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Review

Global sensitivity analysis using polynomial chaos expansions

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Abstract

Global sensitivity analysis (SA) aims at quantifying the respective effects of input random variables (or combinations thereof) onto the variance of the response of a physical or mathematical model. Among the abundant literature on sensitivity measures, the Sobol' indices have received much attention since they provide accurate information for most models. The paper introduces generalized polynomial chaos expansions (PCE) to build surrogate models that allow one to compute the Sobol' indices *analytically* as a post-processing of the PCE coefficients. Thus the computational cost of the sensitivity indices practically reduces to that of estimating the PCE coefficients. An original non intrusive regression-based approach is proposed, together with an experimental design of minimal size. Various application examples illustrate the approach, both from the field of global SA (i.e. well-known benchmark problems) and from the field of stochastic mechanics. The proposed method gives accurate results for various examples that involve up to eight input random variables, at a computational cost which is 2–3 orders of magnitude smaller than the traditional Monte Carlo-based evaluation of the Sobol' indices.

Keywords: Global sensitivity analysis; Sobol' indices; Analysis of variance; Polynomial chaos; Generalized chaos; Regression; Stochastic finite elements

Contents

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1. Introduction

The rational treatment of uncertainties in mechanical models have received much attention in the past decade. Broadly speaking, it is assumed that a model, which is a mathematical representation of physical phenomena, has input parameters which are not well known in practice.

Sensitivity analysis (SA) of a model aims at quantifying the relative importance of each input parameter. Methods of SA are usually classified into two categories:

- *Local SA* concentrates on the local impact of input parameters on the model. It is based on the computation of the gradient of the response with respect to its parameters around a nominal value. Numerous techniques have been developed to compute the gradient efficiently, including finite-difference schemes, direct differentiation or adjoint differentiation methods [1].
- *Global SA* tries to quantify the output uncertainty due to the uncertainty in the input parameters, which are taken singly or in combination with others.

Many papers have been devoted to the latter topic in the last twenty years. A good state-of-the-art of the techniques is available in [2]. Broadly speaking, methods can be gathered into two groups:

- *Regression-based methods*: The standardized regression coefficients (SRC) are based on a linear regression of the output on the input vector. The input/output Pearson correlation coefficients measure the effect of each input variable by the correlation it has with the model output. The partial correlation coefficients (PCC) are based on results of regressions of the model on all input variables except one. These coefficients are useful to measure the effect of the input variables if the model is linear, i.e. if the coefficient of determination R^2 of the regression is close to one. In case of nonlinearity, they fail to represent properly the response sensitivities. However, in case of monotonicity of the model with respect to the input parameters, the rank transformation can be used, leading to the so-called SRRC (standardized rank regression-) and PRCC (partial rank correlation-) coefficients. As a whole, in case of general nonlinear nonmonotonic models, these approaches fail to produce satisfactory sensitivity measures [3].
- *Variance-based methods*: These methods aim at decomposing the variance of the output as a sum of contributions of each input variable, or combinations thereof. There are sometimes called *ANOVA techniques* for "ANalysis Of VAriance". The *correlation ratios* proposed in [4] enter this category. They are formulated as conditional variances and usually evaluated by crude Monte Carlo simulation or Latin hypercube sampling. The Fourier amplitude sensitivity test (FAST) indices [5,6] and the Sobol' indices ([3,7,8], see also the review in [9]) are intended to represent the sensitivities for general models. The Sobol' indices are practically computed using Monte Carlo simulation, which makes them hardly applicable for computationally demanding models, e.g. finite element models in engineering mechanics.

From another viewpoint, the representation of uncertainties of model parameters in engineering mechanics, and their propagation through the models is a long-term story. However, the context is quite far away from the SA problems described above. Indeed, classical methods of probabilistic engineering mechanics can be broadly classified into three categories, according to the type of information on the response they are looking at (see Fig. 1):

- *Response variability methods* such as the *perturbation method* [10,11] and the *weighted integral method* [12–14]

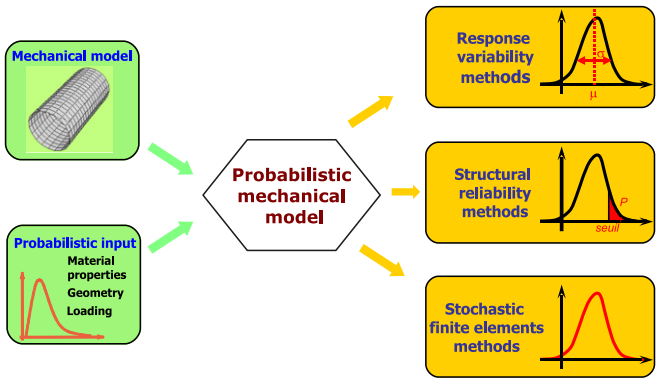

Fig. 1. Classification of methods in probabilistic engineering mechanics.

allow to compute the mean value and variance of the mechanical response of the system. This gives a feeling on the central part of the response probability density function (PDF).

- *Structural reliability methods* allow to investigate the tails of the response PDF by computing the probability of exceedance of a prescribed threshold [15]. Among these methods, directional simulation, FORM/SORM and importance sampling are nowadays of common use both in the academia and in industrial practice.
- *Stochastic finite element methods*, named after the pioneering work by Ghanem and Spanos [16] aim at representing in an intrinsic way the complete response PDF. This is done by expanding the response (which, after proper discretization of the problem, is a random vector of unknown joint PDF) onto a particular basis of the probability space called the *polynomial chaos* (PC). In the last ten years, the literature on the PC-based stochastic finite elements is very rich (see a review by Sudret and Der Kiureghian [17] and many recent papers, among others [18–28]).
  The great advantage of these PC-based approaches is that the full randomness of the response is contained in the set of the expansion coefficients. Thus problems pertaining to the first two classes can be solved as a post-processing of the PC-based analysis. Although the literature has mainly focused on computing the mean value and standard deviation of the response, applications in structural reliability have been shown, see e.g. [21,29–31].

For all three classes of problems (i.e. central part, tail, or full distribution), the Monte Carlo simulation is a versatile tool that can be employed, usually requiring a much higher computational effort than the methods mentioned above. It is thus mainly a means to get a reference solution in specific cases.

PC-based methods have not been used much so far in the context of SA. The interpretation of the first order terms in the PC expansion has been used in [20] in the context of reacting flow simulations. The idea of decomposing the variance of the response into contributions of each random variable or couples thereof can be found in [32].

However, to the author's knowledge, the general link between PC expansions and the Sobol' indices has not been studied so far. After recalling the formalism of variance-based sensitivity methods and Sobol' decomposition, the paper proves that the computation of Sobol' indices of a surrogate PC model is *analytical*. Thus the computational burden reduces to that of computing efficiently the PC coefficients. An original regression-based method is introduced, for which an experimental design of minimal size is proposed.

Application examples are finally presented using: (a) analytical well-known models used in the literature on global SA for benchmarking, and (b) a stochastic finite element model for a foundation problem.

2. Variance-based methods and Sobol' decomposition

Let us consider a mathematical model having n input parameters gathered in a input vector $\boldsymbol{x}$, and a scalar output y:

$$y = f(\boldsymbol{x}), \quad \boldsymbol{x} \in K^n, \tag{1}$$

where the input parameters are defined on the n-dimensional unit cube K^n:

$$K^n = \{\boldsymbol{x}: 0 \leqslant x_i \leqslant 1, i = 1, \ldots, n\}. \tag{2}$$

The Sobol' decomposition of $f(\boldsymbol{x})$ into summands of increasing dimension reads [7]:

$$f(x_1, \ldots, x_n) = f_0 + \sum_{i=1}^{n} f_i(x_i) + \sum_{1 \leqslant i < j \leqslant n} f_{ij}(x_i, x_j) + \cdots + f_{1,2,\ldots,n}(x_1, \ldots, x_n), \tag{3}$$

where f_0 is a constant and the integral of each summand $f_{i_1,\ldots,i_s}(x_{i_1}, \ldots, x_{i_s})$ over any of its independent variables is zero, i.e.:

$$\int_0^1 f_{i_1,\ldots,i_s}(x_{i_1}, \ldots, x_{i_s})\, \mathrm{d}x_{i_k} = 0 \quad \text{for } 1 \leqslant k \leqslant s. \tag{4}$$

The classical properties of this decomposition are the following [33]:

- The sum in Eq. (3) contains a number of summands equal to
$$\sum_{j=1}^{n} \binom{n}{j} = 2^n - 1. \tag{5}$$
- The constant f_0 is the mean value of the function:
$$f_0 = \int_{K^n} f(\boldsymbol{x})\, \mathrm{d}\boldsymbol{x}, \tag{6}$$
where $\mathrm{d}\boldsymbol{x}$ stands for $\mathrm{d}x_1, \ldots, \mathrm{d}x_n$ for the sake of simplicity.
- Due to Eq. (4), the summands are orthogonal to each other in the following sense:
$$\int_{K^n} f_{i_1,\ldots,i_s}(x_{i_1}, \ldots, x_{i_s})\, f_{j_1,\ldots,j_t}(x_{j_1}, \ldots, x_{j_t})\, \mathrm{d}\boldsymbol{x} = 0 \quad \text{for } \{i_1, \ldots, i_s\} \neq \{j_1, \ldots, j_t\}. \tag{7}$$

With the above assumptions, the decomposition in Eq. (3) is *unique* whenever $f(\boldsymbol{x})$ is integrable over K^n. Moreover, the terms in the decomposition may be derived analytically. Indeed, the univariate terms read:

$$f_i(x_i) = \int_{K^{n-1}} f(\boldsymbol{x})\, \mathrm{d}\boldsymbol{x}_{\sim i} - f_0. \tag{8}$$

In this expression, $\int_{K^{n-1}} \mathrm{d}\boldsymbol{x}_{\sim i}$ denotes the integration over all variables except x_i. Similarly, the bivariate terms read:

$$f_{ij}(x_i, x_j) = \int_{K^{n-2}} f(\boldsymbol{x})\, \mathrm{d}\boldsymbol{x}_{\sim \{ij\}} - f_i(x_i) - f_j(x_j) - f_0. \tag{9}$$

Here again, $\int_{K^{n-2}} \mathrm{d}\boldsymbol{x}_{\sim\{ij\}}$ denotes the integration over all parameters except x_i and x_j. More generally, the symbol "$\sim$" means "complementary of" in the sequel. Following this construction, any summand $f_{i_1,\ldots,i_s}(x_{i_1},\ldots,x_{i_s})$ may be written as the difference of a multidimensional integral and summands of lower order.

Consider now that the input parameters are independent random variables uniformly distributed in $[0,1]$:

$$\boldsymbol{X} = \{X_1,\ldots,X_n\}, \quad X_i \sim \mathscr{U}(0,1), \ \ i = 1,\ldots,n. \tag{10}$$

As a consequence, the model response $Y = f(\boldsymbol{X})$ is a random variable, whose variance D (also called *total* variance in the literature on global sensitivity) reads:

$$D = \mathrm{Var}[f(\boldsymbol{X})] = \int_{K^n} f^2(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} - f_0^2. \tag{11}$$

By integrating the square of Eq. (3) and by using (7), it is possible to decompose the total variance (11) as follows:

$$D = \sum_{i=1}^{n} D_i + \sum_{1\leqslant i<j\leqslant n} D_{ij} + \cdots + D_{1,2,\ldots,n}, \tag{12}$$

where the *partial variances* appearing in the above expansion read:

$$D_{i_1,\ldots,i_s} = \int_{K^s} f^2_{i_1,\ldots,i_s}(x_{i_1},\ldots,x_{i_s})\,\mathrm{d}x_{i_1},\ldots,\mathrm{d}x_{i_s}, \quad 1\leqslant i_1<\cdots<i_s\leqslant n, \ \ s=1,\ldots,n. \tag{13}$$

The Sobol' indices are defined as follows:

$$S_{i_1,\ldots,i_s} = D_{i_1,\ldots,i_s}/D. \tag{14}$$

By definition, according to (12), they satisfy

$$\sum_{i=1}^{n} S_i + \sum_{1\leqslant i<j\leqslant n} S_{ij} + \cdots + S_{1,2,\ldots,n} = 1. \tag{15}$$

Thus, each index $S_{i_1,\ldots,i_s}$ is a sensitivity measure describing which amount of the total variance is due to the uncertainties in the set of input parameters $\{i_1,\ldots,i_s\}$. The first order indices S_i give the influence of each parameter taken alone whereas the higher order indices account for possible mixed influence of various parameters.

The *total sensitivity indices* S_{T_i} have been defined in order to evaluate the total effect of an input parameter [33]. They are defined as the sum of all partial sensitivity indices $D_{i_1,\ldots,i_s}$ involving parameter i:

$$S_{T_i} = \sum_{\mathscr{I}_i} D_{i_1,\ldots,i_s}, \quad \mathscr{I}_i = \{(i_1,\ldots,i_s)\colon \exists k, 1\leqslant k\leqslant s, i_k = i\}. \tag{16}$$

It is easy to show that:

$$S_{T_i} = 1 - S_{\sim i}, \tag{17}$$

where $S_{\sim i}$ is the sum of all $S_{i_1,\ldots,i_s}$ that do *not* include index i.

The Sobol' indices are usually computed using Monte Carlo simulation. From Eqs. (6) and (11), the following estimates of the mean value, total and partial variance can be derived using N_{sim} samples [2]:

$$\hat{f}_0 = \frac{1}{N_{sim}}\sum_{m=1}^{N_{sim}} f(\boldsymbol{x}_m), \tag{18}$$

$$\hat{D} = \frac{1}{N_{sim}}\sum_{m=1}^{N_{sim}} f^2(\boldsymbol{x}_m) - \hat{f}_0^2, \tag{19}$$

$$\hat{D}_i = \frac{1}{N_{sim}}\sum_{m=1}^{N_{sim}} f(\boldsymbol{x}^{(1)}_{(\sim i)m}, x^{(1)}_{im}) f(\boldsymbol{x}^{(2)}_{(\sim i)m}, x^{(1)}_{im}) - \hat{f}_0^2. \tag{20}$$

In the latter equations, $\boldsymbol{x}_m = (x_{1m}, x_{2m}, \ldots, x_{nm})$ denotes the mth sample point and:

$$\boldsymbol{x}_{(\sim i)m} = (x_{1m}, x_{2m}, \ldots, x_{(i-1)m}, x_{(i+1)m}, \ldots, x_{nm}). \tag{21}$$

Moreover the superscripts (1) and (2) in Eq. (20) indicate that two different samples are generated and mixed. A similar expression allows to estimate in a single shot the total sensitivity index S_{T_i}:

$$\hat{D}_{\sim i} = \frac{1}{N_{sim}}\sum_{m=1}^{N_{sim}} f(\boldsymbol{x}^{(1)}_{(\sim i)m}, x^{(1)}_{im}) f(\boldsymbol{x}^{(1)}_{(\sim i)m}, x^{(2)}_{im}) - \hat{f}_0^2, \quad \hat{S}_{T_i} = 1 - \hat{D}_{\sim i}/\hat{D}. \tag{22}$$

The Sobol' indices are known to be good descriptors of the sensitivity of the model to its input parameters, since they do not suppose any kind of linearity or monotonicity in the model. However, the full description requires the evaluation of 2^n Monte Carlo integrals, which is not practically feasible unless n is low. In practice, the analyst often computes the first-order and total sensitivity indices, sometimes the second order ones. Note that the first-order indices are equivalent to the sensitivity indices obtained by the FAST method [2,5], whose computation may be more efficient. Moreover, recent work has been devoted to further reduce the computational cost in evaluating the Sobol' indices [34] and obtain "for free" additional indices, see also the accelerated estimation procedure for variance-based measures in [35]. Nevertheless, the computational cost of evaluating *all* the indices by Monte Carlo simulation remains an issue.

3. Polynomial chaos expansion (PCE) of the response

The so-called *PC* decomposition has been developed back in the 30s by Wiener [36]. It has been brought back in the engineering field by Ghanem et al. in the so-called *spectral stochastic finite element analysis* [16]. According to this representation, any second-order random variable may be expanded as follows:

$$Z = \sum_{j=0}^{\infty} Z_j \Psi_j(\{\xi_n\}_{n=1}^{\infty}). \tag{23}$$

In this expression, $\{\xi_n\}_{n=1}^{\infty}$ are independent standard normal random variables and Ψ_j's are the multivariate Hermite polynomials. The set of Ψ_j's is orthogonal with respect to the Gaussian measure. According to the

Cameron–Martin theorem [37], the expansion in Eq. (23) is convergent in the L_2-sense.

The representation in Eq. (23) is useful for dealing with stochastic boundary value problems where input quantities (e.g. coefficients of the stochastic partial differential equations) are random fields. This is the viewpoint of the original work by Ghanem et al. [16] and subsequent contributions [19,38,39].

In this paper, the stochastic models under consideration are thought as (generally nonlinear) functions of a *finite number* of input random variables gathered in a random vector $\boldsymbol{X} = \{X_1, \ldots, X_M\}$:

$$S = f(X_1, \ldots, X_M). \tag{24}$$

Following the viewpoint proposed by Soize et al. [40], the chaos representation of the response S (which is supposed to have finite variance) may be written as

$$S = \sum_{j=0}^{\infty} S_j \phi_j(X_1, \ldots, X_M), \tag{25}$$

where $\{\phi_j(X_1, \ldots, X_M)\}_{j=0}^{\infty}$ is a Hilbertian basis of the suitable Hilbert space containing the response.

When the input random variables are standard normal (the input random vector $\boldsymbol{X}$ is then denoted by $\boldsymbol{\xi}$), a possible Hilbertian basis is the family of multivariate Hermite polynomials, which are orthogonal with respect to the Gaussian measure. Using usual notation for the multivariate Hermite polynomials, Eq. (25) rewrites in this case:

$$S = \sum_{j=0}^{\infty} S_j \Psi_j(\xi_1, \ldots, \xi_M). \tag{26}$$

Eq. (26) appears similar to the Wiener–Hermite representation (23), the difference being in the finiteness of the set of basic random variables, see [40] and associated references for a detailed discussion. In practice, expansion (26) shall be truncated for computational purposes. Considering all M-dimensional Hermite polynomials of degree not exceeding p, the response may be approximated as follows:

$$S \approx \sum_{j=0}^{P-1} S_j \Psi_j(\boldsymbol{\xi}), \quad \boldsymbol{\xi} = \{\xi_1, \ldots, \xi_M\}. \tag{27}$$

The number of unknown (vector) coefficients in this summation is

$$P = \binom{M+p}{p} = \frac{(M+p)!}{M!p!}. \tag{28}$$

The practical construction of a PC of order M and degree p is described in Appendix A.

The formulation presented in [40] allows to build a Hilbertian basis of the response space whatever the joint PDF of the basic random vector $\boldsymbol{X} = \{X_1, \ldots, X_M\}$. However, the construction of such a basis may be computationally complex in the general case. In the case when the components of $\boldsymbol{X}$ are independent, a practical solution consists in transforming first each input random variable into a standard normal variable using the iso-probabilistic transform: denoting by $F_{X_i}(x_i)$ (resp. $\Phi(x)$) the CDF of X_i (resp. a standard normal variable ξ_i), the direct and inverse transform read:

$$\xi_i = \Phi^{-1} \circ F_{X_i}(x_i), \quad X_i = F_{X_i}^{-1} \circ \Phi(\xi_i). \tag{29}$$

If the input random vector has a prescribed joint PDF, it is in general not possible to transform it exactly in a standard normal random vector. However, when only marginal PDF and correlations are known, an approximate representation may be obtained by the Nataf transform [41,42].

As a conclusion, in all cases, the input random vector $\boldsymbol{X}$ may be exactly or approximately represented using a standard normal random vector $\boldsymbol{\xi}$, say:

$$\boldsymbol{X} = T(\boldsymbol{\xi}), \quad \boldsymbol{\xi} = \{\xi_1, \ldots, \xi_M\}. \tag{30}$$

Thus the truncated Hermite PC expansion of the response:

$$S = f \circ T(\boldsymbol{\xi}) \approx \sum_{j=0}^{P-1} S_j \Psi_j(\boldsymbol{\xi}). \tag{31}$$

Note that the choice of transforming the components X_i into standard normal variables (Eq. (29)) is arbitrary at this point. The use of other kinds of basic variables (e.g. uniform) and the associated *generalized PCE* is addressed later on in Section 5.

4. Computation of the response coefficients

4.1. Introduction

The historical approach to computing the response coefficients in stochastic finite element analysis is based on the minimization of the residual in the balance equation in the Galerkin sense [16,24]. This leads to a linear system whose size is the product of the number of degrees of freedom of the system (e.g. size of response vector $\boldsymbol{S}$) by the number of coefficients per response quantity, namely P. This system has a sparse structure and may be solved by appropriate techniques [43,44].

This Galerkin-like solving strategy has been qualified as *intrusive*, in the sense that it requires heavy ad hoc implementation in the finite element code. Alternatively, *non intrusive* methods have been recently proposed, namely the projection and the regression method. The former has been introduced in [45,46] in the context of seismic soil–structure interaction, [47] for problems involving stochastic constitutive relations, and [48] for the study of the eigenmodes of a spatial frame structure. It has been used since in various applications [19,20,49–51]. It is summarized in the next section. Following an early idea proposed in [52], the regression approach has been comprehensively studied in [29] and is detailed in the second next section.

4.2. Projection method

Let us consider the model as a function of the input random vector $\boldsymbol{X}$ so that any scalar response quantity S is given by

$$S = f(\boldsymbol{X}). \tag{32}$$

The *projection* method is based on the orthogonality of the PC. By pre-multiplying Eq. (26) by Ψ_i and taking the expectation of both members, it comes:

$$\mathrm{E}[S\Psi_j] = \mathrm{E}\left[\sum_{i=0}^{\infty} S_j \Psi_i \Psi_j\right]. \tag{33}$$

Due to the orthogonality of the basis, $\mathrm{E}[\Psi_i \Psi_j] = 0$ for any $i \neq j$. Thus,

$$S_j = \frac{\mathrm{E}[S\Psi_j]}{\mathrm{E}[\Psi_j^2]}. \tag{34}$$

In this expression, the denominator is known analytically (see Appendix A) and the numerator may be cast as a multidimensional integral:

$$\mathrm{E}[S\Psi_j] = \int f \circ T(\boldsymbol{\xi}) \Psi_j(\boldsymbol{\xi}) \varphi_M(\boldsymbol{\xi}) \, \mathrm{d}\boldsymbol{\xi}, \tag{35}$$

where φ_M is the M-dimensional multinormal PDF, and where the dependency of S in $\boldsymbol{\xi}$ through the iso-probabilistic transform of the input parameters $\boldsymbol{X} = T(\boldsymbol{\xi})$ (Eq. (30)) has been given for the sake of clarity.

This integral may be computed by crude Monte Carlo simulation [49] or Latin hypercube sampling [31,50]. However the number of samples required in this case should be large enough (say 10,000 for crude MCS) to get a sufficient accuracy. In case when the response S is obtained by a computationally demanding finite element model, this approach is practically not applicable.

An alternative approach presented in [19,24,51] is the use of a Gaussian quadrature scheme to evaluate the integral. Eq. (35) is computed as a weighted summation of the integrands evaluated at selected points (the so-called integration points):

$$\begin{aligned}\mathrm{E}[S\Psi_j] = \sum_{i_1=1}^{K} \cdots \sum_{i_M=1}^{K} \omega_{i_1}, \ldots, \omega_{i_M} f(\boldsymbol{X}(\xi_{i_1}, \ldots, \xi_{i_M})) \\ \times \Psi_j(\boldsymbol{X}(\xi_{i_1}, \ldots, \xi_{i_M})).\end{aligned} \tag{36}$$

In this expression, the integration points $\{\xi_{i_j}, i_j = 1, \ldots, K\}$ and weights $\{\omega_{i_j}, i_j = 1, \ldots, K\}$ in each dimension are computed using the theory of orthogonal polynomials with respect to the Gaussian measure. For a Kth order scheme, the integration points are the roots of the Kth order Hermite polynomial [53].

The proper order of the integration scheme K is selected as follows: if the response S in Eq. (27) was polynomial of order p (i.e. $S_j = 0$ pour $j \geqslant P$), the terms in the integral (35) would be of degree less than or equal to $2p$. Thus an integration scheme of order $K = p + 1$ would give the *exact* value of the expansion coefficients. We take this as a rule in the general case, where the result now is only an approximation of the true value of S_j.

As seen from Eqs. (34) and (36), the projection method allows to compute the expansion coefficients from selected evaluations of the model. Thus the method is qualified as *non intrusive* since the deterministic computation scheme (i.e. a finite element code) is used without any additional implementation or modification.

Note that in finite element analysis, the response is usually a vector (e.g. of nodal displacements, nodal stresses, etc.). The above derivations are strictly valid for a vector response $\boldsymbol{S}$, the expectation in Eq. (36) being computed component by component.

4.3. Regression method

The *regression* method is another approach to computing the response expansion coefficients. It is nothing but the regression of the exact solution S with respect to the PC basis $\{\Psi_j(\boldsymbol{\xi}), j = 1, \ldots, P-1\}$. Let us assume the following expression for a scalar response quantity S:

$$S = f(\boldsymbol{X}) = \tilde{S}(\boldsymbol{\xi}) + \varepsilon, \tag{37}$$

$$\tilde{S}(\boldsymbol{\xi}) = \sum_{j=0}^{P-1} S_j \Psi_j(\boldsymbol{\xi}), \tag{38}$$

where the residual ε is supposed to be a zero-mean variable, and $\mathscr{S} = \{S_j, j = 0, \ldots, P-1\}$ are the unknown coefficients. The minimization of the variance of the residual with respect to the unknown coefficients leads to

$$\mathscr{S} = \mathrm{Argmin}\, \mathrm{E}[(f(\boldsymbol{X}(\boldsymbol{\xi})) - \tilde{S}(\boldsymbol{\xi}))^2]. \tag{39}$$

In order to solve Eq. (39), we choose a set of N regression points in the standard normal space, say $\{\boldsymbol{\xi}^1, \ldots, \boldsymbol{\xi}^N\}$. From these points, the isoprobabilistic transform (30) gives a set of N realizations of the input vector $\boldsymbol{X}$, say $\{\boldsymbol{x}^1, \ldots, \boldsymbol{x}^N\}$. The mean-square minimization (39) leads to solve the following problem:

$$\mathscr{S} = \mathrm{Argmin} \frac{1}{N} \sum_{i=1}^{N} \left\{ f(\boldsymbol{x}^i) - \sum_{j=0}^{P-1} S_j \Psi_j(\boldsymbol{\xi}^i) \right\}^2. \tag{40}$$

Denoting by $\boldsymbol{\Psi}$ the matrix whose coefficients are given by $\boldsymbol{\Psi}_{ij} = \Psi_j(\boldsymbol{\xi}^i)$, $i = 1, \ldots, N$; $j = 0, \ldots, P-1$, and by $\mathscr{S}_{ex}$ the vector containing the exact response values computed by the model $\mathscr{S}_{ex} = \{f(\boldsymbol{x}^i), i = 1, \ldots, N\}$, the solution to Eq. (40) reads:

$$\mathscr{S} = (\boldsymbol{\Psi}^{\mathrm{T}} \boldsymbol{\Psi})^{-1} \cdot \boldsymbol{\Psi}^{\mathrm{T}} \cdot \mathscr{S}_{ex}. \tag{41}$$

The regression approach detailed above is comparable with the so-called *response surface method* used in many domains of science and engineering [54]. In this context, the set of $\{\boldsymbol{x}^1, \ldots, \boldsymbol{x}^N\}$ is the so-called *experimental design*. In Eq. (41), $\boldsymbol{\Psi}^{\mathrm{T}} \boldsymbol{\Psi}$ is the *information matrix*. Computationally speaking, it may be ill-conditioned. Thus a particular solver such as the singular value decomposition method should be employed [55].

It is now necessary to specify the choice of the experimental design. Suppose for a while that the input of the model is scalar (i.e. $M = 1$), and suppose that the approximate polynomial expansion is of degree p (i.e. $P = p + 1$). The optimal design (in the sense of the D-optimality criterion) is given by the roots of the Hermite polynomial He_{p+1}, say $\{r_1, \ldots, r_{p+1}\}$ ([56], as cited in [54,57]).

If the input vector $\boldsymbol{X}$ is now of size M, an optimal design for regression on the tensor product of the polynomial basis (up to order p) is obtained by the tensor product of the unidimensional design $\{r_1, \ldots, r_{p+1}\}$, i.e. the set of M-uplets built using all possible combinations of the roots: $\boldsymbol{r}^k = (r_{i_1}, \ldots, r_{i_M})$, $1 \leqslant i_1 \leqslant \cdots \leqslant i_M \leqslant p+1$, $k = 1, \ldots, (p+1)^M$. Note, however, that the regression problem in Eq. (38) is not exactly equivalent to the latter case, since only the multivariate polynomials of *total* degree less than p are considered in this equation (and not the full tensor product of unidimensional polynomial of degree less than p). Furthermore, the full factorial design of size $(p+1)^M$ is not practically affordable as soon as M and p increase.

This leads to the idea of selecting a subset N of M-uplets among all possible combinations. The choice of regression points that are closest to the origin is originally used in [52,58]. The authors, respectively, selected $N = P + 1$ and $N = 2(P+1)$ points. Investigations by Berveiller et al. showed that this selection schemes do not yield accurate estimations of the PC coefficients in most applications. Numerical experimentation on various examples lead to the following results [29,59]:

- The choice of *M-uplets* of roots that are *closest to the origin* is better than other selection schemes, e.g. selecting randomly the M-uplets among the full factorial design. This can be heuristically understood as follows: the points in the experimental design (which are based on the roots of the Hermite polynomials) are exactly the integration points used in Gauss–Hermite quadrature, see Eq. (36). In this equation, the points that have the greatest weight in the summation are those that are closest to the origin. Thus the idea of using the same "most important" points also for regression. Note that a weighted regression according to the weights in Eq. (36) could also be studied. This discussion can be complemented by the fact that an equivalence between the projection and regression approaches may also be proven, see [60] for details.
- An empirical rule on the optimal number of regression points could be derived:

$$N = (M-1)P. \tag{42}$$

  It was indeed observed that taking more points in the design does not improve the accuracy of the results (this accuracy being measured by comparing the statistical moments and the low quantiles of the response with reference values), although no formal proof for this result has been derived.

The empirical rule (42) allows to considerably reduce the size of the experimental design with respect to the full factorial design. However, in industrial applications for which the unit computational time of the model response is large, this number of calls to the model may still be unaffordable. In the remaining part of this section, a methodology is proposed to compute less large experimental designs (i.e. whose size N is smaller than $(M-1)P$).

A careful investigation of the solution to the regression problem Eq. (41) has shown that the number of points required for an acceptable solution is directly related to the invertibility of the information matrix $\boldsymbol{A} = \boldsymbol{\Psi}^{\mathrm{T}}\boldsymbol{\Psi}$. From this expression, it is seen the generic term of this matrix is

$$\boldsymbol{A}_{ij} = \sum_{k=1}^{N} \Psi_i(\boldsymbol{\xi}^k)\Psi_j(\boldsymbol{\xi}^k). \tag{43}$$

Thus $\boldsymbol{A}$ is a sum of N basic matrices $\boldsymbol{a}^k$, each of them having the generic term $\boldsymbol{a}^k_{ij} = \Psi_i(\boldsymbol{\xi}^k)\Psi_j(\boldsymbol{\xi}^k)$. As the $\boldsymbol{a}^k$ are square matrices of size P and unit rank, it is clear that at least P such matrices should be added in order to get $\boldsymbol{A}$ invertible. However, the sum of P such matrices is usually *not* of rank P. From this remark and the results by Berveiller et al. summarized above, the following strategy is adopted:

- The M-uplets based on the roots of the Hermite polynomials are ordered according to increasing norm.
- The information matrix is iteratively assembled until it becomes invertible according to the algorithm described in Fig. 2.

This strategy allows to define an experimental design of size $N(M,p)$ for any number of input random variables M and degree of PC expansion p. In all cases, the obtained size is smaller than the empirical rule (42). Note that the obtained information matrix, although invertible, may still be ill-conditioned, meaning that the SVD algorithm should be used.

5. PC-based Sobol' indices

5.1. Generalized PCE

Recently, other PCEs called *Wiener–Askey chaos* have been proposed in the literature [61,62]. The idea is to use

Initialization:
  $\boldsymbol{A}^1 = \boldsymbol{a}^1$
  $k = 1$
Repeat until rank($\boldsymbol{A}^k$)=P
  $k \leftarrow k + 1$
  $\boldsymbol{A}^k = \boldsymbol{A}^{k \leftarrow 1} + \boldsymbol{a}^k$
$N = k$
Return N, $\boldsymbol{A}^N$

Fig. 2. Iterative computation of the information matrix $\boldsymbol{\Psi}^{\mathrm{T}}\boldsymbol{\Psi}$ and number of regression points N.

polynomial families that are orthogonal with respect to non Gaussian probability measures. Classical results for orthogonal polynomials [61,63] allow to build e.g. Legendre polynomials for uniform distribution, Laguerre polynomials for gamma distribution, Jacobi polynomials for beta distribution, etc.

The construction of such generalized chaos is formally identical to the construction of the original Hermite chaos. First the family of orthogonal polynomials of a single random variable is determined. Then the multidimensional polynomials are generated using an appropriate algorithm (see Appendix A). A general framework that encompasses the case when the input random vector has correlated components is also given by Soize et al. [40].

In this paper, we are interested in introducing the PCE for the computation of Sobol' indices. As seen in Section 2, the input parameters are supposed to be uniformly distributed in [0,1] in the classical presentation. Thus the Legendre chaos will be used in the sequel, i.e. the Ψ_j's are from now on multivariate Legendre polynomials. Note that the Legendre polynomials are classically defined on $[-1,1]$ as shown in Appendix A. In order to keep up with this definition, the models defined on K^n are first mapped onto $[-1,1]^n$ by a linear transform of the input parameters.

5.2. Statistics of the PCE

Following the above assumptions, it is possible to represent approximately the random response $Y=f(\boldsymbol{X})$ of a system as a Legendre PCE:

$$Y=f(\boldsymbol{X})\approx f_{\mathrm{PC}}(\boldsymbol{X})=\sum_{j=0}^{P-1} f_j\Psi_j(\boldsymbol{X}),\quad \boldsymbol{X}\sim\mathscr{U}([-1,1]^n). \tag{44}$$

Due to the orthogonality of the basis, it is easy to show that the mean and variance of the response respectively read:

$$\bar{Y}=\mathrm{E}[f(\boldsymbol{X})]=f_0, \tag{45}$$

$$D_{\mathrm{PC}}=\mathrm{Var}\left[\sum_{j=0}^{P-1} f_j\Psi_j(\boldsymbol{X})\right]=\sum_{j=1}^{P-1} f_j^2\mathrm{E}[\Psi_j^2(\boldsymbol{X})]. \tag{46}$$

5.3. Sobol' decomposition of the PCE

In order to compute the sensitivity indices based on the PC decomposition of the model, it is necessary to derive the Sobol' decomposition of $f_{\mathrm{PC}}(\boldsymbol{x})=\sum_{j=0}^{P-1} f_j\Psi_j(\boldsymbol{x})$. For this purpose, let us represent each multivariate Legendre polynomial by means of a tuple $\boldsymbol{\alpha}=(\alpha_1,\ldots,\alpha_n)$, as shown in Appendix A (in the sequel, the notation Ψ_j or $\Psi_{\boldsymbol{\alpha}}$ will be used indifferently according to the context):

$$\Psi_j\equiv\Psi_{\boldsymbol{\alpha}}:\ \Psi_j(\boldsymbol{x})=\prod_{i=1}^{n} P_{\alpha_i}(x_i), \tag{47}$$

where $P_k(x)$ is the kth Legendre polynomial (See Appendix A). Let us define by $\mathscr{I}_{i_1,\ldots,i_s}$ the set of $\boldsymbol{\alpha}$ tuples such that only the indices $(i_1,\ldots,i_s)$ are nonzero:

$$\mathscr{I}_{i_1,\ldots,i_s}=\left\{\boldsymbol{\alpha}:\ \begin{array}{lll}\alpha_k>0 & \forall k=1,\ldots,n, & k\in(i_1,\ldots,i_s)\\ \alpha_j=0 & \forall k=1,\ldots,n, & k\notin(i_1,\ldots,i_s)\end{array}\right\}. \tag{48}$$

Note that $\mathscr{I}_i$ corresponds to the polynomials depending only on parameter x_i. Using this notation, the $P-1$ terms in Eq. (44) corresponding to the polynomials $\{\Psi_j, j=1,\ldots,P-1\}$ may now be gathered according the parameters they depend on:

$$\begin{aligned} f_{\mathrm{PC}}(\boldsymbol{x})=f_0&+\sum_{i=1}^{n}\sum_{\boldsymbol{\alpha}\in\mathscr{I}_i} f_{\boldsymbol{\alpha}}\Psi_{\boldsymbol{\alpha}}(x_i)\\ &+\sum_{1\leqslant i_1<i_2\leqslant n}\ \sum_{\boldsymbol{\alpha}\in\mathscr{I}_{i_1,i_2}} f_{\boldsymbol{\alpha}}\Psi_{\boldsymbol{\alpha}}(x_{i_1},x_{i_2})+\cdots\\ &+\sum_{1\leqslant i_1<\cdots<i_s\leqslant n}\ \sum_{\boldsymbol{\alpha}\in\mathscr{I}_{i_1,\ldots,i_s}} f_{\boldsymbol{\alpha}}\Psi_{\boldsymbol{\alpha}}(x_{i_1},\ldots,x_{i_s})\\ &+\cdots+\sum_{\boldsymbol{\alpha}\in\mathscr{I}_{1,2\ldots,n}} f_{\boldsymbol{\alpha}}\Psi_{\boldsymbol{\alpha}}(x_1,\ldots,x_n). \end{aligned} \tag{49}$$

In the above equation, the true dependence of each multidimensional Legendre polynomial to each subset of input parameters has been given for the sake of clarity. It is clear that each term of the form $\sum_{\boldsymbol{\alpha}\in\mathscr{I}_{i_1,\ldots,i_s}} f_{\boldsymbol{\alpha}}\Psi_{\boldsymbol{\alpha}}(x_{i_1},\ldots,x_{i_s})$ in the right-hand side is a polynomial function depending on *all* the input parameters $(i_1,\ldots,i_s)$ and *only* on them. Thus the summands in the Sobol' decomposition of $f_{\mathrm{PC}}(\boldsymbol{x})$ (see Eq. (3)) straightforwardly read:

$$f_{i_1,\ldots,i_s}(x_{i_1},\ldots,x_{i_s})=\sum_{\boldsymbol{\alpha}\in\mathscr{I}_{i_1,\ldots,i_s}} f_{\boldsymbol{\alpha}}\Psi_{\boldsymbol{\alpha}}(x_{i_1},\ldots,x_{i_s}). \tag{50}$$

Due to the uniqueness of the representation in Eq. (3), it may be concluded that Eq. (49) is *the* Sobol' decomposition of $f_{\mathrm{PC}}(\boldsymbol{x})$.

5.4. Sensitivity indices

It is now easy to derive sensitivity indices from the above representation. These indices, called *PC-based Sobol' indices* and denoted by $SU_{i_1,\ldots,i_s}$ are defined as

$$SU_{i_1,\ldots,i_s}=\sum_{\boldsymbol{\alpha}\in\mathscr{I}_{i_1,\ldots,i_s}} f_{\boldsymbol{\alpha}}^2\mathrm{E}[\Psi_{\boldsymbol{\alpha}}^2]/D_{\mathrm{PC}}. \tag{51}$$

Although the above mathematical presentation is quite a burden, the idea behind is simple: once the PC representation of the model is available (see Section 4), the response expansion coefficients are simply gathered according to the dependency of each basis polynomial, square-summed and normalized as shown in Eq. (51).

The total sensitivity indices are also easy to compute. For a given integer sequence $(j_1,\ldots,j_t)$, let us define the following set:

$$\mathscr{J}_{j_1,\ldots,j_t}=\{(i_1,\ldots,i_s),(j_1,\ldots,j_t)\subset(i_1,\ldots,i_s)\}. \tag{52}$$

The *total PC-based sensitivity indices* read:

$$SU^{\mathrm{T}}_{j_1,\ldots,j_t} = \sum_{(i_1,\ldots,i_s)\in \mathscr{I}_{j_1,\ldots,j_t}} SU_{i_1,\ldots,i_s}. \quad (53)$$

As the terms in the summation are the PC-based Sobol indices, whose analytical expression has been given above, the total sensitivity indices may be computed at almost no additional cost.

As a conclusion, this section shows that, once the PC representation of a model is available, the complete list of Sobol indices (i.e. the $2^n - 1$ indices) are available *analytically* with almost no additional cost. Indeed, only elementary mathematical operations are needed to compute these indices from the expansion coefficients $\{f_j\}_{j=1}^{P-1}$. The major computational cost of the approach is the computation of the expansion coefficients, as described in Section 4.

5.5. Tracks to further developments

The above formalism is straightforwardly extended to problems where the input parameters are modeled by random variables of any type (i.e. not of uniform type). In the general case, the system response may be represented onto the Hermite chaos expansion or any generalized PC, following the formulation in [40,61]. The computed coefficients are then gathered as described in Section 5.4. and the sensitivity indices are obtained from Eqs. (51) and (53). The only difference with respect to the previous section is that the analytical coefficients $\mathrm{E}[\Psi_j^2]$ are to be computed with respect to the PC under consideration. An application example related to the elastic analysis of a foundation by means of a Hermite PC is given in Section 6.4.

Additional information is contained in the PC expansion coefficients compared to the classical Sobol' indices. Indeed, sensitivity indices SU_i contain the dependence in input variable X_i whatever its polynomial degree. Looking directly at the terms $f_{\boldsymbol{\alpha}}^2 \mathrm{E}[\Psi_{\boldsymbol{\alpha}}^2]$ in Eq. (51) allows to find out whether the main dependence is linear, quadratic or of greater order. This is shown in an application example in Section 6.3.

6. Application examples

6.1. Example 1: polynomial model

6.1.1. Problem statement

Let us consider the following model:

$$Y = \frac{1}{2^n}\prod_{i=1}^{n}(3X_i^2 + 1), \quad (54)$$

where the input variables X_i, $i = 1, 2, n$ are uniformly distributed over $[0, 1]$. The Sobol' sensitivity indices can be computed analytically [7]:

$$S_{i_1,\ldots,i_s} = \frac{5^{-s}}{(6/5)^n - 1}, \quad s = 1, \ldots, n. \quad (55)$$

The numerical application is carried out for $n = 3$. In this case, the model is polynomial of degree 6.

6.1.2. Exact solution

Knowing *a priori* that the model is polynomial, it is interesting to investigate whether the proposed approach can give exact results. Thus a PC of order $p = 6$ is chosen. The PC expansion contains $\binom{6+3}{6} = 84$ coefficients. Using the approach described in Section 4.3, the experimental design is iteratively augmented until the information matrix is regular. A number of $N = 116$ collocation points (which are closest to the origin among the triplets of roots of Legendre polynomials) is found to be necessary.

Using this experimental design, the following *exact values* of the sensitivity indices are found (12-digit accuracy):

$$\begin{aligned} &S_1 = S_2 = S_3 = 25/91 \ (0.2747),\\ &S_{12} = S_{23} = S_{13} = 5/91 \ (0.0549),\\ &S_{123} = 1/91 \ (0.0110). \end{aligned} \quad (56)$$

6.1.3. Blind solution

In practice, the analyst hardly ever knows the true form of the model, when the latter is an algorithmic sequence. Thus the degree of approximation of the PCE has to be chosen *a priori*. We consider here three cases, namely $p = 3, 4, 5$. In each case, the experimental design is built iteratively according to Section 4.3, until the information matrix is nonsingular. The number N of regression points required for this purpose is reported in Table 1.

From the above results, it appears that the less accurate solution ($p = 3$) already provides a good estimation of the sensitivity indices, since the relative error (compared to the exact solution) is less than 5% for the first-order indices, 12% for the second-order indices and 25% for the third-order index (which is close to zero). These results are obtained at a cost of 29 calls to the model evaluation. Using a fourth order PCE ($p = 4$), these relative errors decrease down to 1%, 4% and 2%, respectively, at a cost

Table 1
Example 1—Polynomial model—influence of the degree of the PC representation

Sensitivity index	Order of PC expansion			
	$p = 3$	$p = 4$	$p = 5$	$p = 6$[a]
SU_1	0.2879	0.2725	0.2747	0.2747
SU_2	0.2773	0.2733	0.2747	0.2747
SU_3	0.2773	0.2737	0.2747	0.2747
SU_{12}	0.0506	0.0564	0.0550	0.0549
SU_{13}	0.0506	0.0564	0.0550	0.0549
SU_{23}	0.0481	0.0569	0.0550	0.0549
SU_{123}	0.0081	0.0108	0.0110	0.0110
P	20	35	56	84
N	29	44	77	116

[a]The values obtained for $p = 6$ are the exact analytical values.

of 44 calls to the model evaluation. Finally, the relative error obtained with $p = 5$ is less than 0.1% for all sensitivity indices at a cost of 77 calls to the model evaluation. Note that the *exact values* are obtained as soon as the degree of the PCE is that of the true response function.

6.2. Example 2: Ishigami function

Let us consider now the so-called Ishigami function [2, Chapter 2]:

$$Y = \sin X_1 + a \sin^2 X_2 + b X_3^4 \sin X_1, \tag{57}$$

where the input variables $X_i, i = 1, 2, 3$ are uniformly distributed over $[-\pi, \pi]$. This function, which is nonlinear and nonmonotonic has been used in the literature to benchmark sensitivity methods. The variance D of Y and the Sobol' sensitivity indices can be computed analytically [64]:

$$\begin{aligned} D &= \frac{a^2}{8} + \frac{b\pi^4}{5} + \frac{b^2\pi^8}{18} + \frac{1}{2}, \\ D_1 &= \frac{b\pi^4}{5} + \frac{b^2\pi^8}{50} + \frac{1}{2}, \quad D_2 = \frac{a^2}{8}, \quad D_3 = 0, \\ D_{12} &= D_{23} = 0, \quad D_{13} = \frac{8b^2\pi^8}{225}, \quad D_{123} = 0. \end{aligned} \tag{58}$$

The application example is carried out using the numerical values $\{a = 7, b = 0.1\}$. PC expansions of increasing degree ($p = 3, 5, 7, 9$) are used. Since the number of input random variables is equal to 3, the PC expansions contain $P = 20$, 56, 120, 220 unknown coefficients, respectively. The corresponding minimal number of regression points used according to Section 4.3 is $N = 29$, 77, 157, 291, respectively. The results are gathered in Table 2.

It is observed that the respective influence of X_2 and (X_1, X_3) is miscomputed if the PC degree is too low. However, convergence is obtained as soon as $p \geqslant 7$. Note that the zero value indices are computed exactly, even at a low degree of expansion.

It may now be useful to decompose the unidimensional indices according to the increasing powers of the related input variable. Let us look as an example at the decomposition of SU_1 according to Eq. (51), in the case when $p = 7$ ($SU_1 = 0.3114$). The coefficients $f_{\boldsymbol{\alpha}}$ that contribute to SU_1 correspond to the basis polynomials of the form X_1^q, $q = 1, \ldots, 7$. The corresponding contribution are $\{0.1364, 0.0000, 0.1736, 0.0000, 0.0014, 0.0000, 0.0000\}$ respectively (which add up to 0.3114). Looking at the nonzero contributions, it is clear that the dependence of the model in X_1 is an odd function, and that it is mainly the sum of a linear and a cubic term, the latter being predominant.

If we consider now $SU_2 = 0.4434$, the contributions of the terms of increasing power of X_2 are $\{0.0000, 0.0267, 0.0000, 0.2868, 0.0000, 0.1299, 0.0000\}$. It appears here that the dependence of the model in X_2 is an even function with a main contribution in X_2^4.

Table 2
Example 2—Ishigami function—influence of the degree of the PC representation

Index	Analytical value	Order of PC expansion			
		$p = 3$	$p = 5$	$p = 7$	$p = 9$
SU_1	0.3138	0.3941	0.3550	0.3114	0.3146
SU_2	0.4424	0.1330	0.1846	0.4434	0.4396
SU_3	0	0.0000	0.0000	0.0000	0.0000
SU_{12}	0	0.0000	0.0000	0.0000	0.0000
SU_{13}	0.2436	0.4729	0.4603	0.2452	0.2459
SU_{23}	0	0.0000	0.0000	0.0000	0.0000
SU_{123}	0	0.0000	0.0000	0.0000	0.0000
SU_1^{T}	0.5574	0.8670	0.8154	0.5566	0.5604
SU_2^{T}	0.4424	0.1330	0.1846	0.4434	0.4396
SU_3^{T}	0.2436	0.4729	0.4603	0.2452	0.2459
# Unknown coefficients P		20	56	120	220
# Regression points N		29	77	157	291

As a conclusion, this academic example shows the potential of the PC-based SA to investigate the dependencies of the response with respect to the input parameters in a manner deeper than the usual Sobol' indices. Note that this problem is particularly challenging in SA. Indeed all three input variables are important, either when taken alone (e.g. X_1) or as a couple (e.g. (X_1, X_3)). This is an uncommon situation in real engineering problems, and this is the reason why a relatively high order of expansion ($p = 7$) is required to get accurate results. Despite these difficulties, the proposed approach allows to find the analytical solution if the degree of expansion is sufficiently large.

6.3. Example 3: Sobol' function

Let us consider now the so-called Sobol' function [65]:

$$Y = \prod_{i=1}^{q} \frac{|4X_i - 2| + a_i}{1 + a_i}, \tag{59}$$

where the input variables X_i, $i = 1, \ldots, q$ are uniformly distributed over $[0, 1]$ and a_i's are nonnegative. The variance D of Y and the Sobol' sensitivity indices can be computed analytically.

$$D = \prod_{i=1}^{q} (D_i + 1) - 1, \quad D_i = \frac{1}{3(1 + a_i)^2}, \tag{60}$$

$$S_{i_1, \ldots, i_s} = \frac{1}{D} \prod_{i=1}^{s} D_i. \tag{61}$$

For numerical application, $q = 8$ is selected together with $\boldsymbol{a} = [1, 2, 5, 10, 20, 50, 100, 500]$. It is intended to show that the few important variables in this model are catched by a low-order PC analysis. For this purpose, a second order PC

expansion is used ($p=2$). There are $P=\binom{8+2}{2}=45$ unknown coefficients in the PC expansion. The regression method requires 72 regression points. Results are reported in Table 3, together with the analytical Sobol' indices.

It clearly appears from the numbers in Table 3 that only the three or four first parameters have a significant influence on the response variance. Thus an approximate model is now built by representing the first four parameters $\{X_1, X_2, X_3, X_4\}$ as random variables uniformly distributed over $[0,1]$, and by setting $X_5 = X_6 = X_7 = X_8 = \frac{1}{2}$ (i.e. their mean value). The PC-based SA is carried out using this simplified model ($M=4$) together with different values of p. The results are reported in Table 4, as well as the number of unknown coefficients P and regression points N used in each case.

It appears that the simplified model provides a two-digit accuracy in the first order, second order, and total Sobol' indices, as soon as the PC degree is greater than 5. Considering here only those indices that are greater than 0.1, a maximal relative error of 3.8% is observed when using $p=5$ (this relative error is computed by comparison to the analytical indices obtained from the 8-parameter model, which are recalled in Table 4, Column #2). This error reduces to less than 1% when using $p=7$. Greater relative errors are observed for other indices, which is however not a problem since the absolute value of these indices make the associated input variable unimportant.

Table 3
Example 3—Sobol' function—analytical and PC-based Sobol' indices ($p=2$)

Index	Analytical solution	PC-based solution ($p=2$)
SU_1	0.6037	0.5986
SU_2	0.2683	0.3045
SU_3	0.0671	0.0426
SU_4	0.0200	0.0091
SU_5	0.0055	0.0041
SU_6	0.0009	0.0034
SU_7	0.0002	0.0001
SU_8	0.0000	0.0002
$SU_{1,2}$	0.0224	0.0140
$SU_{1,3}$	0.0056	0.0004
$SU_{1,4}$	0.0017	0.0005
$SU_{1,5}$	0.0005	0.0015
$SU_{1,6}$	0.0001	0.0019
$SU_{1,7}$	0.0000	0.0000
$SU_{1,8}$	0.0000	0.0000
SU_1^T	0.6342	0.6170
SU_2^T	0.2945	0.3229
SU_3^T	0.0756	0.0473
SU_4^T	0.0227	0.0140
SU_5^T	0.0062	0.0122
SU_6^T	0.0011	0.0129
SU_7^T	0.0003	0.0055
SU_8^T	0.0000	0.0057

Table 4
Example 3—Sobol' function—approximated model with four parameters—PC-based Sobol' indices

Index	Full model (eight parameters)	Approximate model (four parameters)		
	Analytical	$p=3$	$p=5$	$p=7$
SU_1	0.6037	0.6644	0.5994	0.5999
SU_2	0.2683	0.2616	0.2748	0.2677
SU_3	0.0671	0.0581	0.0676	0.0729
SU_4	0.0200	0.0164	0.0198	0.0226
$SU_{1,2}$	0.0224	0.0000	0.0283	0.0191
$SU_{1,3}$	0.0056	0.0000	0.0058	0.0069
$SU_{1,4}$	0.0017	0.0000	0.0016	0.0023
$SU_{2,3}$	0.0004	0.0000	0.0021	0.0043
$SU_{2,4}$	0.0005	0.0000	0.0006	0.0013
$SU_{3,4}$	0.0005	0.0000	0.0001	0.0004
SU_1^T	0.6342	0.6644	0.6350	0.6308
SU_2^T	0.2945	0.2611	0.3057	0.2950
SU_3^T	0.0756	0.0581	0.0756	0.0866
SU_4^T	0.0227	0.0164	0.0220	0.0272
# Unknown coefficients P		35	126	330
# Regression points N		73	233	533

As a conclusion, using the two-step strategy, the main sensitivity indices (i.e. greater than 0.1) of the original eight-parameter model could be evaluated with a relative accuracy of 3–4% at a cost of $72+233=305$ model evaluations.

6.4. Example 4: finite element model of a foundation

Let us consider an elastic soil mass made of two layers of different isotropic linear elastic materials lying on a rigid substratum. A foundation on this soil mass is modeled by a uniform pressure P_1 applied over a length $2B_1 = 10\,\mathrm{m}$ of the free surface. An additional load P_2 is applied over a length $2B_2 = 5\,\mathrm{m}$ (Fig. 3a).

Due to the symmetry, half of the structure is modeled by finite element (Fig. 3b). The mesh comprises 80 QUAD4 elements. The model parameters are listed in Table 5. The geometry is considered as deterministic. Only the elastic material properties and the applied loads are random parameters, whose PDF are specified in Table 5. All six random variables are supposed to be independent.

The model response of interest is the maximum settlement, i.e. the vertical displacement of the upper-left node of the mesh. This displacement v_A is an algorithmic function f_{FE} of the six input parameters:

$$v_A = f_{FE}(E_1, E_2, \nu_1, \nu_2, P_1, P_2). \tag{62}$$

The PC-based Sobol' indices of v_A are computed using a PC expansion of degree $p=2$ (resp. $p=3$). The usual total Sobol' indices are obtained by Monte Carlo simulation as described in Section 2 using $N_{sim} = 10,000$ samples.

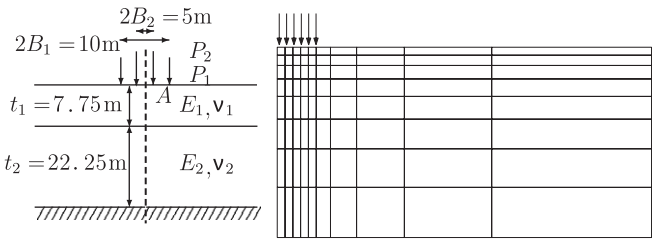

Fig. 3. Example 4: foundation on a two-layer soil layer mass: scheme of the foundation (left); and mesh (right).

Table 5
Two-layer soil layer mass: parameters of the model

Parameter	Notation	Type of PDF	Mean value	Coef. of variation (%)
Upper layer soil thickness	t_1	Deterministic	7.75 m	–
Lower layer soil thickness	t_2	Deterministic	22.25 m	–
Upper layer Young's modulus	E_1	Lognormal	50 MPa	20
Lower layer Young's modulus	E_2	Lognormal	100 MPa	20
Upper layer Poisson's ratio	ν_1	Uniform	0.3	15
Lower layer Poisson's ratio	ν_2	Uniform	0.3	15
Load #1	P_1	Gamma	0.2 MPa	20
Load #2	P_2	Weibull	0.4 MPa	20

Table 6
Example 4: foundation on a two-layer soil layer mass—PC-based Sobol' indices and Monte Carlo-based Sobol' indices

Index	Approximate model		Monte Carlo simulation (10,000 samples)
	$p = 2$	$p = 3$	
SU_1	0.3944	0.3849	–
SU_2	0.0360	0.0460	–
SU_3	0.1049	0.1018	–
SU_4	0.0010	0.0011	–
SU_5	0.1553	0.1561	–
SU_6	0.2938	0.2969	–
$SU_{1,2}$	0.0028	0.0020	–
$SU_{1,3}$	0.0000	0.0000	–
$SU_{1,4}$	0.0000	0.0000	–
$SU_{1,5}$	0.0037	0.0023	–
$SU_{1,6}$	0.0059	0.0058	–
$SU_{2,3}$	0.0000	0.0000	–
$SU_{2,4}$	0.0000	0.0000	–
$SU_{2,5}$	0.0002	0.0004	–
$SU_{2,6}$	0.0002	0.0006	–
$SU_{3,4}$	0.0001	0.0000	–
$SU_{3,5}$	0.0009	0.0010	–
$SU_{3,6}$	0.0008	0.0010	–
$SU_{4,5}$	0.0000	0.0000	–
$SU_{4,6}$	0.0000	0.0000	–
$SU_{5,6}$	0.0000	0.0000	–
SU_1^{T}	0.4068	0.3951	$ST_1 = 0.3844$
SU_2^{T}	0.0392	0.0490	$ST_2 = 0.0424$
SU_3^{T}	0.1067	0.1039	$ST_3 = 0.0684$
SU_4^{T}	0.0010	0.0011	$ST_4 = 0.0030$
SU_5^{T}	0.1601	0.1597	$ST_5 = 0.1827$
SU_6^{T}	0.3007	0.3044	$ST_6 = 0.2520$

From the results in Table 6, it is concluded that the second- and third-order PC expansion provide almost the same results, at a respective cost of 72 and 417 evaluations of the model function. The Monte Carlo simulation provides similar results at a cost of 70,000 evaluations of the model function (for each sample, there is one evaluation of the model which enters the computation of the mean value $\hat{f}_0$ and as many evaluations of the model as the number of model parameters for computing the total indices). The important parameters are ranked in the same order by both methods, i.e. Young's modulus of the upper layer, load #2, load #1, Young's modulus of the lower layer. The Poisson's ratio of both layers appear unimportant in the decomposition of the response of the variance.

Slight discrepancies in the values of certain indices are observed (this is due to the statistical uncertainty associated with Monte Carlo simulation). In order to check if the Monte Carlo simulation is accurate, the evolution of the estimates of the total Sobol' indices with respect to the number of simulation is plotted in Fig. 4. This figure shows that 10,000 samples may not be enough to get converged results. This implies that the most accurate results in Table 6 are probably those obtained by the PC expansion, although they are based on an approximate model.

Fig. 4 also shows that the number of simulation required to get at least the correct ordering of the important variables is already large (around 5000 samples). In particular, if the simulation had been limited to 3000 samples (i.e. 21,000 calls to the model function), the relative role of variables #1 (Young's modulus of the upper layer) and #6 (Load $P2$) would have been misunderstood.

As a conclusion, this example shows that the PC-based Sobol' indices are able to evaluate the global sensitivity of a finite element model, whatever the PDF of the input parameters, at a cost which is 3–4 orders of magnitude lower than the usual Monte Carlo-based Sobol' indices. Moreover, the PC-based indices, even computed with a low-order PC expansion (such as $p = 2$) appear more reliable than the Monte Carlo based indices, when a sample set of limited size is used due to computation cost.

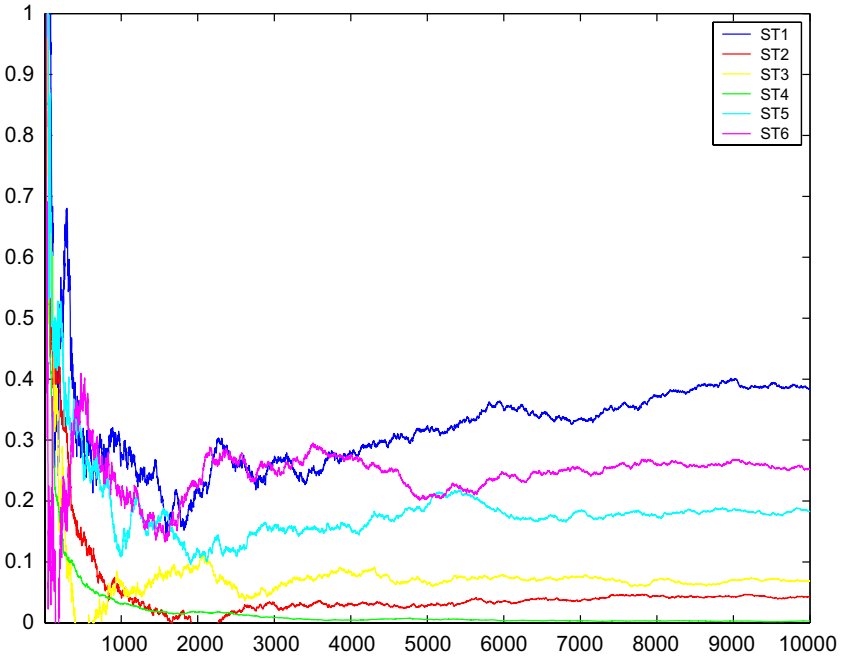

Fig. 4. Example 4: foundation on a two-layer soil layer mass—convergence of the Monte Carlo simulation of the total Sobol' indices.

7. Conclusions

SA has received much attention in the literature in the past decade. Versatile sensitivity indices for nonlinear nonmonotonic problems are known to be based on Sobol' decomposition of functions. However, the usual way to compute practically the Sobol' indices is Monte Carlo simulation, which is unaffordable when the model under consideration is a time-consuming algorithmic sequence (e.g. finite element code).

On the other hand, the PCEs have proven efficiency and accuracy in computational stochastic mechanics. The aim of this paper is to make a bridge between these approaches. It is shown that the computation of Sobol' indices after a proper PC expansion is *analytical*. The computation cost is thus transferred to the obtention of the PC coefficients, the subsequent post-processing being almost costless.

Two methods are presented for computing the PC expansion coefficients from selected *deterministic* evaluations of the model function, namely the projection and the regression method. For the second one, which is similar to a response surface method in the probabilistic space, a strategy is proposed, which aims at limiting the number of model evaluation, in order to make the approach applicable to time-consuming computational models.

The approach is applied to several benchmark problems found in the literature on SA. This allows to demonstrate the accuracy of the proposed approach and its efficiency (limited number of model evaluations compared to Monte Carlo simulation). Indeed, a full set of Sobol' indices are obtained in tens to a few hundred evaluations of the function in the presented applications, which is 2–4 orders of magnitude less than the usual computational cost of Sobol' indices.

The method is particularly efficient when the number of random input parameters is low, say less than 10, while the cost of each model evaluation is large, making the use of direct Monte Carlo simulation unaffordable.

In case of problems having a large number of input parameters, the proposed regression method may be computationally expensive. However, it is always possible to compute the PC expansion coefficients using the *projection method* (see Section 4.2) together with Monte Carlo simulation. The advantage of using MCS for computing the PC coefficients instead of directly computing the Sobol' indices is that a single set of, say 5000–10,000 samples (i.e. 5000–10,000 model evaluations), will allow to compute *all* PC expansion coefficients, and thus all sensitivity indices by an analytical post-processing (whatever the number of input parameters). The statistical uncertainty on the evaluated PC coefficients (whose estimates are normally distributed) may then be propagated to the sensitivity indices.

It has been shown in Example 3 that a two-step strategy may be successfully applied using the PC expansions: first, a low order expansion (say, $p = 2$) allows to find the most important variables; second, a higher order expansion (say, $p = 5$) of a reduced model allows to compute the main sensitivity indices. This two-step strategy should be further improved. It may eventually be possible to extend iteratively the PC basis starting from a low order expansion *only* along the relevant dimensions.

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Appendix A

A.1. Orthogonal polynomials

Several families of univariate polynomials are of current use in the theory of numerical integration [53]. We focus here on two families, namely the Legendre and Hermite polynomials.

A.1.1. Legendre polynomials

The Legendre polynomials $P_n(x)$ are solution of the following differential equation:

$$(1-x^2)y'' - 2xy' + n(n+1)y = 0, \quad n \in \mathbb{N}. \tag{63}$$

They may be generated in practice by the following recurrence relationship:

$$P_0(x) = 1, \tag{64}$$

$$(n+1)P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x). \tag{65}$$

They are orthogonal with respect to the uniform probability measure over $[-1,1]$:

$$\int_{-1}^{1} P_m(x)P_n(x)\,\mathrm{d}x = \frac{2}{2n+1}\delta_{mn}, \tag{66}$$

where δ_{mn} is the Kronecker symbol: $\delta_{mn} = 1$ if $m = n$ and 0 otherwise. If U is a random variable with uniform PDF over $[-1,1]$, the following relationship holds:

$$\mathrm{E}[P_m(U)P_n(U)] = \frac{1}{2n+1}\delta_{mn}, \tag{67}$$

where E[.] is the mathematical expectation. The first three Legendre polynomials are

$$P_1(x) = x, \quad P_2(x) = \tfrac{1}{2}(3x^2-1), \quad P_3(x) = \tfrac{1}{2}(5x^3-3x). \tag{68}$$

A.1.2. Hermite polynomials

The Hermite polynomials $He_n(x)$ are solution of the following differential equation:

$$y'' - xy' + ny = 0, \quad n \in \mathbb{N}. \tag{69}$$

They may be generated in practice by the following recurrence relationship:

$$He_0(x) = 1, \tag{70}$$

$$He_{n+1}(x) = xHe_n(x) - nHe_{n-1}(x). \tag{71}$$

They are orthogonal with respect to the Gaussian probability measure:

$$\int_{-\infty}^{\infty} He_m(x)He_n(x)\varphi(x)\,\mathrm{d}x = n!\delta_{mn}, \tag{72}$$

where $\varphi(x) = 1/\sqrt{2\pi}e^{-x^2/2}$ is the standard normal PDF. If ξ is a standard normal random variable, the following relationship holds:

$$\mathrm{E}[He_m(\xi)He_n(\xi)] = n!\delta_{mn}. \tag{73}$$

The first three Hermite polynomials are

$$He_1(x) = x, \quad He_2(x) = x^2 - 1, \quad He_3(x) = x^3 - 3x. \tag{74}$$

A.2. Construction of the PC

Let us consider a family of univariate polynomials $\{K_n(x), n \in \mathbb{N}\}$. The generalized PC of order M and degree p based on this family is the set of multivariate polynomials obtained by products of univariate polynomials so that the maximal degree is less than or equal to than p. Let us define the following integer sequence $\boldsymbol{\alpha}$:

$$\boldsymbol{\alpha} = \{\alpha_i, i = 1,\ldots,M\}, \quad \alpha_i \geqslant 0, \quad \sum_{i=1}^{M} \alpha_i \leqslant p. \tag{75}$$

The multivariate polynomial $\Psi_{\boldsymbol{\alpha}}$ is defined by

$$\Psi_{\boldsymbol{\alpha}}(x_1,\ldots,x_M) = \prod_{i=1}^{M} K_{\alpha_i}(x_i). \tag{76}$$

The number of such polynomials of degree not exceeding p is

$$P = \frac{(M+p)!}{M!p!}. \tag{77}$$

An original algorithm to determine the set of $\boldsymbol{\alpha}$'s is detailed in [26]. Let $\boldsymbol{Z}$ be a random vector of size M, whose components are independent and distributed according to the PDF related to the family $\{K_n(x), n \in \mathbb{N}\}$. It is clear that

$$\mathrm{E}[\Psi_{\boldsymbol{\alpha}}\Psi_{\boldsymbol{\beta}}] = \prod_{i=1}^{M} \mathrm{E}[K_{\alpha_i}(Z_i)K_{\beta_i}(Z_i)] = \delta_{\boldsymbol{\alpha}\boldsymbol{\beta}} \prod_{i=1}^{M} \mathrm{E}[K^2_{\alpha_i}(Z_i)]. \tag{78}$$

The latter equation shows that the PC basis is orthogonal.

More generally, if $\boldsymbol{Z}$ is a random vector with independent components, each of them having a prescribed PDF, it is possible to define a generalized PC by tensor products of the univariate polynomials of each related family [61].

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