendre and Laguerre polynomials. In order to carry out the computation efficiently the derivative polynomials shall be represented onto the orthonormal basis of the same family, which can be done once and for all. Note that the derivatives of classical orthogonal polynomial expansions is also an asset of this paper, which can be reused in other contexts including gradient-based optimization algorithms.

The proposed PCE/DGSM technique is illustrated on two well-known benchmark functions. By comparing with Monte Carlo simulation, the PCE

approach is shown to provide sensitivity indices with smaller uncertainty at a computational cost that is one to two orders of magnitude smaller. The gain is even larger in high dimensions since the finite difference computation of the gradients leads to a linear increase of the computational cost with respect to the input dimension for MCS-based DGSMs, whereas the use of sparse polynomial chaos expansions makes the approach rather insensitive to that dimension.

As an outlook, the capacity of PC expansions to estimate DGSM indices using very small experimental designs shall be investigated, in order to have a real screening method that only makes use of limited information to rank qualitatively the input parameters according to their importance. This work is currently in progress.

References

Reuter, U., Liebscher, M.. Global sensitivity analysis in view of nonlinear structural behavior. LSDYNA Anwenderforum, Bamberg 2008;.

Hasofer, A.M.. Modern sensitivity analysis of the CESARE-Risk computer fire model. Fire Safety J 2009;44(3):330–338.

Campolongo, F., Cariboni, J., Saltelli, A.. An effective screening design for sensitivity analysis of large models. Environmental modelling & software 2007;22(10):1509–1518.

Patelli, E., Pradlwarter, H.J.. Monte Carlo gradient estimation in high dimensions. Int J Numer Meth Engng 2010;81(2):172–188.

Sudret, B., Mai, C.V.. Computing seismic fragility curves using polynomial chaos expansions. In: Deodatis, G., editor. Proc. 11th Int. Conf. Struct. Safety and Reliability (ICOSSAR'2013), New York, USA. 2013,.

Sudret, B.. Uncertainty propagation and sensitivity analysis in mechanical models - Contributions to structural reliability and stochastic spectral methods. Ph.D. thesis; Université BLAISE PASCAL - Clermont II; 2007.

de Rocquigny, E.. Modelling Under Risk and Uncertainty. Wiley Series in Probability and Statistics; Chichester, UK: John Wiley & Sons, Ltd; 2012.

Saltelli, A., Chan, K., Scott, E.. Sensitivity analysis. J. Wiley & Sons; 2000.

Saltelli, A., Tarantola, S., Campolongo, F., Ratto, M.. Sensitivity analysis in practice: a guide to assessing scientific models. J. Wiley & Sons; 2004.

Saltelli, A., Ratto, M., Andres, T., Campolongo, F., Cariboni, J., Gatelli, D., et al. Global Sensitivity Analysis – The Primer. Wiley; 2008.

Pappenberger, F., Beven, K.J., Ratto, M., Matgen, P.. Multi-method global sensitivity analysis of flood inundation models. Adv Water Resour 2008;31(1):1–14.

Kala, Z.. Sensitivity analysis of steel plane frames with initial imperfections. Eng Struct 2011;33(8):2342–2349.

Fassò, A.. Sensitivity Analysis of Computer Models. John Wiley & Sons, Ltd; 2013,.

Borgonovo, E., Peccati, L.. Uncertainty and global sensitivity analysis in the evaluation of investment projects. Int J Prod Econ 2006;104(1):62–73.

Marino, S., Hogue, I.B., Ray, C.J., Kirschner, D.E.. A methodology for performing global uncertainty and sensitivity analysis in systems biology. J Theor Biol 2008;254(1):178–196.

Abraham, A.K., Krzyzanski, W., Mager, D.E.. Partial derivative-based sensitivity analysis of models describing target-mediated drug disposition. The AAPS journal 2007;9(2):E181–E189.

Ditlevsen, O., Madsen, H.O.. Structural reliability methods. J.˜Wiley and Sons, Chichester; 1996.

Kucherenko, S., Rodriguez-Fernandez, M., Pantelides, C., Shah, N.. Monte Carlo evaluation of derivative-based global sensitivity measures. Reliab Eng Sys Safety 2009;94(7):1135–1148.

Morris, M.D.. Factorial Sampling Plans for Preliminary Copmputational Experiments. Technometrics 1991;33(2):161–174.

Cukier, R.I., Fortuin, C.M., Shuler, K.E., Petschek, A.G., Schaibly, J.H.. Study of the sensitivity of coupled reaction systems to uncertainties in rate coefficients - theory. J Chem Phys 1973;59:38,73–3878.

Cukier, H., Levine, R.I., Shuler, K.. Nonlinear sensitivity analysis of multiparameter model systems. J Comput Phys 1978;26:1–42.

Mara, T.A.. Extension of the RBD-FAST method to the computation of global sensitivity indices. Reliab Eng Sys Safety 2009;94(8):1274–1281.

Sobol', I.M.. Sensitivity estimates for nonlinear mathematical models. Math Modeling & Comp Exp 1993;1:407–414.

Sobol, I.. Global sensitivity indices for nonlinear mathematical models and their Monte Carlo estimates. Mathematics and Computers in Simulation 2001;55(1-3):271–280.

Sobol', I.M., Kucherenko, S.S.. Global sensitivity indices for nonlinear mathematical models. Review. Wilmott magazine 2005;1:56–61.

Archer, G.E., Saltelli, A., Sobol', I.M.. Sensitivity measures, ANOVA-like techniques and the use of bootstrap. J Stat Comput Simul 1997;58:99–120.

Saltelli, A.. Making best use of model evaluations to compute sensitivity indices. Comput Phys Comm 2002;145:280–297.

Saltelli, A., Annoni, P., Azzini, V., Campolongo, F., Ratto, M., Tarantola, S.. Variance based sensitivity analysis of model output. Design and estimator for the total sensitivity index. Comput Phys Comm 2010;181:259–270.

Sathyanarayanamurthy, H., Chinnam, R.B.. Metamodels for variable importance decomposition with applications to probabilistic engineering design. Comput Ind Eng 2009;57(3):996–1007.

Zhang, X., Pandey, M.D.. An effective approximation for variance-based global sensitivity analysis. Reliab Eng Sys Safety 2014;121(0):164–174.

Sudret, B.. Global sensitivity analysis using polynomial chaos expansions. In: Spanos, P., Deodatis, G., editors. Proc. 5th Int. Conf. on Comp. Stoch. Mech (CSM5), Rhodos, Greece. 2006,.

Sudret, B.. Global sensitivity analysis using polynomial chaos expansions. Reliab Eng Sys Safety 2008;93:964–979.

Blatman, G., Sudret, B.. Efficient computation of global sensitivity indices using sparse polynomial chaos expansions. Reliab Eng Sys Saf 2010a;95(11):1216–1229.

Sobol', I.M., Kucherenko, S.. Derivative based global sensitivity measures and their link with global sensitivity indices. Math Comput Simul 2009;79(10):3009–3017.

Sobol', I.M., Kucherenko, S.. A new derivative based importance criterion for groups of variables and its link with the global sensitivity index. Comput Phys Comm 2010;181(7):1212–1217.

Lamboni, M., Iooss, B., Popelin, A.L., Gamboa, F.. Derivative-based global sensitivity measures: general links with Sobol' indices and numerical tests. Math Comput Simul 2013;87:44–54.

Sobol', I.M., Tarantola, S., Gatelli, D., Kucherenko, S., Mauntz, W.. Estimating the approximation error when fixing unessential factors in global sensitivity analysis. Reliab Eng Sys Safety 2007;92(7):957–960.

Monod, H., Naud, C., Makowski, D.. Uncertainty and sensitivity analysis for crop models. Working with Dynamic Crop Models: Evaluation, Analysis, Parameterization, and Applications, Elsevier 2006;:55–100.

Janon, A., Klein, T., Lagnoux, A., Nodet, M., Prieur, C.. Asymptotic normality and efficiency of two Sobol index estimators. ESAIM: Probability and Statistics 2013;:1–20.

Ghanem, R., Spanos, P.. Stochastic Finite Elements : A Spectral Approach. Courier Dover Publications; 2003.

Soize, C., Ghanem, R.. Physical systems with random uncertainties: chaos representations with arbitrary probability measure. SIAM J Sci Comput 2004;26(2):395–410.

Le Maître, O.P., Reagan, M., Najm, H.N., Ghanem, R.G., Knio, O.M.. A stochastic projection method for fluid flow – II. Random process. J Comput Phys 2002;181:9–44.

Matthies, H.G., Keese, A.. Galerkin methods for linear and nonlinear elliptic stochastic partial differential equations. Comput Methods Appl Mech Engrg 2005;194:1295–1331.

Xiu, D.. Fast numerical methods for stochastic computations: a review. Comm Comput Phys 2009;5(2-4):242–272.

Berveiller, M., Sudret, B., Lemaire, M.. Presentation of two methods for computing the response coefficients in stochastic finite element analysis. In: Proc. 9th ASCE Specialty Conference on Probabilistic Mechanics and Structural Reliability, Albuquerque, USA. 2004,.

Berveiller, M., Sudret, B., Lemaire, M.. Stochastic finite elements: a non intrusive approach by regression. Eur J Comput Mech 2006;15(1-3):81–92.

Blatman, G.. Adaptive sparse polynomial chaos expansions for uncertainty propagation and sensitivity analysis. Ph.D. thesis; Université Blaise Pascal, Clermont-Ferrand; 2009.

Blatman, G., Sudret, B.. An adaptive algorithm to build up sparse polynomial chaos expansions for stochastic finite element analysis. Prob Eng Mech 2010b;25(2):183–197.

Blatman, G., Sudret, B.. Adaptive sparse polynomial chaos expansion based on Least Angle Regression. J Comput Phys 2011;230:2345–2367.

Xiu, D., Karniadakis, G.E.. The Wiener-Askey polynomial chaos for stochastic differential equations. SIAM J Sci Comput 2002;24(2):619–644.

Pujol, G., Iooss, B., Janon, A.. sensitivity: Sensitivity Analysis; 2013.

Oakley, J., O'Hagan, A.. Probabilistic sensitivity analysis of complex models: a Bayesian approach. J Royal Stat Soc, Series B 2004;66:751–769.

Abramovitz, M., Stegun, I.A.. Handbook of mathematical functions. New York: Dover Publications Inc.; 1965.

As seen in Section 4, the computation of polynomial chaos expansions derivative-based global sensitivity measures (PCE-DGSMs) consists of two steps. The first step is to represent the derivative of the PCE in terms of orthonormal polynomials from the same families. It essentially requires to construct the matrices of coefficients $\boldsymbol{C}$ that are used for differentiating the classical orthonormal polynomials. The second step is to post-process this "PCE" of the derivative. A general solution to compute the mean squared derivative using the coefficients matrices $\boldsymbol{C}$ was presented in Section 4.3.

A Hermite polynomial chaos expansions

The classical Hermite polynomials $\{He_n, n \in \mathbb{N}\}$, where n determines the degree of the polynomial, are defined on the set of real numbers$\mathbb{R}$ so as to be orthogonal with respect to the Gaussian probability measure and associated inner product:

$$\langle He_m,\, He_n\rangle \stackrel{\text{def}}{=} \int_{\mathbb{R}} He_m(z) He_n(z) \frac{e^{-z^2/2}}{\sqrt{2\pi}}\,\mathrm{d}z = n!\,\delta_{mn} \tag{67}$$

The Hermite polynomials satisfy the following differential equation (Abramovitz and Stegun, 1965, Chap. 22)

$$\frac{\mathrm{d}}{\mathrm{d}z} He_n(z) = n He_{n-1}(z) \tag{68}$$

From Eq. (67) the norm of Hermite polynomials reads:

$$\langle He_n,\, He_n\rangle = n! \tag{69}$$

so that the *orthonormal Hermite polynomials* are defined by:

$$\tilde{He}_n(z) = \frac{1}{\sqrt{n!}} He_n(z) \tag{70}$$

Substituting for Eq. (70) in Eq. (68), one gets the derivative of orthonormal Hermite polynomial $\tilde{He}_n^{'}(z) \stackrel{\text{def}}{=} \dfrac{\mathrm{d}\tilde{He}(z)}{\mathrm{d}z}$:

$$\tilde{He}_n^{'}(z) = \sqrt{n}\,\tilde{He}_{n-1}(z) \tag{71}$$

For computational purposes the following matrix notation is introduced:

$$\left\{\tilde{He}_1^{'}(z), \ldots, \tilde{He}_n^{'}(z)\right\}^{\mathsf{T}} = \boldsymbol{C}^{\mathcal{H}} \cdot \{\tilde{He}_0(z), \ldots, \tilde{He}_{n-1}(z)\}^{\mathsf{T}} \tag{72}$$

which allows one to cast the derivative of the orthonormal Hermite polynomials in the initial basis. From Eq. (71), $\boldsymbol{C}^{\mathcal{H}}$ is obviously diagonal:

$$\boldsymbol{C}^{\mathcal{H}}_{i,j} = \sqrt{i}\,\delta_{ij} \tag{73}$$

B Legendre polynomial chaos expansions

The classical Legendre polynomials $\{Le_n, n \in \mathbb{N}\}$ are defined over $[-1, 1]$ so as to be orthogonal with respect to the uniform probability measure and associated inner product:

$$\langle Le_m,\, Le_n\rangle \stackrel{\text{def}}{=} \int_{-1}^{1} Le_m(z) Le_n(z) \frac{\mathrm{d}z}{2} = \frac{1}{2\,n+1}\,\delta_{mn} \tag{74}$$

They satisfy the following differential equation (Abramovitz and Stegun, 1965, Chap. 22)

$$\frac{\mathrm{d}}{\mathrm{d}z}\left[Le_{n+1}(z) - Le_{n-1}(z)\right] = (2n+1) Le_n(z) \tag{75}$$

Using the notation $Le_n^{'}(z) \stackrel{\text{def}}{=} \dfrac{\mathrm{d}Le_n(z)}{\mathrm{d}z}$ one can transform Eq. (75) into the equation:

$$\begin{aligned} Le_{n+1}^{'}(z) &= (2n+1) Le_n(z) + Le_{n-1}^{'}(z) \\ &= (2n+1) Le_n(z) + (2(n-2)+1) Le_{n-2}(z) + Le_{n-3}^{'}(z) \\ &= \cdots \end{aligned} \tag{76}$$

From Eq. (74), the norm of Legendre polynomials reads:

$$\langle Le_n,\, Le_n\rangle = \frac{1}{2\,n+1} \tag{77}$$

so that the *orthonormal Legendre polynomials* read:

$$\tilde{Le}_n(z) = \sqrt{2n+1}\, Le_n(z) \tag{78}$$

Substituting for Eq. (78) in Eq. (76) one obtains:

$$\tilde{Le}_{n+1}^{'}(z) = \sqrt{2n+3}\left[\sqrt{2n+1}\,\tilde{Le}_n(z) + \sqrt{2(n-2)+1}\,\tilde{Le}_{n-2}(z) + \sqrt{2(n-4)+1}\,\tilde{Le}_{n-4}(z) + \dots\right] \tag{79}$$

Introducing the matrix notation:

$$\left\{\tilde{Le}_1^{'}(z), \dots, \tilde{Le}_n^{'}(z)\right\}^{\mathsf{T}} = \boldsymbol{C}^{\mathcal{L}e} \cdot \{\tilde{Le}_0(z), \dots, \tilde{Le}_{n-1}(z)\}^{\mathsf{T}} \tag{80}$$

the matrix $\boldsymbol{C}^{\mathcal{L}e}$ reads:

$$\boldsymbol{C}^{\mathcal{L}e} = \begin{bmatrix} \sqrt{3} & 0 & 0 & 0 & \dots & \\ 0 & \sqrt{5}\sqrt{3} & 0 & 0 & \dots & \\ \sqrt{7}\cdot 1 & 0 & \sqrt{7}\sqrt{5} & 0 & \dots & \\ \vdots & & & & & \\ 0 & \sqrt{4p+1}\sqrt{3} & 0 & \sqrt{4p+1}\sqrt{7} & \dots & \sqrt{4n+1}\sqrt{4n-1} \end{bmatrix} \tag{81}$$

when $n = 2p$ is even and

$$\boldsymbol{C}^{\mathcal{L}e} = \begin{bmatrix} \sqrt{3} & 0 & 0 & 0 & \dots & & \\ 0 & \sqrt{5}\sqrt{3} & 0 & 0 & \dots & & \\ \sqrt{7}\cdot 1 & 0 & \sqrt{7}\sqrt{5} & 0 & \dots & & \\ \vdots & & & & & & \\ \sqrt{4p+3}\cdot 1 & 0 & \sqrt{4p+3}\sqrt{5} & 0 & \dots & 0 & \sqrt{4p+3}\sqrt{4p+1} \end{bmatrix} \tag{82}$$

when $n = 2p+1$ is odd.

C Generalized Laguerre polynomial chaos expansions

Consider a model $Y = \mathcal{M}(\boldsymbol{X})$ where the input vector $\boldsymbol{X}$ contains M independent random variables with Gamma distribution $X_i \sim \Gamma(\alpha_i, \beta_i)$, $(\alpha_i, \beta_i > 0)$ with prescribed probability density functions:

$$f_{X_i}(x_i) = {\beta_i}^{\alpha_i}\,\frac{1}{\Gamma(\alpha_i)} x^{\alpha_i - 1} e^{-\beta_i x_i} \tag{83}$$

where $\Gamma(\cdot)$ is the Gamma function. We first use an isoprobabilistic transform to convert the input factors into a random vector $\boldsymbol{Z} = \{Z_i, \dots, Z_M\}$ as

follows:

$$Z_i = \beta_i \, X_i \tag{84}$$

One can prove that:

$$f_{Z_i}(z_i) = \left| \frac{\mathrm{d}x_i}{\mathrm{d}z_i} \right| f_{X_i}(x_i) = \frac{1}{\Gamma(\alpha)} {z_i}^{\alpha-1} e^{-z_i} \tag{85}$$

which means $Z_i \sim \Gamma(\alpha_i, 1)$.

By definition, the generalized Laguerre polynomials $\left\{ L_n^{(\alpha-1)}(z),\, n \in \mathbb{N} \right\}$, where n is the degree of the polynomial, are orthogonal with respect to the weight function $w(z) = z^{\alpha-1} e^{-z}$ over $(0, \infty)$:

$$\langle L_n^{(\alpha-1)}(z), L_m^{(\alpha-1)}(z) \rangle \overset{\text{def}}{=} \int_0^{+\infty} z^{\alpha-1} e^{-z} L_n^{(\alpha-1)}(z) L_m^{(\alpha-1)}(z) \mathrm{d}z = \frac{\Gamma(n+\alpha)}{n!} \delta_{mn} \tag{86}$$

The derivative of $L_n^{(\alpha-1)}$ reads:

$$L_n'^{(\alpha-1)}(z) = -\sum_{k=0}^{n-1} L_k^{(\alpha-1)}(z) \tag{87}$$

Recall that one obtains the Gamma distribution by scaling the weight function $w(z)$ by $1/\Gamma(\alpha)$. Therefore in the context of PCE, we use the generalized Laguerre polynomials functions orthonormalized as follows:

$$\tilde{L}_n^{(\alpha-1)}(z) = \sqrt{\frac{n! \Gamma(\alpha)}{\Gamma(n+\alpha)}} L_n^{(\alpha-1)}(z) = \sqrt{n \, B(n, \alpha)} \, L_n^{(\alpha-1)}(z) \tag{88}$$

where $B(x, y) = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)}$ is the beta function. Substituting for Eq. (88) in Eq. (87) one obtains:

$$\tilde{L}_n'^{(\alpha-1)}(z) = -\sum_{k=0}^{n-1} \sqrt{\frac{\Gamma(k+\alpha+1)\, n!}{\Gamma(n+\alpha+1)\, k!}} \tilde{L}_k^{(\alpha-1)}(z) = -\sum_{k=1}^{n} \sqrt{\frac{B(n+1, \alpha)}{B(k, \alpha)}} \tilde{L}_{k-1}^{(\alpha-1)}(z) \tag{89}$$

Introducing the matrix notation:

$$\left\{ \tilde{L}_1'(z), \ldots, \tilde{L}_n'(z) \right\}^{\mathsf{T}} = \boldsymbol{C}^{\mathcal{L}a} \cdot \{ \tilde{L}_0(z), \ldots, \tilde{L}_{n-1}(z) \}^{\mathsf{T}} \tag{90}$$

the constant matrix $\boldsymbol{C}^{\mathcal{L}a}$ is a lower triangular matrix whose generic term reads:

$$\boldsymbol{C}_{i,j}^{\mathcal{L}a} = -\sqrt{\frac{B(i+1, \alpha)}{B(j, \alpha)}} \tag{91}$$