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POLYNOMIAL CHAOS EXPANSIONS AND STOCHASTIC  
FINITE ELEMENT METHODS

B.Sudret



## Data Sheet

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# Polynomial chaos expansions and stochastic finite element methods

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## 1 Introduction

Soil and rock masses naturally present heterogeneity at various scales of description. This heterogeneity may be of two kinds. At a large scale soil properties may be considered piecewise homogeneous once regions (*e.g.* layers) have been identified. At a lower scale the local spatial variability of the properties shall be accounted for. In any case, the use of deterministic values for representing the soil characteristics is poor, since it ignores the natural randomness of the medium. Alternatively, this randomness may be properly modelled using probabilistic models.

In the first of the two cases identified above, the material properties (*e.g.* Young's modulus, cohesion, friction angle, etc.) may be modelled in each region as *random variables* whose distributions (and possibly mutual correlation) have to be specified. In the second case, the introduction of random fields is necessary. In this respect probabilistic soil modelling is a long-term story, see *e.g.* Vanmarcke (1977); DeGroot and Baecher (1993); Fenton (1999a,b); Rackwitz (2000); Popescu et al. (2005).

Usually soil characteristics are investigated in order to feed models of geotechnical structures in the context of engineering design. Examples of such structures are dams, embankments, pile or raft foundations, tunnels, etc. The design then consists in choosing characteristics of the structure (dimensions, material properties) so that the latter fulfills some requirements (*e.g.* retain water, support a building, etc.) under a given set of environmental actions that we will call "loading". The design is practically carried out by satisfying some *design criteria* which usually apply onto model response quantities (*e.g.* global equilibrium equation, settlements, bearing capacity, etc.). The conservatism of the design according to codes of practice is ensured first by introducing safety coefficients,

second by using penalized values of the model parameters. In this approach, the natural spatial variability of the soil is completely hidden.

From another point of view, when the uncertainties and variability of the soil properties have been identified, methods that allow to *propagate* these uncertainties throughout the model have to be used. Perturbation methods used in the 80's and 90's (Baecher and Ingra, 1981; Phoon et al., 1990) allow to estimate the mean value and standard deviation of the system response. First/Second-order reliability methods (FORM/SORM) are used for assessing the probability of failure of the system with respect to performance criteria (Ditlevsen and Madsen, 1996). Numerous applications of the latter can be found *e.g.* in Phoon (2003); Low (2005); Low and Tang (2007); Li and Low (2010) among others.

In the early 90's a new approach called *stochastic finite element method* (SFEM) has emerged, which allows one to solve boundary value problems with uncertain coefficients and is especially suited to spatially variable inputs (Ghanem and Spanos, 1991). The key ingredient in this approach is so-called *polynomial chaos expansions* (PCE), which allows one to represent a random output (*e.g.* the nodal displacement vector resulting from a finite element analysis) as a polynomial series in the input variables. Early applications of such a SFEM to geotechnics can be found in Ghanem and Brzkala (1996); Sudret and Der Kiureghian (2000); Ghiocel and Ghanem (2002); Clouteau and Lafargue (2003); Sudret et al. (2004); Sudret et al. (2006); Berveiller et al. (2006).

During the last ten years, polynomial chaos expansions have become a cross-field key approach to uncertainty quantification in engineering problems ranging from computational fluid dynamics and heat transfer problems to electromagnetism. The associated computational methods have also been somewhat simplified due to the emergence of *non intrusive* spectral approaches, as shown later.

The goal of this chapter is to give an overview on stochastic finite element analysis using polynomial chaos expansions, focusing more specifically on non intrusive computation schemes. The chapter is organized as follows. Section 2 presents a versatile uncertainty quantification framework which is now widely used by both researchers and practitioners (Sudret, 2007; De Rocquigny, 2012). Section 3 presents the machinery of polynomial chaos expansions in a step-by-step approach: how to construct the polynomial chaos basis, how to compute the coefficients, how to estimate the quality of obtained series, how to address large dimensional problems using *sparse* expansions? Section 4 shows how to post-process a PC expansion for different applications, *i.e.* compute statistical moments of the response quantities, estimate the model output distribution or carry out sensitivity analysis. Finally, Section 5 presents different application examples in the field of geotechnics.

## 2 Uncertainty propagation framework

### 2.1 Introduction

Let us consider a physical system (*e.g.* a foundation on a soft soil layer, a retaining wall, etc.) whose mechanical behaviour is represented by a computational model  $\mathcal{M}$ :

$$\mathbf{x} \in \mathcal{D}_X \subset \mathbb{R}^M \mapsto y = \mathcal{M}(\mathbf{x}) \in \mathbb{R}. \quad (1)$$

In this equation,  $\mathbf{x} = \{x_1, \dots, x_M\}^\top$  gathers the  $M$  input parameters of the model while  $y$  is the *quantity of interest* (QoI) in the analysis, *e.g.* a load carrying capacity, a limit state equation for stability, etc. In the sequel only models having a single (scalar) quantity of interest are presented, although the derivations hold componentwise in case of vector-valued models  $\mathbf{y} = \mathcal{M}(\mathbf{x}) \in \mathbb{R}^q$ .

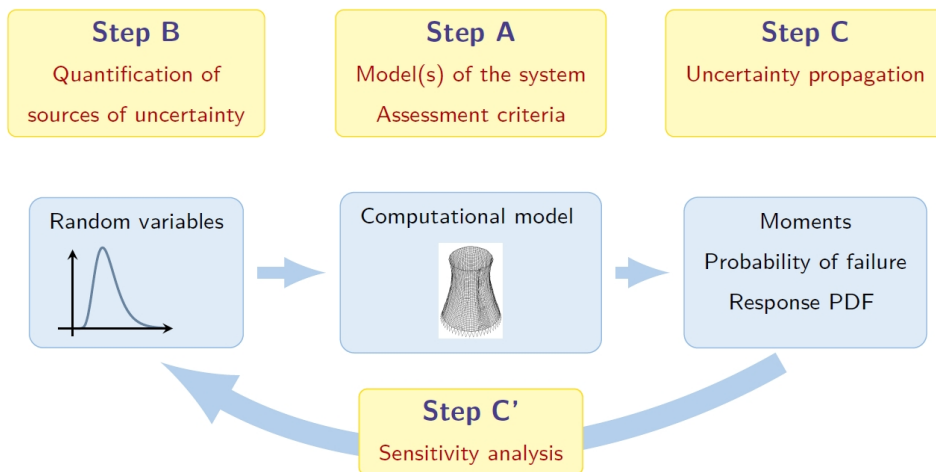


Figure 1: Uncertainty quantification framework

As shown in Figure 1, once a computational model  $\mathcal{M}$  is chosen to evaluate the performance of the system of interest (Step A), the sources of uncertainty are to be quantified (Step B): in this step the available information (expert judgment on the problem, data bases and literature, existing measurements) are used to build a proper probabilistic model of the input parameters, which is eventually cast as a random vector  $\mathbf{X}$  described by a joint probability density function  $f_{\mathbf{X}}$ . When the parameters are assumed statistically independent, this joint distribution is equivalently defined by the set of marginal distribution of all input parameters, say  $\{f_{X_i}, i = 1, \dots, M\}$ . If dependence exists, the copula formalism may be used, see Nelsen (1999); Caniou (2012). As a consequence, the quantity of interest becomes a random variable

$$Y = \mathcal{M}(\mathbf{X}), \quad (2)$$

whose properties are implicitly defined by the *propagation* of the uncertainties described by the joint distribution  $f_{\mathbf{X}}$  through the computational model (Step C). This step consists in characterizing the probabilistic content of  $Y$ , *i.e.* its statistical moments, quantiles or

full distribution, in order to derive confidence intervals around the mean QoI for robust predictions, or to carry out reliability assessment.

When the spatial variability of soil properties is to be modelled, *random fields* have to be used. The mathematical description of random fields and their discretization is beyond the scope of this chapter. For an overview the interested reader is referred to Vanmarcke (1983); Sudret and Der Kiureghian (2000); Sudret and Berveiller (2007). In any case, and whatever the random field discretization technique (*e.g.* Karhunen-Love expansion, EOLE, etc.), the problem eventually reduces to an input random vector (which is usually Gaussian) appearing in the discretization. Then the uncertainty propagation issue identically suits the framework described above. For the sake of illustration an application example involving spatial variability will be addressed in Section 5.3.

## 2.2 Monte Carlo simulation

Monte Carlo simulation (MCS) is a well-known technique for estimating statistical properties of the random response  $Y = \mathcal{M}(\mathbf{X})$ : realizations of the input vector  $\mathbf{X}$  are sampled according to the input distribution  $f_{\mathbf{X}}$ , then the computational model  $\mathcal{M}$  is run for each sample and the resulting set of QoI is post-processed (Rubinstein and Kroese, 2008). Although rather universal, MCS suffers from a low efficiency. Typically  $10^{3-4}$  samples are required to reach an acceptable accuracy. The cost even blows up when probabilities of failure are to be computed for the sake of reliability assessment, since  $10^{k+2}$  samples are required when estimating a probability of  $10^{-k}$ . Thus alternative methods have to be devised for addressing uncertainty quantification problems which involve computationally demanding models such as finite element models. In the last decade polynomial chaos expansions have become a popular approach in this respect.

## 3 Polynomial chaos expansions

### 3.1 Mathematical setting

Consider a computational model  $\mathcal{M}$  whose input parameters are represented by a random vector  $\mathbf{X}$ , and the associated (random) quantity of interest  $Y = \mathcal{M}(\mathbf{X})$ . Assuming that  $Y$  has a finite variance (which is a physically meaningful assumption when dealing with geotechnical systems), it belongs to the so-called Hilbert space of second order random variables, which allows for the following representation (Soize and Ghanem, 2004):

$$Y = \sum_{j=0}^{\infty} y_j Z_j. \quad (3)$$

In the latter equation, the random variable  $Y$  is cast as an infinite series, in which  $\{Z_j\}_{j=0}^{\infty}$  is a numerable set of random variables (which form a basis of the Hilbert space), and  $\{y_j\}_{j=0}^{\infty}$  are coefficients. The latter may be interpreted as the *coordinates* of  $Y$  in this basis. Hilbertian analysis guarantees the existence of such bases and representation,

however many choices are possible. In the sequel we focus on *polynomial chaos expansions*, in which the basis terms  $\{Z_j\}_{j=0}^\infty$  are multivariate orthonormal polynomials in the input vector  $\mathbf{X}$ , *i.e.*  $Z_j = \Psi_j(\mathbf{X})$ .

## 3.2 Construction of the basis

### 3.2.1 Univariate orthonormal polynomials

For the sake of simplicity we assume that the input random vector has *independent* components denoted by  $\{X_i, i = 1, \dots, M\}$ , meaning that the joint distribution is simply the product of the  $M$  marginal distributions  $\{f_{X_i}\}_{i=1}^M$ :

$$f_{\mathbf{X}}(\mathbf{x}) = \prod_{i=1}^M f_{X_i}(x_i), \quad x_i \in \mathcal{D}_{X_i}, \quad (4)$$

where  $\mathcal{D}_{X_i}$  is the support of  $X_i$ . For each single variable  $X_i$  and any two functions  $\phi_1, \phi_2 : x \in \mathcal{D}_{X_i} \mapsto \mathbb{R}$ , we define a functional inner product by the following integral (provided it exists):

$$\langle \phi_1, \phi_2 \rangle_i = \int_{\mathcal{D}_{X_i}} \phi_1(x) \phi_2(x) f_{X_i}(x) dx. \quad (5)$$

The latter is nothing but the expectation  $\mathbb{E}[\phi_1(X_i) \phi_2(X_i)]$  with respect to the marginal distribution  $f_{X_i}$ . Two such functions are said *orthogonal* with respect to the probability measure  $\mathbb{P}(dx) = f_{X_i}(x) dx$  if  $\mathbb{E}[\phi_1(X_i) \phi_2(X_i)] = 0$ . Using the above notation, classical algebra allows one to build a family of *orthogonal polynomials*  $\{\pi_k^{(i)}, k \in \mathbb{N}\}$  satisfying

$$\left\langle \pi_j^{(i)}, \pi_k^{(i)} \right\rangle_i \stackrel{\text{def}}{=} \mathbb{E} \left[ \pi_j^{(i)}(X_i) \pi_k^{(i)}(X_i) \right] = \int_{\mathcal{D}_{X_i}} \pi_j^{(i)}(x) \pi_k^{(i)}(x) f_{X_i}(x) dx = a_j^i \delta_{jk}, \quad (6)$$

where subscript  $k$  denotes the degree of the polynomial  $\pi_k^{(i)}$ ,  $\delta_{jk}$  is the Kronecker symbol equal to 1 when  $j = k$  and 0 otherwise, and  $a_j^i$  corresponds to squared norm of  $\pi_j^{(i)}$ :

$$a_j^i \stackrel{\text{def}}{=} \|\pi_j^{(i)}\|_i^2 \stackrel{\text{def}}{=} \left\langle \pi_j^{(i)}, \pi_j^{(i)} \right\rangle_i \quad (7)$$

This family can be obtained by applying the Gram-Schmidt orthogonalization procedure to the canonical family of monomials  $\{1, x, x^2, \dots\}$ . For standard distributions, the associated family of orthogonal polynomials is well-known. For instance, if  $X_i \sim \mathcal{U}(-1, 1)$  has a uniform distribution over  $[-1, 1]$ , the resulting family is that of so-called *Legendre polynomials*. If  $X_i \sim \mathcal{N}(0, 1)$  has a standard normal distribution with zero mean value and unit standard deviation, the resulting family is that of *Hermite polynomials*. The families associated to standard distributions are summarized in Table 1 (Xiu and Karniadakis, 2002).

Note that the obtained family is usually not orthonormal. By enforcing the normalization, an *orthonormal family*  $\{\psi_j^{(i)}\}_{j=0}^\infty$  is obtained from Eqs.(6),(7) by

$$\psi_j^{(i)} = \pi_j^{(i)} / \sqrt{a_j^i} \quad i = 1, \dots, M, \quad j \in \mathbb{N}, \quad (8)$$

The normalizing coefficients are listed in Table 1 for the standard families. For the sake of illustration Hermite polynomials up to degree 4 are plotted in Figure 2.



Table 1: Classical families of orthogonal polynomials

Type of variable	Distribution	Orthogonal polynomials	Hilbertian basis $\psi_k(x)$
Uniform $\mathcal{U}(-1, 1)$	$\mathbf{1}_{[-1,1]}(x)/2$	Legendre $P_k(x)$	$P_k(x)/\sqrt{\frac{1}{2k+1}}$
Gaussian $\mathcal{N}(0, 1)$	$\frac{1}{\sqrt{2\pi}}e^{-x^2/2}$	Hermite $H_{e_k}(x)$	$H_{e_k}(x)/\sqrt{k!}$
Gamma $\Gamma(a, \lambda = 1)$	$x^a e^{-x} \mathbf{1}_{\mathbb{R}^+}(x)$	Laguerre $L_k^a(x)$	$L_k^a(x)/\sqrt{\frac{\Gamma(k+a+1)}{k!}}$
Beta $\mathcal{B}(a, b)$	$\mathbf{1}_{[-1,1]}(x) \frac{(1-x)^a(1+x)^b}{B(a)B(b)}$	Jacobi $J_k^{a,b}(x)$	$J_k^{a,b}(x)/\mathfrak{J}_{a,b,k}$

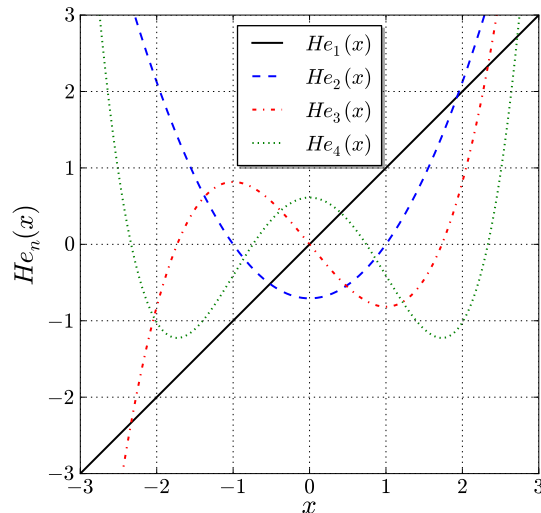
$$\mathfrak{J}_{a,b,k}^2 = \frac{2^{a+b+1}}{2k+a+b+1} \frac{\Gamma(k+a+1)\Gamma(k+b+1)}{\Gamma(k+a+b+1)\Gamma(k+1)}$$


Figure 2: Univariate Hermite polynomials

### 3.2.2 Multivariate polynomials

In order to build up a basis such as in (3), *tensor products* of univariate orthonormal polynomials are built up. For this purpose let us define multi-indices (also called tuples)  $\boldsymbol{\alpha} \in \mathbb{N}^M$  which are ordered lists of integers

$$\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_M), \quad \alpha_i \in \mathbb{N}. \quad (9)$$

One can associate a multivariate polynomial  $\Psi_{\boldsymbol{\alpha}}$  to any multi-index  $\boldsymbol{\alpha}$  by

$$\Psi_{\boldsymbol{\alpha}}(\mathbf{x}) \stackrel{\text{def}}{=} \prod_{i=1}^M \psi_{\alpha_i}^{(i)}(x_i), \quad (10)$$

where the univariate polynomials  $\{\psi_k^{(i)}, k \in \mathbb{N}\}$  are defined according to the  $i$ -th marginal distribution, see Eqs.(6),(8). By virtue of Eq.(6) and the above tensor product construc-

tion, the multivariate polynomials in the input vector  $\mathbf{X}$  are also orthonormal, *i.e.*

$$\mathbb{E} [\Psi_{\alpha}(\mathbf{X}) \Psi_{\beta}(\mathbf{X})] \stackrel{\text{def}}{=} \int_{\mathcal{D}_{\mathbf{X}}} \Psi_{\alpha}(\mathbf{x}) \Psi_{\beta}(\mathbf{x}) f_{\mathbf{X}}(\mathbf{x}) d\mathbf{x} = \delta_{\alpha\beta} \quad \forall \alpha, \beta \in \mathbb{N}^M, \quad (11)$$

where  $\delta_{\alpha\beta}$  is the Kronecker symbol which is equal to 1 if  $\alpha = \beta$  and zero otherwise. With this notation, it can be proven that the set of all multivariate polynomials in the input random vector  $\mathbf{X}$  forms a basis of the Hilbert space in which  $Y = \mathcal{M}(\mathbf{X})$  is to be represented (Soize and Ghanem, 2004):

$$Y = \sum_{\alpha \in \mathbb{N}^M} y_{\alpha} \Psi_{\alpha}(\mathbf{X}). \quad (12)$$

This equation may be interpreted as an intrinsic representation of the random response  $Y$  in an abstract space through an orthonormal basis and coefficients that are the *coordinates* of  $Y$  in this basis.

### 3.3 Practical implementation

#### 3.3.1 Isoprobabilistic transform

In practical uncertainty quantification problems the random variables which model the input parameters (*e.g.* material properties, loads, etc.) are usually *not* standardized as those shown in Table 1. Thus it is necessary to first transform random vector  $\mathbf{X}$  into a set of *reduced variables*  $\mathbf{U}$  through an isoprobabilistic transform

$$\mathbf{X} = \mathcal{T}(\mathbf{U}). \quad (13)$$

Depending on the marginal distribution of each input variable  $X_i$ , the associated reduced variable  $U_i$  may be standard normal  $\mathcal{N}(0, 1)$ , standard uniform  $\mathcal{U}(-1, 1)$ , etc. Then the random model response  $Y$  is cast as a function of the reduced variables by composing the computational model  $\mathcal{M}$  and the transform  $\mathcal{T}$ :

$$Y = \mathcal{M}(\mathbf{X}) = \mathcal{M} \circ \mathcal{T}(\mathbf{U}) = \sum_{\alpha \in \mathbb{N}^M} y_{\alpha} \Psi_{\alpha}(\mathbf{U}). \quad (14)$$

Note that the isoprobabilistic transform also allows one to address the case of correlated input variables through *e.g.* Nataf transform (Ditlevsen and Madsen, 1996).

**Example 1** Suppose  $\mathbf{X} = \{X_1, \dots, X_M\}^T$  is a vector of independent Gaussian variables  $X_i \sim \mathcal{N}(\mu_i, \sigma_i)$  with respective mean value  $\mu_i$  and standard deviation  $\sigma_i$ . Then a one-to-one mapping  $\mathbf{X} = \mathcal{T}(\mathbf{U})$  is obtained by:

$$X_i = \mu_i + \sigma_i U_i, \quad i = 1, \dots, M. \quad (15)$$

where  $\mathbf{U} = \{U_1, \dots, U_M\}^T$  is a standard normal vector.

**Example 2** Suppose  $\mathbf{X} = \{X_1, X_2\}^T$  where  $X_1 \sim \mathcal{LN}(\lambda, \zeta)$  is a lognormal variable and  $X_2 \sim \mathcal{U}(a, b)$  is a uniform variable. It is natural to transform  $X_1$  into a standard normal variable and  $X_2$  into a standard uniform variable. The isoprobabilistic transform  $\mathbf{X} = \mathcal{T}(\mathbf{U})$  then reads:

$$\begin{cases} X_1 &= e^{\lambda + \zeta U_1} \\ X_2 &= \frac{b-a}{2}U_2 + \frac{b+a}{2} \end{cases} \quad (16)$$

### 3.3.2 Truncation scheme

The representation of the random response in Eq.(12) is exact when the infinite series is considered. However, in practice, only a finite number of terms may be computed. For this purpose a *truncation scheme* has to be adopted. Since the polynomial chaos basis is made of polynomials, it is natural to consider as a truncated series all polynomials up to a certain degree. Let us define the *total degree* of a multivariate polynomial  $\Psi_{\boldsymbol{\alpha}}$  by:

$$|\boldsymbol{\alpha}| \stackrel{\text{def}}{=} \sum_{i=1}^M \alpha_i. \quad (17)$$

The standard truncation scheme consists in selecting all polynomials such that  $|\boldsymbol{\alpha}|$  is smaller than a given  $p$ , *i.e.*

$$\mathcal{A}^{M,p} = \{\boldsymbol{\alpha} \in \mathbb{N}^M : |\boldsymbol{\alpha}| \leq p\}. \quad (18)$$

The number of terms in the truncated series is

$$\text{card } \mathcal{A}^{M,p} = \binom{M+p}{p} = \frac{(M+p)!}{M! p!}. \quad (19)$$

The maximal polynomial degree  $p$  may typically be equal to 3 – 5 in practical applications. The question on how to define the suitable  $p$  for obtaining a given accuracy in the truncated series will be addressed later in Section 3.6. Note that the cardinality of  $\mathcal{A}^{M,p}$  increases polynomially with  $M$  and  $p$ . Thus the number of terms in the series, *i.e.* the number of coefficients to be computed, increases dramatically when  $M > 10$ , say. This complexity is referred to as the *curse of dimensionality*. Other advanced truncation schemes that allow one to bypass this problem will be considered later on in Section 3.6. As a conclusion, the construction of a truncated PC expansion requires to:

- transform the input random vector  $\mathbf{X}$  into reduced variables;
- compute the associated families of univariate orthonormal polynomials;
- compute the set of multi-indices corresponding to the truncation set (Eq.(18)). For this purpose, two different algorithms may be found in Sudret et al. (2006, Appendix I) and Blatman (2009, Appendix C).

### 3.3.3 Application example

Let us consider a computational model  $y = \mathcal{M}(x_1, x_2)$  involving two random parameters  $\{X_1, X_2\}^\top$  that are modelled by *lognormal* distributions, *e.g.* the load carrying capacity of a foundation in which the soil cohesion and friction angle are considered uncertain. Denoting by  $(\lambda_i, \zeta_i)$  the parameters of each distribution (*i.e.* the mean and standard deviation of the logarithm of  $X_i$ ,  $i = 1, 2$ ), the input variables may be transformed into reduced standard normal variables  $\mathbf{X} = \mathcal{T}(\mathbf{U})$  as follows:

$$\begin{aligned} X_1 &\sim \mathcal{LN}(\lambda_1, \zeta_1) & X_1 &= e^{\lambda_1 + \zeta_1 U_1} \\ X_2 &\sim \mathcal{LN}(\lambda_2, \zeta_2) & X_2 &= e^{\lambda_2 + \zeta_2 U_2} \end{aligned} \quad (20)$$

The problem reduces to representing a function of two standard normal variables onto a polynomial chaos expansion:

$$Y = \mathcal{M}(\mathcal{T}(U_1, U_2)) = \sum_{\alpha \in \mathbb{N}^2} y_\alpha \Psi_\alpha(U_1, U_2). \quad (21)$$

Since the reduced variables are standard normal, Hermite polynomials are used. Their derivation is presented in details in Appendix A. For the sake of illustration the orthonormal Hermite polynomials up to degree  $p = 3$  read (see Eq.(8)):

$$\psi_0(x) = 1 \quad \psi_1(x) = x \quad \psi_2(x) = (x^2 - 1)/\sqrt{2} \quad \psi_3(x) = (x^3 - 3x)/\sqrt{6}. \quad (22)$$

Suppose a standard truncation scheme of maximal degree  $p = 3$  is selected. This leads to a truncation set  $\mathcal{A}^{2,3}$  of size  $P = \binom{2+3}{3} = 10$ . The set of multi-indices  $(\alpha_1, \alpha_2)$  such that  $\{\alpha_i \geq 0, \alpha_1 + \alpha_2 \leq 3\}$  is given in Table 2 together with the expression of the resulting multivariate polynomials.

Table 2: Hermite polynomial chaos basis –  $M = 2$  standard normal variables,  $p = 3$

$j$	$\alpha$	$\Psi_\alpha \equiv \Psi_j$
0	(0, 0)	$\Psi_0 = 1$
1	(1, 0)	$\Psi_1 = U_1$
2	(0, 1)	$\Psi_2 = U_2$
3	(2, 0)	$\Psi_3 = (U_1^2 - 1)/\sqrt{2}$
4	(1, 1)	$\Psi_4 = U_1 U_2$
5	(0, 2)	$\Psi_5 = (U_2^2 - 1)/\sqrt{2}$
6	(3, 0)	$\Psi_6 = (U_1^3 - 3U_1)/\sqrt{6}$
7	(2, 1)	$\Psi_7 = (U_1^2 - 1)U_2/\sqrt{2}$
8	(1, 2)	$\Psi_8 = (U_2^2 - 1)U_1/\sqrt{2}$
9	(0, 3)	$\Psi_9 = (U_2^3 - 3U_2)/\sqrt{6}$

As a conclusion, the random response of our computational model  $Y = \mathcal{M}(\mathcal{T}(U_1, U_2))$

will be approximated by a 10-term polynomial series expansion in  $(U_1, U_2)$ :

$$\begin{aligned} \tilde{Y} \stackrel{\text{def}}{=} \mathcal{M}^{\text{PC}}(U_1, U_2) &= y_0 + y_1 U_1 + y_2 U_2 + y_3 (U_1^2 - 1)/\sqrt{2} + y_4 U_1 U_2 \\ &+ y_5 (U_2^2 - 1)/\sqrt{2} + y_6 (U_1^3 - 3U_1)/\sqrt{6} + y_7 (U_1^2 - 1)U_2/\sqrt{2} \\ &+ y_8 (U_2^2 - 1)U_1/\sqrt{2} + y_9 (U_2^3 - 3U_2)/\sqrt{6}. \end{aligned} \quad (23)$$

### 3.4 Computation of the coefficients

#### 3.4.1 Introduction

Once the truncated basis has been selected the coefficients  $\{y_\alpha\}_{\alpha \in \mathcal{A}^{M,p}}$  shall be computed. Historically, so-called *intrusive* computation schemes have been developed in the context of stochastic finite element analysis (Ghanem and Spanos, 1991). In this setup the constitutive equations of the physical problem (*e.g.* linear elasticity for estimating the settlement of foundations) are discretized both in the physical space (using standard finite element techniques) and in the random space using the polynomial chaos expansion. This results in coupled systems of equations which require ad-hoc solvers, thus the term “intrusive”. The application of such approaches to geotechnical problems may be found in Ghiocel and Ghanem (2002); Berveiller et al. (2004b); Sudret et al. (2004); Sudret et al. (2006), Sudret and Berveiller (2007, Chap. 7).

In the last decade alternative approaches termed *non-intrusive* have been developed for computing the expansion coefficients. The common point of these techniques is that they rely upon the *repeated run* of the computational model for selected realizations of random vector  $\mathbf{X}$ , exactly as in Monte-Carlo simulation. Thus the computational model may be used without modification. The main techniques are now reviewed with an emphasis on *least-square minimization*.

#### 3.4.2 Projection

Due to the orthogonality of the PC basis (Eq.(11)) one can compute each expansion coefficient as follows:

$$\mathbb{E}[Y \Psi_\alpha(\mathbf{X})] = \mathbb{E} \left[ \Psi_\alpha(\mathbf{X}) \cdot \sum_{\beta \in \mathbb{N}^M} y_\beta \Psi_\beta(\mathbf{X}) \right] = \sum_{\beta \in \mathbb{N}^M} y_\beta \overbrace{\mathbb{E}[\Psi_\alpha(\mathbf{X}) \Psi_\beta(\mathbf{X})]}^{\delta_{\alpha\beta}} = y_\alpha. \quad (24)$$

Thus each coefficient  $y_\alpha$  is nothing but the *orthogonal projection* of the random response  $Y$  onto the corresponding basis function  $\Psi_\alpha(\mathbf{X})$ . The latter may be further elaborated as

$$y_\alpha = \mathbb{E}[Y \Psi_\alpha(\mathbf{X})] = \int_{\mathcal{D}_\mathbf{X}} \mathcal{M}(\mathbf{x}) \Psi_\alpha(\mathbf{x}) f_\mathbf{X}(\mathbf{x}) d\mathbf{x}. \quad (25)$$

The numerical estimation of  $y_\alpha$  may be carried with either one of the two expressions, namely:

- by Monte Carlo simulation (MCS) allowing one to estimate the expectation in Eq.(25) (Ghiocel and Ghanem, 2002). This technique however shows low efficiency, as does MCS in general;

- by a the numerical integration of the right-hand side of Eq.(25) using Gaussian quadrature (Le Maître et al., 2002; Berveiller et al., 2004a; Matthies and Keese, 2005).

The quadrature approach has been extended using *sparse grids* for a more efficient integration, especially in large dimensions. So-called *stochastic collocation methods* have also been developed. The reader is referred to the review paper by Xiu (2009) for more details.

### 3.4.3 Least-square minimization

Instead of devising numerical methods that directly estimate each coefficient from the expression  $y_\alpha = \mathbb{E}[Y \Psi_\alpha(\mathbf{X})]$ , an alternative approach based on least-square minimization and originally termed “regression approach” has been proposed in Berveiller et al. (2004b, 2006). The problem is set up as follows. Once a truncation scheme  $\mathcal{A} \subset \mathbb{N}^M$  is chosen (for instance,  $\mathcal{A} = \mathcal{A}^{M,p}$  as in Eq.(18)), the infinite series is recast as the sum of the truncated series and a residual:

$$Y = \mathcal{M}(\mathbf{X}) = \sum_{\alpha \in \mathcal{A}} y_\alpha \Psi_\alpha(\mathbf{X}) + \varepsilon, \quad (26)$$

in which  $\varepsilon$  corresponds to all those PC polynomials whose index  $\alpha$  is *not* in the truncation set  $\mathcal{A}$ . The least-square minimization approach consists in finding the set of coefficients  $\mathbf{y} = \{y_\alpha, \alpha \in \mathcal{A}\}$  which minimizes the mean square error

$$\mathbb{E}[\varepsilon^2] \stackrel{\text{def}}{=} \mathbb{E} \left[ \left( Y - \sum_{\alpha \in \mathcal{A}} y_\alpha \Psi_\alpha(\mathbf{X}) \right)^2 \right], \quad (27)$$

that is:

$$\mathbf{y} = \arg \min_{\mathbf{y} \in \mathbb{R}^{\text{card}(\mathcal{A})}} \mathbb{E} \left[ \left( \mathcal{M}(\mathbf{X}) - \sum_{\alpha \in \mathcal{A}} y_\alpha \Psi_\alpha(\mathbf{X}) \right)^2 \right]. \quad (28)$$

The residual in Eq.(27) is nothing but a quadratic function of the (still unknown) coefficients  $\{y_\alpha\}_{\alpha \in \mathcal{A}}$ . By simple algebra it can be proven that the solution is identical to that obtained by projection in Eq.(25). However, the setup in Eq.(28) which is similar to regression opens to new computational schemes.

For this purpose, the discretized version of the problem is obtained by replacing the expectation operator in Eq.(28) by the empirical mean over a sample set:

$$\hat{\mathbf{y}} = \arg \min_{\mathbf{y} \in \mathbb{R}^{\text{card}(\mathcal{A})}} \frac{1}{n} \sum_{i=1}^n \left( \mathcal{M}(\mathbf{x}^{(i)}) - \sum_{\alpha \in \mathcal{A}} y_\alpha \Psi_\alpha(\mathbf{x}^{(i)}) \right)^2. \quad (29)$$

In this expression,  $\mathcal{X} = \{\mathbf{x}^{(i)}, i = 1, \dots, n\}$  is a sample set of points, (also called *experimental design* (ED)) that is typically obtained by Monte Carlo simulation of the input random vector  $\mathbf{X}$ . The least-square minimization problem in Eq.(29) is solved as follows:

- The computational model  $\mathcal{M}$  is run for each point in the ED, and the results are stored in a vector

$$\mathcal{Y} = \{y^{(1)} = \mathcal{M}(\mathbf{x}^{(1)}), \dots, y^{(n)} = \mathcal{M}(\mathbf{x}^{(n)})\}^\top. \quad (30)$$

- The *information matrix* is calculated from the evaluation of the basis polynomials onto each point in the ED:

$$\mathbf{A} = \left\{ \mathbf{A}_{ij} \stackrel{\text{def}}{=} \Psi_j(\mathbf{x}^{(i)}), i = 1, \dots, n, j = 1, \dots, \text{card } \mathcal{A} \right\}. \quad (31)$$

- The solution of the least-square minimization problem reads

$$\hat{\mathbf{y}} = (\mathbf{A}^\top \mathbf{A})^{-1} \mathbf{A}^\top \mathcal{Y}. \quad (32)$$

In order to be well-posed the least-square minimization requires that the number of unknown  $P = \text{card } \mathcal{A}$  is smaller than the size of the experimental design  $n = \text{card } \mathcal{X}$ . The empirical thumb rule  $n \approx 2P - 3P$  is often mentioned (Sudret, 2007; Blatman, 2009). To overcome the potential ill-conditioning of the information matrix, a singular value decomposition shall be used (Press et al., 2001).

The points used in the experimental design may be obtained from crude Monte Carlo simulation. However other types of designs are of common use, especially Latin Hypercube sampling (LHS), see McKay et al. (1979), or quasi-random sequences such as the Sobol' or Halton sequence (Niederreiter, 1992). From the author's experience the latter types of design provide rather equivalent accuracy in terms of resulting mean-square error, for the same sample size  $n$ . Note that deterministic designs based on the roots of the orthogonal polynomials have also been proposed earlier in Berveiller et al. (2006) based on Isukapalli (1999).

Once the coefficients have been evaluated (Eq.(32)) the approximation of the random response is the random variable

$$\hat{Y} = \mathcal{M}^{\text{PC}}(\mathbf{X}) = \sum_{\alpha \in \mathcal{A}} \hat{y}_\alpha \Psi_\alpha(\mathbf{X}). \quad (33)$$

The above equation may also be interpreted as a response surface, *i.e.* a function  $\mathbf{x} \mapsto \mathcal{M}^{\text{PC}}(\mathbf{x}) = \sum_{\alpha \in \mathcal{A}} \hat{y}_\alpha \Psi_\alpha(\mathbf{x})$  that allows one to surrogate (fast, although approximately) the original model  $y = \mathcal{M}(\mathbf{x})$ .

## 3.5 Validation

### 3.5.1 Error estimators

As mentioned already, it is not possible to know in advance how to choose the maximal polynomial degree in the standard truncation scheme Eq.(18). A crude approach would consist in testing several truncation schemes of increasing degree (*e.g.*  $p = 2, 3, 4$ ) and observe if there is some convergence for the quantities of interest. Recently, *a posteriori* error estimates have been proposed by Blatman and Sudret (2010) that allow for an objective evaluation of the accuracy of any truncated PCE.

First of all it is reminded that a good measure of the error committed by using a truncated series expansion is the mean-square error of the residual (which is also called

generalization error in statistical learning theory):

$$Err_G \stackrel{\text{def}}{=} \mathbb{E} [\varepsilon^2] = \mathbb{E} \left[ \left( Y - \sum_{\alpha \in \mathcal{A}} \hat{y}_\alpha \Psi_\alpha(\mathbf{X}) \right)^2 \right]. \quad (34)$$

In practice the latter is not known analytically, yet it may be estimated by a Monte Carlo simulation using a large sample set, say  $\mathcal{X}_{\text{val}} = \{\mathbf{x}_1, \dots, \mathbf{x}_{n_{\text{val}}}\}$ :

$$\widehat{Err}_G \stackrel{\text{def}}{=} \frac{1}{n_{\text{val}}} \sum_{i=1}^{n_{\text{val}}} \left( \mathcal{M}(\mathbf{x}_i) - \sum_{\alpha \in \mathcal{A}} \hat{y}_\alpha \Psi_\alpha(\mathbf{x}_i) \right)^2. \quad (35)$$

The so-called *validation set*  $\mathcal{X}_{\text{val}}$  shall be large enough to get an accurate estimation, *e.g.*  $n_{\text{val}} = 10^3$ – $5$ . However, as the computation of  $\widehat{Err}_G$  requires evaluating  $\mathcal{M}$  for each point in  $\mathcal{X}_{\text{val}}$ , this is not affordable in real applications and would ruin the efficiency of the approach. Indeed the purpose of using polynomial chaos expansions is to avoid Monte Carlo simulation, *i.e.* to limit the number of runs of  $\mathcal{M}$  in Eq.(30) to the smallest possible number, typically  $n = 50$  to a few hundreds.

As a consequence, in order to get an estimation of the generalization error Eq.(34) at an affordable computational cost, the points in the experimental design  $\mathcal{X}$  could be used in Eq.(35) instead of the validation set, leading to the so-called *empirical error*  $\widehat{Err}_E$  defined by

$$\widehat{Err}_E \stackrel{\text{def}}{=} \frac{1}{n} \sum_{i=1}^n \left( \mathcal{M}(\mathbf{x}^{(i)}) - \sum_{\alpha \in \mathcal{A}} \hat{y}_\alpha \Psi_\alpha(\mathbf{x}^{(i)}) \right)^2, \quad \mathbf{x}^{(i)} \in \mathcal{X} \quad (36)$$

This empirical error now only uses the values  $\mathcal{M}(\mathbf{x}^{(i)})$  that are already available from Eq.(30) and is thus readily computable. Note that the normalized quantity

$$R^2 = 1 - \frac{\widehat{Err}_E}{\text{Var}[\mathcal{Y}]}, \quad (37)$$

where  $\text{Var}[\mathcal{Y}]$  is the empirical variance of the set of response quantities in Eq.(30), is the well-known *coefficient of determination* in regression analysis.

However  $\widehat{Err}_E$  usually underestimates (sometimes severely) the real generalization error  $Err_G$ . As an example, in the limit case when an interpolating polynomial would be fitted to the experimental design,  $\widehat{Err}_E$  would be exactly zero while  $Err_G$  in Eq.(34) would probably not: this phenomenon is known as *overfitting*.

### 3.5.2 Leave-one-out cross-validation

A compromise between fair error estimation and affordable computational cost may be obtained by *leave-one-out* (LOO) cross-validation, which was originally proposed by Allen (1971); Geisser (1975). The idea is to use different sets of points to (i) build a PC expansion and (ii) compute the error with the original computational model. Starting from the full experimental design  $\mathcal{X}$ , LOO cross-validation sets one point apart, say  $\mathbf{x}^{(i)}$



and builds a PC expansion denoted by  $\mathcal{M}^{\text{PC}\setminus i}(\cdot)$  from the  $n - 1$  remaining points, *i.e.* from the ED  $\mathcal{X}\setminus\mathbf{x}^{(i)} \stackrel{\text{def}}{=} \{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(i-1)}, \mathbf{x}^{(i+1)}, \dots, \mathbf{x}^{(n)}\}$ . The predicted residual error at that point reads:

$$\Delta_i \stackrel{\text{def}}{=} \mathcal{M}(\mathbf{x}^{(i)}) - \mathcal{M}^{\text{PC}\setminus i}(\mathbf{x}^{(i)}). \quad (38)$$

The PRESS coefficient (*predicted residual sum of squares*) and the *leave-one-out error* respectively read:

$$PRESS = \sum_{i=1}^n \Delta_i^2, \quad (39)$$

$$\widehat{Err}_{LOO} = \frac{1}{n} \sum_{i=1}^n \Delta_i^2. \quad (40)$$

Similar to the determination coefficient in Eq.(37) the  $Q^2$  indicator defined by

$$Q^2 = 1 - \frac{\widehat{Err}_{LOO}}{\text{Var}[\mathcal{Y}]} \quad (41)$$

is a normalized measure of the accuracy of the meta-model. From the above equations one could think that evaluating  $\widehat{Err}_{LOO}$  is computationally demanding since it is based on the sum of  $n$  predicted residuals, each of them obtained from a *different* PC expansion. However algebraic derivations may be carried out to compute  $\widehat{Err}_{LOO}$  from a *single* PC expansion analysis using the full original experimental design  $\mathcal{X}$  (details may be found in Blatman (2009, Appendix D)) as follows. The predicted residual in Eq.(38) eventually reads:

$$\Delta_i = \mathcal{M}(\mathbf{x}^{(i)}) - \mathcal{M}^{\text{PC}\setminus i}(\mathbf{x}^{(i)}) = \frac{\mathcal{M}(\mathbf{x}^{(i)}) - \mathcal{M}^{\text{PC}}(\mathbf{x}^{(i)})}{1 - h_i}, \quad (42)$$

where  $h_i$  is the  $i$ -th diagonal term of matrix  $\mathbf{A}(\mathbf{A}^\top \mathbf{A})^{-1} \mathbf{A}^\top$ . The LOO error estimate eventually reads

$$\widehat{Err}_{LOO} = \frac{1}{n} \sum_{i=1}^n \left( \frac{\mathcal{M}(\mathbf{x}^{(i)}) - \mathcal{M}^{\text{PC}}(\mathbf{x}^{(i)})}{1 - h_i} \right)^2, \quad (43)$$

where  $\mathcal{M}^{\text{PC}}$  has been built up from the *full* experimental design. As a conclusion, from a single resolution of a least-square problem using the ED  $\mathcal{X}$ , a fair error estimate of the mean-square error is available *a posteriori* using Eq.(43). Note that in practice, a normalized version of the LOO error is obtained by dividing  $\widehat{Err}_{LOO}$  by the sample variance  $\text{Var}[\mathcal{Y}]$ . A correction factor that accounts for the limit size of the experimental design is also added (Chapelle et al., 2002) which eventually leads to:

$$\widehat{\epsilon}_{LOO} = \frac{1}{n - P} \left( \frac{1 + \frac{1}{n} \text{tr} \mathbf{C}_{emp}^{-1}}{\text{Var}[\mathcal{Y}]} \right) \sum_{i=1}^n \left( \frac{\mathcal{M}(\mathbf{x}^{(i)}) - \mathcal{M}^{\text{PC}}(\mathbf{x}^{(i)})}{1 - h_i} \right)^2, \quad (44)$$

where  $\text{tr}(\cdot)$  is the trace,  $P = \text{card } \mathcal{A}$  and  $\mathbf{C}_{emp} = \frac{1}{n} \mathbf{\Psi}^\top \mathbf{\Psi}$ .

### 3.6 Curse of dimensionality

Common engineering problems are solved with computational models having typically  $M = 10$  to  $50$  input parameters. Even using a low-order PC expansion, this leads to a large number of unknown coefficients (size of the truncation set  $P = \text{card } \mathcal{A}^{M,p}$ ), which is equal to *e.g.*  $286 - 23,426$  terms when choosing  $p = 3$ . As explained already the suitable size of the experimental design shall be two to three times those numbers, which may reveal unaffordable when the computational model  $\mathcal{M}$  is *e.g.* a finite element model.

On the other hand, most of the terms in this large truncation set  $\mathcal{A}^{M,p}$  correspond to polynomials representing *interactions* between input variables. Yet it has been observed in many practical applications that only the low-interaction terms have coefficients that are significantly non zero. Taking again the example  $\{M = 50, p = 3\}$ , the number of *univariate polynomials* in the input variables (*i.e.* depending *only* on  $U_1$ , on  $U_2$ , etc.) is equal to  $p \cdot M = 150$ , *i.e.* less than 1% of the total number of terms in  $\mathcal{A}^{50,3}$ . As a conclusion, the common truncation scheme in Eq.(18) leads to compute a large number of coefficients, whereas most of them may reveal negligible once the computation has been carried out.

Due to this *sparsity-of-effect principle* Blatman (2009) has proposed to use truncation schemes that favor the low-interaction (also called low-rank) polynomials. Let us define the *rank*  $r$  of a multi-index  $\alpha$  by the number of non zero integers in  $\alpha$ , *i.e.*

$$r \stackrel{\text{def}}{=} \|\alpha\|_0 = \sum_{i=1}^M \mathbf{1}_{\{\alpha_i > 0\}} \quad (45)$$

This rank corresponds to the number of input variables a polynomial  $\Psi_\alpha$  depends on. For instance,  $\Psi_1$ ,  $\Psi_3$  and  $\Psi_9$  in Table 2 are of rank 1 (they only depend on one single variable) whereas  $\Psi_4$ ,  $\Psi_7$  and  $\Psi_8$  are of rank 2. Blatman and Sudret (2010) propose to fix *a priori* the maximum rank  $r_{max}$  and define truncation sets as follows:

$$\mathcal{A}^{M,p,r_{max}} = \{\alpha \in \mathbb{N}^M : |\alpha| \leq p, \|\alpha\|_0 \leq r_{max}\} \quad (46)$$

Another approach which has proven to be more relevant in the context of adaptive algorithms has been introduced in Blatman and Sudret (2011a) and is referred to as the *hyperbolic truncation scheme*. Let us define for any multi-index  $\alpha$  and  $0 < q \leq 1$  the  $q$ -norm:

$$\|\alpha\|_q \stackrel{\text{def}}{=} \left( \sum_{i=1}^M \alpha_i^q \right)^{1/q} \quad (47)$$

The hyperbolic truncation scheme corresponds to selecting all multi-indices of  $q$ -norm less than or equal to  $p$ :

$$\mathcal{A}^{M,p,q} = \{\alpha \in \mathbb{N}^M : \|\alpha\|_q \leq p\} \quad (48)$$

As shown in Figure 3 for a two-dimensional problem ( $M = 2$ ), such a truncation set contains all univariate polynomials up to degree  $p$  (since tuples of the form  $(0, \dots, \alpha_i \neq 0, \dots, 0)$  belong to it as long as  $\alpha_i \leq p$ ). The case  $q = 1$  corresponds to the standard truncation set

$\mathcal{A}^{M,p}$  defined in Eq.(18). When  $q < 1$  though, the polynomials of rank  $r > 1$  (corresponding to the blue points that are not on the axes in Figure 3) are less numerous than in  $\mathcal{A}^{M,p}$ . The gain in the basis size is all the more important when  $q$  is small and  $M$  is large. In the limit when  $q \rightarrow 0^+$  only univariate polynomials (rank 1, no interaction terms) are retained leading to an additive surrogate model, *i.e.* a sum of univariate functions. As shown in Blatman and Sudret (2011a) the size of the truncation set in Eq.(48) may be smaller by 2 to 3 orders of magnitude than that of the standard truncation scheme for large  $M$  and  $p \geq 5$ .

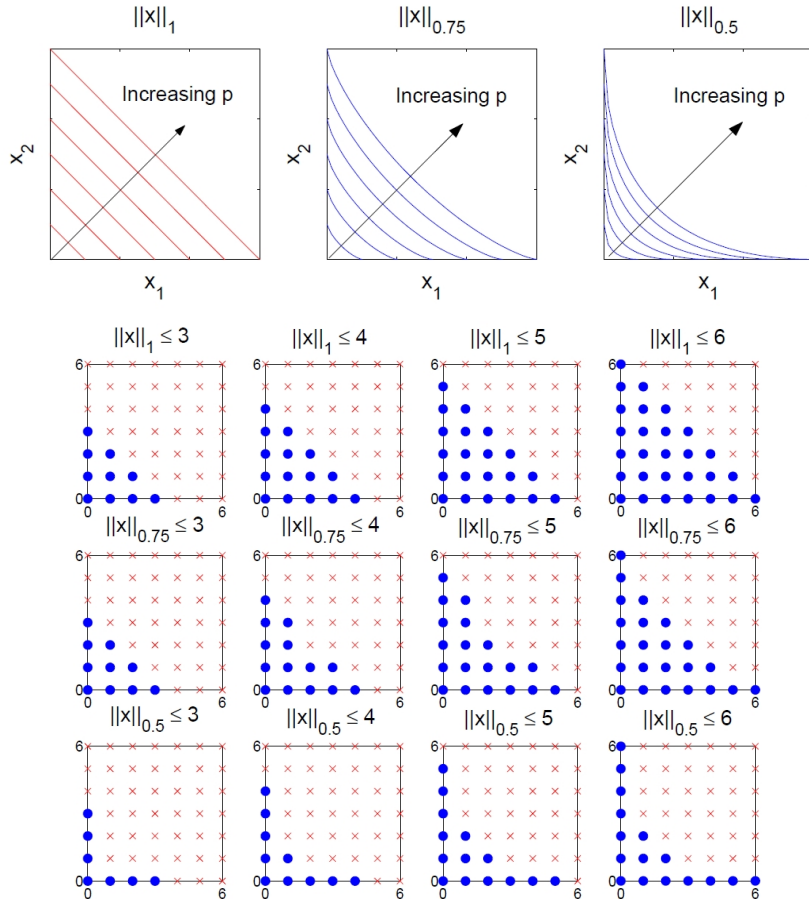


Figure 3: Hyperbolic truncation scheme (after Blatman and Sudret (2011a))

### 3.7 Adaptive algorithms

The use of hyperbolic truncation schemes  $\mathcal{A}^{M,p,q}$  as described above allows one to *a priori* decrease the number of coefficients to be computed in a truncated series expansion. This automatically reduces the computational cost since the minimal size of the experimental design  $\mathcal{X}$  shall be equal to  $k \cdot \text{card } \mathcal{A}^{M,p,q}$ , where  $k = 2$  to  $3$ . However this may remain too costly when large-dimensional, highly non linear problems are to be addressed.

Moreover, it is often observed *a posteriori* that the non zero coefficients in the expansion form a *sparse* subset of  $\mathcal{A}^{M,p,q}$ . Thus came the idea to build on-the-fly the suitable

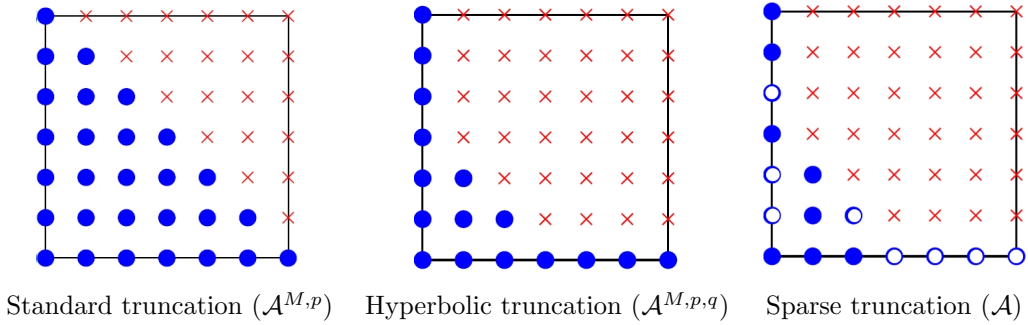


Figure 4: Sketch of the different truncation sets (blue points)

sparse basis instead of computing useless terms in the expansion which are eventually negligible. For this purpose adaptive algorithms have been introduced in Blatman and Sudret (2008) and further improved in Blatman and Sudret (2010, 2011a). In the latter publication the question of finding a suitable truncated basis is interpreted as a *variable selection* problem. The so-called *least-angle regression* (LAR) algorithm (Efron et al., 2004) has proven remarkable efficiency in this respect (see also Hastie et al. (2007)).

The principle of LAR is to (i) select a *candidate set* of polynomials  $\mathcal{A}$ , e.g. a given hyperbolic truncation set as in Eq.(48), and (ii) build up from scratch a sequence of sparse bases having 1, 2, , . . . , card  $\mathcal{A}$  terms. The algorithm is initialized by looking for the basis term  $\Psi_{\alpha_1}$  which is the most correlated with the response vector  $Y$ . The correlation is practically computed from the realizations of  $Y$  (i.e. the set  $\mathcal{Y}$  of QoI in Eq.(30)) and the realizations of the  $\Psi_{\alpha}$ 's, namely the information matrix in Eq.(31). This is carried out by normalizing each column vector into a zero-mean, unit variance vector, such that the correlation is then obtained by a mere scalar product of the normalized vector. Once the first basis term  $\Psi_{\alpha_1}$  is identified, the associated coefficient is computed such that the residual  $Y - y_{\alpha_1}^{(1)} \Psi_{\alpha_1}(\mathbf{X})$  becomes equicorrelated with two basis terms ( $\Psi_{\alpha_1}, \Psi_{\alpha_2}$ ). This will define the best one-term expansion. Then the current approximation is improved by moving along the direction  $(\Psi_{\alpha_1} + \Psi_{\alpha_2})$  up to a point where the residual becomes equi-correlated with a third polynomial  $\Psi_{\alpha_3}$ , and so on.

In the end the LAR algorithm has produced a sequence of less and less sparse expansions. The leave-one-out error of each expansion can be evaluated by Eq.(43). The sparse model providing the smallest error is retained. The great advantage of LAR is that it can be applied also in the case when the size of the candidate basis  $\mathcal{A}$  is larger than the size of the ED, card  $\mathcal{X}$ . Usually the size of the optimal sparse truncation is smaller than card  $\mathcal{X}$  in the end. Thus the coefficients of the associated PC expansion may be recomputed by least-square minimization for a better accuracy (Efron et al., 2004).

Note that all the above calculations are conducted from a prescribed initial experimental design  $\mathcal{X}$ . It may happen though that this size is too small to address the complexity of the problem, meaning that there is not enough information to find a sparse expansion with a sufficiently small LOO error. In this case overfitting appears, which can be detected automatically as shown in Blatman and Sudret (2011a). At that point the ED shall be enriched by adding new points (Monte Carlo samples or nested Latin Hypercube

sampling).

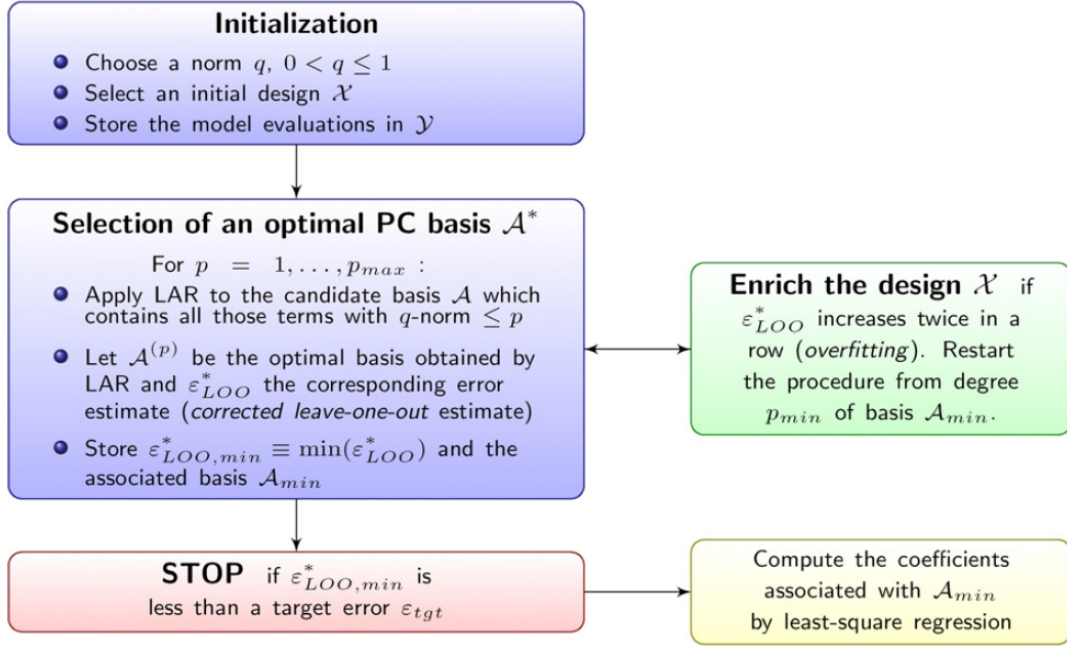


Figure 5: Basis-and-ED adaptive algorithm for sparse PC expansions (after Blatman and Sudret (2011a))

All in all a fully automatic “basis-and-ED” adaptive algorithm may be devised that will only require to prescribe the target accuracy of the analysis, *i.e.* the maximal tolerated LOO error, and an initial experimental design. The algorithm then automatically runs LAR analysis with increasingly large candidate sets  $\mathcal{A}$ , and possibly by increasing large experimental designs so as to reach the prescribed accuracy (see Figure 5). Note that extensions to vector-valued models have been proposed recently in Blatman and Sudret (2011b, 2013).

## 4 Post-processing for engineering applications

The polynomial chaos expansion technique presented in the previous sections leads to represent the quantity of interest (QoI) of a computational model  $Y = \mathcal{M}(\mathbf{X})$  through a somewhat abstract representation by a polynomial series  $\hat{Y} = \sum_{\alpha \in \mathcal{A}} \hat{y}_{\alpha} \Psi_{\alpha}(\mathbf{X})$  (Eq.(33)). Once the PC basis has been set up (*a priori* or using an adaptive algorithm such as LAR) and once the coefficients have been calculated, the series expansion shall be post-processed so as to provide engineeringwise meaningful numbers and statements: what is the mean behaviour of the system (mean QoI), scattering (variance of the QoI), confidence intervals or probability of failure (*i.e.* the probability that the QoI exceeds an admissible threshold)? In this section the various ways of post-processing a PC expansion are reviewed.

## 4.1 Moment analysis

From the orthonormality of the PC basis shown in Eq.(11) one can easily compute the mean and standard deviation of a truncated series  $\hat{Y} = \sum_{\alpha \in \mathcal{A}} \hat{y}_\alpha \Psi_\alpha(\mathbf{X})$ . Indeed, each polynomial shall be orthogonal to  $\Psi_{\mathbf{0}} \equiv 1$ , meaning that  $\mathbb{E}[\Psi_\alpha(\mathbf{X})] = 0 \quad \forall \alpha \neq \mathbf{0}$ . Thus the mean value of  $\hat{Y}$  is the first term of the series:

$$\mathbb{E}[\hat{Y}] = \mathbb{E}\left[\sum_{\alpha \in \mathcal{A}} \hat{y}_\alpha \Psi_\alpha(\mathbf{X})\right] = y_0 \quad (49)$$

Similarly, due to Eq.(11) the variance reads

$$\sigma_{\hat{Y}}^2 \stackrel{\text{def}}{=} \text{Var}[\hat{Y}] = \mathbb{E}\left[\left(\hat{Y} - y_0\right)^2\right] = \sum_{\substack{\alpha \in \mathcal{A} \\ \alpha \neq \mathbf{0}}} \hat{y}_\alpha^2 \quad (50)$$

Higher order moments such as the skewness and kurtosis coefficients  $\delta_{\hat{Y}}$  and  $\kappa_{\hat{Y}}$  may also be computed, which however requires the expectation of products of three (resp. four) multivariate polynomials:

$$\begin{aligned} \delta_{\hat{Y}} &\stackrel{\text{def}}{=} \frac{1}{\sigma_{\hat{Y}}^3} \mathbb{E}\left[(\hat{Y} - y_0)^3\right] = \frac{1}{\sigma_{\hat{Y}}^3} \sum_{\alpha \in \mathcal{A}} \sum_{\beta \in \mathcal{A}} \sum_{\gamma \in \mathcal{A}} \mathbb{E}[\Psi_\alpha(\mathbf{X})\Psi_\beta(\mathbf{X})\Psi_\gamma(\mathbf{X})] \hat{y}_\alpha \hat{y}_\beta \hat{y}_\gamma \\ \kappa_{\hat{Y}} &\stackrel{\text{def}}{=} \frac{1}{\sigma_{\hat{Y}}^4} \mathbb{E}\left[(\hat{Y} - y_0)^4\right] = \frac{1}{\sigma_{\hat{Y}}^4} \sum_{\alpha \in \mathcal{A}} \sum_{\beta \in \mathcal{A}} \sum_{\gamma \in \mathcal{A}} \sum_{\delta \in \mathcal{A}} \mathbb{E}[\Psi_\alpha(\mathbf{X})\Psi_\beta(\mathbf{X})\Psi_\gamma(\mathbf{X})\Psi_\delta(\mathbf{X})] \hat{y}_\alpha \hat{y}_\beta \hat{y}_\gamma \hat{y}_\delta \end{aligned} \quad (51)$$

The above expectations of products can be given analytical expressions only when Hermite polynomials are used (see Sudret et al. (2006, Appendix I)). Otherwise they may be computed numerically by quadrature.

## 4.2 Distribution analysis and confidence intervals

As shown from Eq.(33) the PC expansion  $\mathcal{M}^{\text{PC}}$  can be used as a polynomial response surface. Thus the output probability density function of  $\hat{Y} = \sum_{\alpha \in \mathcal{A}} \hat{y}_\alpha \Psi_\alpha(\mathbf{X})$  can be obtained by merely sampling the input random vector  $\mathbf{X}$ , say  $\mathcal{X}_{\text{MCS}} = \{\mathbf{x}_1, \dots, \mathbf{x}_{n_{\text{MCS}}}\}$  and evaluating the PC expansion onto this sample, *i.e.*

$$\mathcal{Y}_{\text{MCS}}^{\text{PC}} = \{\mathcal{M}^{\text{PC}}(\mathbf{x}_1), \dots, \mathcal{M}^{\text{PC}}(\mathbf{x}_{n_{\text{MCS}}})\}. \quad (52)$$

Using a sufficiently large sample set (*e.g.*  $n_{\text{MCS}} = 10^{5-6}$ ), one can then compute and plot the almost exact PDF of  $\hat{Y}$  by using a kernel density estimator (Wand and Jones, 1995):

$$\hat{f}_{\hat{Y}}(y) = \frac{1}{n_{\text{MCS}} h} \sum_{i=1}^{n_{\text{MCS}}} K\left(\frac{y - \mathcal{M}^{\text{PC}}(\mathbf{x}_i)}{h}\right). \quad (53)$$

In this equation the *kernel function*  $K$  is a positive definite function integrating to one (*e.g.* the standard normal PDF  $\varphi(y) = e^{-y^2/2}/\sqrt{2\pi}$ ) and  $h$  is the *bandwidth*. The latter can be taken for instance from Silverman's equation:

$$h = 0.9 n_{\text{MCS}}^{-1/5} \min(\hat{\sigma}_{\hat{Y}}, (Q_{0.75} - Q_{0.25})/1.34), \quad (54)$$

where  $\sigma_{\hat{y}}$  (resp.  $Q_{0.25}$ ,  $Q_{0.75}$ ) is the empirical standard deviation of  $\mathcal{Y}_{\text{MCS}}^{\text{PC}}$  (resp. the first and third quartile of  $\mathcal{Y}_{\text{MCS}}^{\text{PC}}$ ). Note that these quantiles as well as any other can be obtained from the large sample set in Eq.(52). Having first reordered it in ascending order, say  $\{\hat{y}_{(1)}, \dots, \hat{y}_{(n_{\text{MCS}})}\}$ , the empirical  $p$ -quantile  $Q_{p\%}$ ,  $0 < p < 1$  is the  $\lfloor p\% \cdot n_{\text{MCS}} \rfloor$ -th point in the ordered sample set, *i.e.*

$$Q_{p\%} = \hat{y}_{(\lfloor p\% \cdot n_{\text{MCS}} \rfloor)}, \quad (55)$$

where  $\lfloor u \rfloor$  is the largest integer that is smaller than  $u$ . This allows one to compute confidence intervals (CI) on the quantity of interest  $\hat{Y}$ . For instance the 95% centered confidence interval, whose bounds are defined by the 2.5% and 97.5% quantile, is

$$CI_{\hat{Y}}^{95\%} = [\hat{y}_{(\lfloor 2.5\% \cdot n_{\text{MCS}} \rfloor)}, \hat{y}_{(\lfloor 97.5\% \cdot n_{\text{MCS}} \rfloor)}]. \quad (56)$$

Note that all the above post-processing may be carried out on large Monte Carlo samples since the function to evaluate in Eq.(52) is the polynomial surrogate model and not the original model  $\mathcal{M}$ . Such an evaluation is nowadays a matter of seconds on standard computers, even with  $n_{\text{MCS}} = 10^{5-6}$ .

### 4.3 Reliability analysis

Reliability analysis aims at computing the probability of failure associated to a performance criterion related to the quantity of interest (QoI)  $Y = \mathcal{M}(\mathbf{X})$ . In general the failure criterion under consideration is represented by a *limit state function*  $g(\mathbf{X})$  defined in the space of parameters as follows (Ditlevsen and Madsen, 1996):

- $\mathcal{D}_s = \{\mathbf{x} \in \mathcal{D}_{\mathbf{X}} : g(\mathbf{x}) > 0\}$  is the *safe domain* of the structure;
- $\mathcal{D}_f = \{\mathbf{x} \in \mathcal{D}_{\mathbf{X}} : g(\mathbf{x}) < 0\}$  is the *failure domain*;
- The set of realizations  $\{\mathbf{x} \in \mathcal{D}_{\mathbf{x}} : g(\mathbf{x}) = 0\}$  is the so-called *limit state surface*.

Typical performance criteria are defined by the fact that the QoI shall be smaller than an admissible threshold  $y_{\text{adm}}$ . According to the above definition the limit state function then reads

$$g(\mathbf{x}) = y_{\text{adm}} - \mathcal{M}(\mathbf{x}). \quad (57)$$

Then the probability of failure of the system is defined as the probability that  $\mathbf{X}$  belongs to the failure domain:

$$P_f = \int_{\{\mathbf{x}: y_{\text{adm}} - \mathcal{M}(\mathbf{x}) \leq 0\}} f_{\mathbf{X}}(\mathbf{x}) d\mathbf{x} = \mathbb{E} [\mathbf{1}_{\{\mathbf{x}: y_{\text{adm}} - \mathcal{M}(\mathbf{x}) \leq 0\}}(\mathbf{X})] \quad (58)$$

where  $f_{\mathbf{X}}$  is the joint probability density function of  $\mathbf{X}$  and  $\mathbf{1}_{\{\mathbf{x}: y_{\text{adm}} - \mathcal{M}(\mathbf{x}) \leq 0\}}$  is the indicator function of the failure domain. In all but academic cases, this integral cannot be computed analytically, since the failure domain is defined from a quantity of interest  $Y = \mathcal{M}(\mathbf{X})$  (*e.g.* displacements, strains, stresses, etc.), which is obtained by means of a computer code (*e.g.* finite element code) in industrial applications.

Once a PC expansion of the QoI is available though, the probability of failure may be obtained by substituting  $\mathcal{M}$  by  $\mathcal{M}^{\text{PC}}$  in Eq.(57):

$$P_f^{\text{PC}} = \int_{\{\mathbf{x}: y_{\text{adm}} - \mathcal{M}^{\text{PC}}(\mathbf{x}) \leq 0\}} f_{\mathbf{X}}(\mathbf{x}) d\mathbf{x} = \mathbb{E} \left[ \mathbf{1}_{\{\mathbf{x}: \mathcal{M}^{\text{PC}}(\mathbf{x}) \geq y_{\text{adm}}\}}(\mathbf{X}) \right] \quad (59)$$

The latter can be estimated by crude Monte Carlo simulation. Using the sample set in Eq.(52) one computes the number  $n_f$  of samples such that  $\mathcal{M}^{\text{PC}}(\mathbf{x}_i) \geq y_{\text{adm}}$ . Then the estimate of the probability of failure reads:

$$\widehat{P}_f^{\text{PC}} = \frac{n_f}{n_{\text{MCS}}} \quad (60)$$

This crude Monte Carlo approach will typically work efficiently if  $P_f \leq 10^{-4}$ , *i.e.* if at most  $10^6$  runs of PC expansion are required. Note that any standard reliability method such as importance sampling or subset simulation could be also used.

## 4.4 Sensitivity analysis

### 4.4.1 Sobol' decomposition

Global sensitivity analysis (GSA) aims at quantifying which input parameters  $\{X_i, i = 1, \dots, M\}$  or combinations thereof explain at best the variability of the quantity of interest  $Y = \mathcal{M}(\mathbf{X})$  (Saltelli et al., 2000, 2008). This variability being well described by the variance of  $Y$ , the question reduces to apportioning  $\text{Var}[Y]$  to each input parameter  $\{X_1, \dots, X_M\}$ , second-order interactions  $X_i X_j$ , etc. For this purpose variance decomposition techniques have gained interest since the mid 90's. The Sobol' decomposition (Sobol', 1993) states that any square integrable function  $\mathcal{M}$  with respect to a probability measure associated with a PDF  $f_{\mathbf{X}}(\mathbf{x}) = \prod_{i=1}^M f_{X_i}(x_i)$  (independent components) may be cast as:

$$\mathcal{M}(\mathbf{x}) = \mathcal{M}_0 + \sum_{i=1}^M \mathcal{M}_i(x_i) + \sum_{1 \leq i < j \leq M} \mathcal{M}_{ij}(x_i, x_j) + \dots + \mathcal{M}_{12\dots M}(\mathbf{x}) \quad (61)$$

that is, as a sum of a constant, univariate functions  $\{\mathcal{M}_i(x_i), 1 \leq i \leq M\}$ , bivariate functions  $\{\mathcal{M}_{ij}(x_i, x_j), 1 \leq i < j \leq M\}$ , etc. Using the *set notation* for indices

$$\mathbf{u} \stackrel{\text{def}}{=} \{i_1, \dots, i_s\} \subset \{1, \dots, M\}, \quad (62)$$

the Sobol' decomposition in Eq.(61) reads:

$$\mathcal{M}(\mathbf{x}) = \mathcal{M}_0 + \sum_{\substack{\mathbf{u} \subset \{1, \dots, M\} \\ \mathbf{u} \neq \emptyset}} \mathcal{M}_{\mathbf{u}}(\mathbf{x}_{\mathbf{u}}) \quad (63)$$

where  $\mathbf{x}_{\mathbf{u}}$  is a subvector of  $\mathbf{x}$  which only contains the components that belong to the index set  $\mathbf{u}$ . It can be proven that the Sobol' decomposition is unique when the orthogonality between summands is required, namely:

$$\mathbb{E}[\mathcal{M}_{\mathbf{u}}(\mathbf{x}_{\mathbf{u}}) \mathcal{M}_{\mathbf{v}}(\mathbf{x}_{\mathbf{v}})] = 0 \quad \forall \mathbf{u}, \mathbf{v} \subset \{1, \dots, M\}, \quad \mathbf{u} \neq \mathbf{v} \quad (64)$$



A recursive construction is obtained by the following recurrence relationship:

$$\begin{aligned}\mathcal{M}_0 &= \mathbb{E}[\mathcal{M}(\mathbf{X})] \\ \mathcal{M}_i(x_i) &= \mathbb{E}[\mathcal{M}(\mathbf{X})|X_i = x_i] - \mathcal{M}_0 \\ \mathcal{M}_{ij}(x_i, x_j) &= \mathbb{E}[\mathcal{M}(\mathbf{X})|X_i, X_j = x_i, x_j] - \mathcal{M}_i(x_i) - \mathcal{M}_j(x_j) - \mathcal{M}_0\end{aligned}\tag{65}$$

The latter equation is of little interest in practice since the integrals required to compute the various conditional expectations are cumbersome. Nevertheless the existence and unicity of Eq.(61) together with the orthogonality property in Eq.(64) now allow one to decompose the variance of  $Y$  as follows:

$$D \stackrel{\text{def}}{=} \text{Var}[Y] = \text{Var}\left[\sum_{\substack{\mathbf{u} \subset \{1, \dots, M\} \\ \mathbf{u} \neq \emptyset}} \mathcal{M}_{\mathbf{u}}(\mathbf{x}_{\mathbf{u}})\right] = \sum_{\substack{\mathbf{u} \subset \{1, \dots, M\} \\ \mathbf{u} \neq \emptyset}} \text{Var}[\mathcal{M}_{\mathbf{u}}(\mathbf{X}_{\mathbf{u}})]\tag{66}$$

where the *partial variances* read:

$$D_{\mathbf{u}} \stackrel{\text{def}}{=} \text{Var}[\mathcal{M}_{\mathbf{u}}(\mathbf{X}_{\mathbf{u}})] = \mathbb{E}[\mathcal{M}_{\mathbf{u}}^2(\mathbf{X}_{\mathbf{u}})].\tag{67}$$

#### 4.4.2 Sobol' indices

The so-called *Sobol' indices* are defined as the ratio of the partial variances  $D_{\mathbf{u}}$  to the total variance  $D$ . The so-called *first-order indices* correspond to single input variables, *i.e.*  $\mathbf{u} = \{i\}$ :

$$S_i = \frac{D_i}{D} = \frac{\text{Var}[\mathcal{M}_i(X_i)]}{\text{Var}[Y]}\tag{68}$$

The second-order indices ( $\mathbf{u} = \{i, j\}$ ) read:

$$S_{ij} = \frac{D_{ij}}{D} = \frac{\text{Var}[\mathcal{M}_{ij}(X_i, X_j)]}{\text{Var}[Y]}\tag{69}$$

etc. Note that the *total Sobol' index*  $S_i^T$ , which quantifies the total impact of a given parameter  $X_i$  including all interactions, may be computed by the sum of the Sobol' indices of any order that contain  $X_i$ :

$$S_i^T = \sum_{i \in \mathbf{u}} S_{\mathbf{u}}\tag{70}$$

#### 4.4.3 Sobol' indices from PC expansions

Sobol' indices have proven to be the most efficient sensitivity measures for general computational models (Saltelli et al., 2008). However they are traditionally evaluated by Monte Carlo simulation (possibly using quasi-random sequences) (Sobol' and Kucherenko, 2005), which make them difficult to use when costly computational models  $\mathcal{M}$  are used. In order to bypass the problem Sudret (2006, 2008) has proposed an original post-processing of polynomial chaos expansions for sensitivity analysis. Indeed, the Sobol' decomposition of

a truncated PC expansion  $\hat{Y} = \mathcal{M}^{\text{PC}}(\mathbf{X}) = \sum_{\alpha \in \mathcal{A}} \hat{y}_\alpha \Psi_\alpha(\mathbf{X})$  can be established *analytically*, as shown below.

For any subset of variables  $\mathbf{u} = \{i_1, \dots, i_s\} \subset \{1, \dots, M\}$  let us define the set of multivariate polynomials  $\Psi_\alpha$  which depend *only* on  $\mathbf{u}$ :

$$\mathcal{A}_\mathbf{u} = \{\alpha \in \mathcal{A} : \alpha_k \neq 0 \text{ if and only if } k \in \mathbf{u}\}. \quad (71)$$

It is clear that the  $\mathcal{A}_\mathbf{u}$ 's form a partition of  $\mathcal{A}$  since

$$\bigcup_{\mathbf{u} \subset \{1, \dots, M\}} \mathcal{A}_\mathbf{u} = \mathcal{A}. \quad (72)$$

Thus a truncated PC expansion such as in Eq.(33) may be rewritten as follows by simple reordering of the terms:

$$\mathcal{M}^{\text{PC}}(\mathbf{x}) = y_0 + \sum_{\substack{\mathbf{u} \subset \{1, \dots, M\} \\ \mathbf{u} \neq \emptyset}} \mathcal{M}_\mathbf{u}^{\text{PC}}(\mathbf{x}_\mathbf{u}) \quad (73)$$

where:

$$\mathcal{M}_\mathbf{u}^{\text{PC}}(\mathbf{x}_\mathbf{u}) \stackrel{\text{def}}{=} \sum_{\alpha \in \mathcal{A}_\mathbf{u}} y_\alpha \Psi_\alpha(\mathbf{x}) \quad (74)$$

Consequently, due to the orthogonality of the PC basis, the partial variance  $D_\mathbf{u}$  reduces to:

$$D_\mathbf{u} = \text{Var} [\mathcal{M}_\mathbf{u}^{\text{PC}}(\mathbf{X}_\mathbf{u})] = \sum_{\alpha \in \mathcal{A}_\mathbf{u}} y_\alpha^2 \quad (75)$$

In other words, from a given PC expansion, the Sobol' indices *at any order* may be obtained by a mere combination of the squares of the coefficients. As an illustration the first-order PC-based Sobol' indices read:

$$S_i^{\text{PC}} = \sum_{\alpha \in \mathcal{A}_i} y_\alpha^2 / D \quad \mathcal{A}_i = \{\alpha \in \mathcal{A} : \alpha_i > 0, \alpha_{j \neq i} = 0\} \quad (76)$$

whereas the total PC-based Sobol' indices are:

$$S_i^{T, \text{PC}} = \sum_{\alpha \in \mathcal{A}_i^T} y_\alpha^2 / D \quad \mathcal{A}_i^T = \{\alpha \in \mathcal{A} : \alpha_i > 0\} \quad (77)$$

Polynomial chaos expansions and the various types of post-processing presented above are now applied to different classical geotechnical problems.

## 5 Application examples

### 5.1 Load carrying capacity of a strip footing

#### 5.1.1 Independent input variables

Let us consider the strip footing of width  $B = 10$  m sketched in Figure 6 which is embedded at depth  $D$ . We assume that the ground water table is far below the surface.

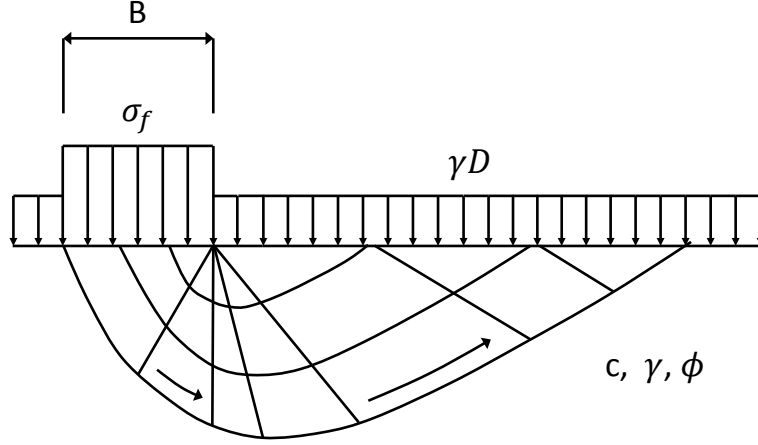


Figure 6: Example #1 : Strip footing

The soil layer is assumed homogeneous with cohesion  $c$ , friction angle  $\phi$  and unit weight  $\gamma$ .

The ultimate bearing capacity reads (Lang et al., 2007):

$$q_u = c N_c + \gamma D N_q + \frac{1}{2} B \gamma N_\gamma \quad (78)$$

where the bearing capacity factors read:

$$\begin{aligned} N_q &= e^{\pi \tan \phi} \tan^2(\pi/4 + \phi/2) \\ N_c &= (N_q - 1) \cot \phi \\ N_\gamma &= 2(N_q - 1) \tan \phi \end{aligned} \quad (79)$$

The soil parameters and the foundation depth are considered as independent random variables, whose properties are listed in Table 3. Let us denote the model input vector by  $\mathbf{X} = \{D, \gamma, c, \phi\}^T$ . The associated random bearing capacity is  $q_u(\mathbf{X})$ .

Table 3: Ultimate bearing capacity of a strip foundation – probabilistic model

Parameter	Notation	Type of PDF	Mean value	Coef. of variation
Foundation width	$B$	Deterministic	10 m	-
Foundation depth	$D$	Gaussian	1 m	15%
Unit soil weight	$\gamma$	Lognormal	20 kN/m <sup>3</sup>	10 %
Cohesion	$c$	Lognormal	20 kPa	25%
Friction angle	$\phi$	Beta	Range:[0, 45] <sup>°</sup> , $\mu = 30^\circ$	=10%

Using the mean values of the parameters in Table 3 the ultimate bearing capacity is equal to  $\bar{q}_u = 2.78$  MPa. We consider now several design situations with applied loads  $q_{des} = \bar{q}_u/SF$  where  $SF = 1.5, 2, 2.5, 3$  would be the global safety factor obtained from a deterministic design. Then we consider the reliability of the foundation with respect to

the ultimate bearing capacity. The limit state function reads:

$$g(\mathbf{X}) = q_u(\mathbf{X}) - q_{des} = q_u(\mathbf{X}) - \bar{q}_u/SF \quad (80)$$

Classical reliability methods are used, namely FORM, SORM and crude Monte Carlo simulation (MCS) with  $10^7$  samples in order to get a reference solution. The uncertainty quantification software UQLab is used (Marelli and Sudret, 2014). Alternatively a PC expansion  $q_u^{PC}(\mathbf{X})$  of the ultimate bearing capacity is first computed using a LHS experimental design of size  $n = 500$ . Then the PC expansion is substituted for in Eq.(80) and the associated probability of failure is computed by Monte Carlo simulation ( $10^7$  samples), now using the PC expansion only (and for the different values of SF). The results are reported in Table 4.

Table 4: Ultimate bearing capacity of a strip foundation – Probability of failure (resp. generalized reliability index  $\beta_{gen} = -\Phi^{-1}(P_f)$  between parentheses) – Case of independent variables

$SF$	FORM	SORM	MCS ( $10^7$ runs)	PCE +MCS <sup>†</sup>
1.5	$1.73 \cdot 10^{-1}$ (0.94)	$1.70 \cdot 10^{-1}$ (0.96)	$1.69 \cdot 10^{-1}$ (0.96)	$1.70 \cdot 10^{-1}$ (0.96)
2.0	$5.49 \cdot 10^{-2}$ (1.60)	$5.30 \cdot 10^{-2}$ (1.62)	$5.30 \cdot 10^{-2}$ (1.62)	$5.29 \cdot 10^{-2}$ (1.62)
2.5	$1.72 \cdot 10^{-2}$ (2.11)	$1.65 \cdot 10^{-2}$ (2.13)	$1.63 \cdot 10^{-2}$ (2.14)	$1.65 \cdot 10^{-2}$ (2.13)
3.0	$5.54 \cdot 10^{-3}$ (2.54)	$5.23 \cdot 10^{-3}$ (2.56)	$5.24 \cdot 10^{-3}$ (2.56)	$5.20 \cdot 10^{-3}$ (2.56)

<sup>†</sup>  $n = 500, n_{MCS} = 10^7$

From Table 4 it is clear that the results obtained by PC expansion are almost equal to those obtained by the reference Monte Carlo simulation. The relative error in terms of the probability of failure is all in all less than one 1% (the corresponding error on the generalized reliability index  $\beta_{gen} = -\Phi^{-1}(P_f)$  is negligible).

The number of runs associated to FORM (resp. SORM) are 31 for  $SF=1.5$  and 2, and 35 for  $SF =2.5$  and 3 (resp. 65 for  $SF=1.5$  and 2, and 69 for  $SF =2.5$  and 3). Note that for each value of  $SF$  a new analysis FORM/SORM analysis shall be run. In contrast to FORM/SORM, a *single* PC expansion has been used to obtain the reliability associated to all safety factors. Using 500 points in the experimental design, *i.e.* 500 evaluations of  $q_u(\mathbf{X})$ , the obtained PC expansion provides a normalized LOO error equal to  $1.7 \cdot 10^{-7}$  (the maximal PC degree is 6 and the number of terms in the sparse expansion is 140).

### 5.1.2 Correlated input variables

For a more realistic modelling of the soil properties one now considers the statistical dependence between the cohesion  $c$  and the friction angle  $\phi$ . From the literature (see a review in Al Bittar and Soubra (2013)) the correlation between these parameters is negative with a value around  $-0.5$ . In this section we model the dependence between  $c$  and  $\phi$  by a Gaussian copula which is parametrized by the *rank correlation coefficient*

$\rho_R = -0.5$ . Due to the choice of marginal distributions in Table 3 this corresponds to a linear correlation of  $-0.512$ . Using 500 points in the experimental design, *i.e.* 500 evaluations of  $q_u(\mathbf{X})$ , the obtained PC expansion provides a LOO error equal to  $6.8 \cdot 10^{-7}$  (the maximal PC degree is 6 and the number of terms in the sparse expansion is 172). The reliability results accounting for correlation are reported in Table 5.

Table 5: Ultimate bearing capacity of a strip foundation – Probability of failure (resp. generalized reliability index  $\beta_{gen} = \Phi^{-1}(P_f)$  between parentheses) – Case of dependent  $(c, \phi)$

$SF$	FORM	SORM	MCS ( $10^7$ runs.)	PCE +MCS <sup>†</sup>
1.5	$1.55 \cdot 10^{-1}$ (1.01)	$1.52 \cdot 10^{-1}$ (1.03)	$1.51 \cdot 10^{-1}$ (1.03)	$1.52 \cdot 10^{-1}$ (1.03)
2.0	$4.02 \cdot 10^{-2}$ (1.75)	$3.85 \cdot 10^{-2}$ (1.77)	$3.85 \cdot 10^{-2}$ (1.77)	$3.85 \cdot 10^{-2}$ (1.77)
2.5	$9.60 \cdot 10^{-3}$ (2.34)	$8.98 \cdot 10^{-3}$ (2.37)	$8.98 \cdot 10^{-3}$ (2.37)	$8.99 \cdot 10^{-3}$ (2.37)
3.0	$2.20 \cdot 10^{-3}$ (2.85)	$2.00 \cdot 10^{-3}$ (2.88)	$2.01 \cdot 10^{-3}$ (2.88)	$2.00 \cdot 10^{-3}$ (2.88)

<sup>†</sup>  $n = 500, n_{MCS} = 10^7$

These results show that polynomial chaos expansions may be applied to solve reliability problems also when the variables in the limit state function are correlated. In terms of accuracy, the PCE results compare very well with the reference results obtained by MCS, the error on the probability of failure being again less than 1%. SORM provides accurate results as well, at a cost of 65, 65, 72 and 83 runs when SF=1.5, 2, 2.5, 3 (the associated FORM analysis required 31, 31, 38 and 49 runs). Moreover, it clearly appears that neglecting the correlation between  $c$  and  $\phi$  leads to a conservative estimation of the probability of failure, *e.g.* by a factor 2.5 for  $SF = 3$  (10% underestimation of the generalized reliability index).

## 5.2 Settlement of a foundation on an elastic 2-layer soil mass

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  $2B_1 = 10\text{ m}$  of the free surface. An additional load  $P_2$  is applied over a length  $2B_2 = 5\text{ m}$  (Figure 7-(a)).

Due to the symmetry, half of the structure is modeled by finite elements (Figure 7-(b)). The mesh comprises 500 QUAD4 isoparametric elements. A plane strain analysis is carried out. The geometry is considered as deterministic. The elastic material properties of both layers and the applied loads are modelled by random variables, whose PDF are specified in Table 6. All six random variables are supposed to be independent.

The quantity of interest is the maximum vertical displacement  $u_A$  at point A, *i.e.* on the symmetry axis of the problem. The finite element model is thus considered a black-box  $\mathcal{M}^{FE}$  that computes  $u_A$  as a function of the six input parameters  $\mathbf{X} =$

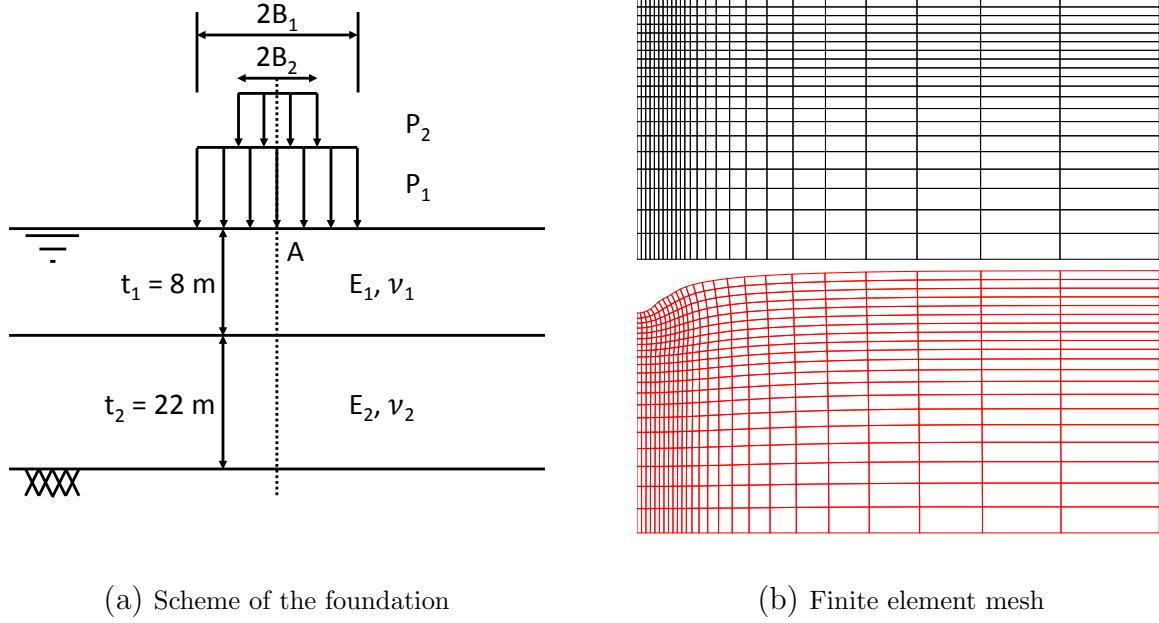


Figure 7: Example #2 : Foundation on a two-layer soil mass

Table 6: Example #1 : 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	8 m	-
Lower layer soil thickness	$t_2$	Deterministic	22 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 ratio	$\nu_1$	Uniform	0.3	15 %
Lower layer Poisson ratio	$\nu_2$	Uniform	0.3	15 %
Load #1	$P_1$	Gamma	0.2 MPa	20 %
Load #2	$P_2$	Weibull	0.4 MPa	20 %

$\{E_1, E_2, \nu_1, \nu_2, P_1, P_2\}^T$ :

$$u_A = \mathcal{M}^{\text{FE}}(E_1, E_2, \nu_1, \nu_2, P_1, P_2). \quad (81)$$

The serviceability of this foundation on a layered soil mass vis-à-vis an admissible settlement is studied. The limit state function is defined by:

$$g(\mathbf{X}) = u_{\text{adm}} - u_A = u_{\text{adm}} - \mathcal{M}^{\text{FE}}(E_1, E_2, \nu_1, \nu_2, P_1, P_2), \quad (82)$$

in which the admissible settlement is chosen to 12, 15, 20 and 21 cm. First FORM and SORM are applied, together with importance sampling (IS) at the design point using  $n_{\text{MCS}} = 10^4$  samples. The latter is considered as the reference solution. Results are reported in Table 7.

Then PC expansions of the maximal settlement  $\mathcal{M}^{\text{PC}}$  are computed using different experimental designs (ED) of increasing size, namely  $n = 100, 200, 500, 1000$  using the

Table 7: Settlement of a foundation on a two-layer soil mass – reliability results

Threshold	FORM		SORM		Importance Sampling	
$u_{\text{adm}}$	$P_{f,\text{FORM}}$	$\beta$	$P_{f,\text{SORM}}$	$\beta$	$P_{f,\text{IS}}$	$\beta$
12 cm	$1.54 \cdot 10^{-1}$	1.02	$1.38 \cdot 10^{-1}$	1.09	$1.42 \cdot 10^{-1}$ [CoV = 1.27%]	1.07
15 cm	$1.64 \cdot 10^{-2}$	2.13	$1.36 \cdot 10^{-2}$	2.21	$1.43 \cdot 10^{-2}$ [CoV = 1.67%]	2.19
20 cm	$1.54 \cdot 10^{-4}$	3.61	$1.17 \cdot 10^{-4}$	3.68	$1.23 \cdot 10^{-4}$ [CoV = 2.23%]	3.67
21 cm	$5.57 \cdot 10^{-5}$	3.86	$4.14 \cdot 10^{-5}$	3.94	$4.53 \cdot 10^{-5}$ [CoV = 2.27%]	3.91

UQLab platform (Marelli and Sudret, 2014). The obtained expansion is then substituted for in the limit state function Eq.(82) and the associated reliability problem is solved using crude Monte Carlo simulation ( $n_{\text{MCS}} = 10^6$  samples). The results are reported in Table 8.

Table 8: Settlement of a foundation on a two-layer soil mass – reliability results from PC expansion (MCS with  $n_{\text{MCS}} = 10^7$ )

Threshold	$n = 100$		$n = 200$		$n = 500$		$n = 1000$	
$u_{\text{adm}}$	$P_f$	$\beta$	$P_f$	$\beta$	$P_f$	$\beta$	$P_f$	$\beta$
12 cm	$1.44 \cdot 10^{-1}$	1.06	$1.45 \cdot 10^{-1}$	1.06	$1.44 \cdot 10^{-01}$	1.06	$1.44 \cdot 10^{-1}$	1.06
	[CoV = 0.08%]		[CoV = 0.08%]		[CoV = 0.08%]		[CoV = 0.08%]	
15 cm	$1.33 \cdot 10^{-2}$	2.22	$1.44 \cdot 10^{-2}$	2.19	$1.45 \cdot 10^{-02}$	2.18	$1.45 \cdot 10^{-2}$	2.18
	[CoV = 0.27%]		[CoV = 0.26%]		[CoV = 0.26%]		[CoV = 0.26%]	
20 cm	$5.84 \cdot 10^{-5}$	3.85	$1.13 \cdot 10^{-4}$	3.69	$1.26 \cdot 10^{-04}$	3.66	$1.24 \cdot 10^{-4}$	3.66
	[CoV = 4.14%]		[CoV = 2.97%]		[CoV = 2.82%]		[CoV = 2.84%]	
21 cm	$1.66 \cdot 10^{-5}$	4.15	$3.64 \cdot 10^{-5}$	3.97	$4.72 \cdot 10^{-05}$	3.90	$4.56 \cdot 10^{-5}$	3.91
	[CoV = 7.76%]		[CoV = 5.24%]		[CoV = 4.60%]		[CoV = 4.68%]	

It can be observed that the results obtained from the PC expansion compare very well to the reference as soon as  $n = 200$  points are used in the experimental design. The error is less than 1% in the generalized reliability index, for values as large as  $\beta = 4$ , *i.e.* for probabilities of failure in the order of  $10^{-5}$ . The detailed features of the PC expansions built for each experimental design of size  $n = 100, 200, 500, 1,000$  are reported in Table 9.

Again the sparsity of the expansions is clear: a full expansion with all polynomials up to degree  $p = 4$  in  $M = 6$  variables has  $P = \binom{6+4}{4} = 210$  terms, which would typically require an experimental design of size  $2 \times 210 = 440$ . Using only  $n = 100$  points a sparse PC expansion having 59 terms could be built up. It is also observed that the classical (normalized) empirical error  $1 - R^2$  is typically one order of magnitude smaller than the

Table 9: Settlement of a foundation on a two-layer soil mass – PC expansion features ( $p$  stands for the maximal degree of polynomials and  $P$  is the number of non zero terms polynomials in the sparse expansion)

	$n = 100$	$n = 200$	$n = 500$	$n = 1000$
$1 - R^2$ (Eq.(37))	$8.45 \cdot 10^{-5}$	$6.76 \cdot 10^{-6}$	$1.25 \cdot 10^{-6}$	$1.14 \cdot 10^{-7}$
$\hat{\epsilon}_{LOO}$ (Eq.(44))	$1.20 \cdot 10^{-3}$	$2.39 \cdot 10^{-4}$	$1.33 \cdot 10^{-5}$	$2.08 \cdot 10^{-6}$
$p$	4	4	4	5
$P$	59	126	152	225

leave-one-out normalized error, the latter being a closer estimate of the real generalization error.

### 5.3 Settlement of a foundation on soil mass with spatially varying Young’s modulus (after Blatman (2009))

Let us now consider a foundation on an elastic soil layer showing spatial variability in its material properties. A structure to be founded on this soil mass is idealized as a uniform pressure  $P$  applied over a length  $2B = 20$  m of the free surface (Figure 8).

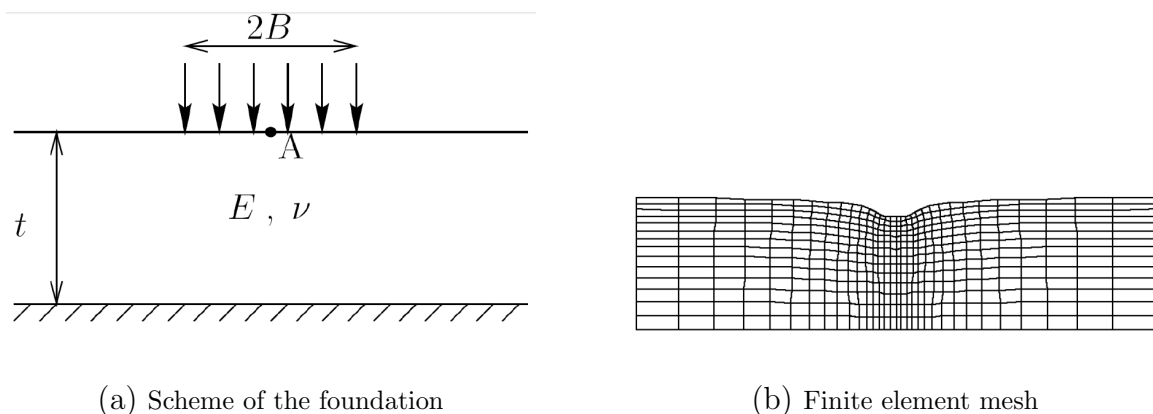


Figure 8: Example #3: Foundation on a soil mass with spatially varying Young’s modulus

The soil layer thickness is equal to 30 m. The soil mesh width is equal to 120 m. The soil layer is modelled as an elastic linear isotropic material with Poisson’s ratio equal to 0.3. A plane strain analysis is carried out. The finite element mesh is made of 448 QUAD4-elements. The Young’s modulus is modelled by a two-dimensional homogeneous *lognormal* random field with mean value  $\mu_E = 50$  MPa and a coefficient of variation of 30%. The underlying Gaussian random field  $\log E(\mathbf{x}, \omega)$  has a square-exponential autocorrelation function:

$$\rho_{\log E}(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{\|\mathbf{x} - \mathbf{x}'\|^2}{\ell^2}\right), \quad (83)$$

where  $\ell = 15$  m. The Gaussian random field  $\log E(\mathbf{x}, \omega)$  is discretized using the Karhunen-Loève (KL) expansion (Loève, 1978; Sudret and Der Kiureghian, 2000), (Sudret and



Berveiller, 2007, Chap. 7):

$$\log E(\mathbf{x}, \omega) = \mu_{\log E} + \sigma_{\log E} \sum_{i=1}^{\infty} \sqrt{\lambda_i} \xi_i(\omega) \phi_i(\mathbf{x}) \quad (84)$$

where  $\{\xi_i(\omega)\}_{i=1}^{\infty}$  are independent standard normal variables and the pairs  $\{(\lambda_i, \phi_i)\}_{i=1}^{\infty}$  are solution of the following eigenvalue problem (Fredholm integral of the second kind):

$$\int \rho_{\log E}(\mathbf{x}, \mathbf{x}') \varphi_i(\mathbf{x}') d\mathbf{x}' = \lambda_i \varphi_i(\mathbf{x}) \quad (85)$$

As no analytical solution to the Fredholm equation exists for this type of autocorrelation function, the latter is solved by expanding the eigenmodes onto an orthogonal polynomial basis, see details in Blatman (2009, Appendix B). Note that other numerical methods have been proposed in the literature (Phoon et al., 2002b,a, 2005; Li et al., 2007). Eventually 38 modes are retained in the truncated expansion:

$$\log E(\mathbf{x}, \omega) \approx \mu_{\log E} + \sigma_{\log E} \sum_{i=1}^{38} \sqrt{\lambda_i} \xi_i(\omega) \phi_i(\mathbf{x}), \quad (86)$$

where  $\mu_{\log E} = 3.8689$  and  $\sigma_{\log E} = 0.2936$  in the present application. The 9 first eigenmodes are plotted in Figure 9 for the sake of illustration. Note that these 38 modes allow one to account for 99% of the variance of the Gaussian field.

The *average settlement under the foundation* is computed by finite element analysis. It may be considered as a random variable  $Y = \mathcal{M}(\boldsymbol{\xi})$ , where  $\boldsymbol{\xi}$  is the standard normal vector of dimension 38 that enters the truncated KL expansion. Of interest is the sensitivity of this average settlement to the various modes appearing in the KL expansion. To address this problem, a sparse PC expansion is built using a LHS experimental design of size  $n = 200$ . It allows one to get a LOO error less than 5%. From the obtained expansion the total Sobol' indices related to each input variable  $\xi_i$  (*i.e.* each mode in the KL expansion) are computed and plotted in Figure 10

It appears that only 7 modes contribute to the variability of the settlement. This may be explained by the fact that the model response is an averaged quantity over the domain of application of the load, which is therefore rather insensitive to small-scale fluctuations of the spatially variable random Young's modulus. Note that some modes have a zero total Sobol' index, namely modes #2, 4, 7 and 8. From Figure 10 it appears that they correspond to *antisymmetric modes* with respect to the vertical axis (see Figure 9). This means that the symmetry of the problem is accounted for in the analysis. It is now clear why the PC expansion is sparse since roughly half of the modes (*i.e.* half of the input variables of the uncertainty quantification problem) do not play any role in the analysis.

## 5.4 Conclusions

In this section three different problems of interest in geotechnical engineering have been addressed, namely the bearing capacity of a strip footing, the maximal settlement of a

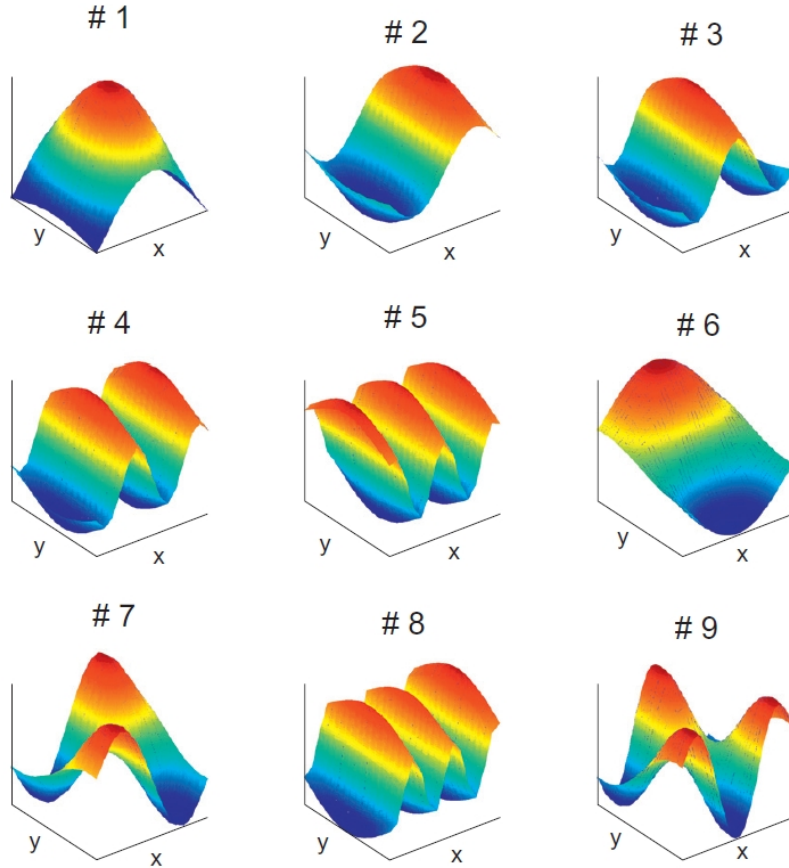


Figure 9: Example #3: First modes of the Karhunen-Loève expansion of the Young's modulus (after Blatman and Sudret (2011a))

foundation on a two-layer soil mass, and the settlement in case of a single layer with spatially-varying Young's modulus. In the two first cases reliability analysis is carried out as a post-processing of a PC expansion. The results in terms of probability of failure compare very well with those obtained by reference methods such as importance sampling at the design point. From a broader experience in structural reliability analysis, it appears that PC expansions are suitable for reliability analysis as long as the probability of failure to be computed is smaller than  $10^{-5}$ . For very small probabilities, suitable methods such as adaptive Kriging shall be rather used (Dubourg et al., 2011; Sudret, 2012)

In the last example the spatial variability of the soil properties is introduced. The purpose is to show that problems involving a large number of random input variables (here, 38) may be solved at an affordable cost using sparse PC expansions (here, 200 samples in the experimental design). Recent applications of this approach to the bearing capacity of 2D and 3D foundations can be found in Al Bittar and Soubra (2013); Mao et al. (2012).

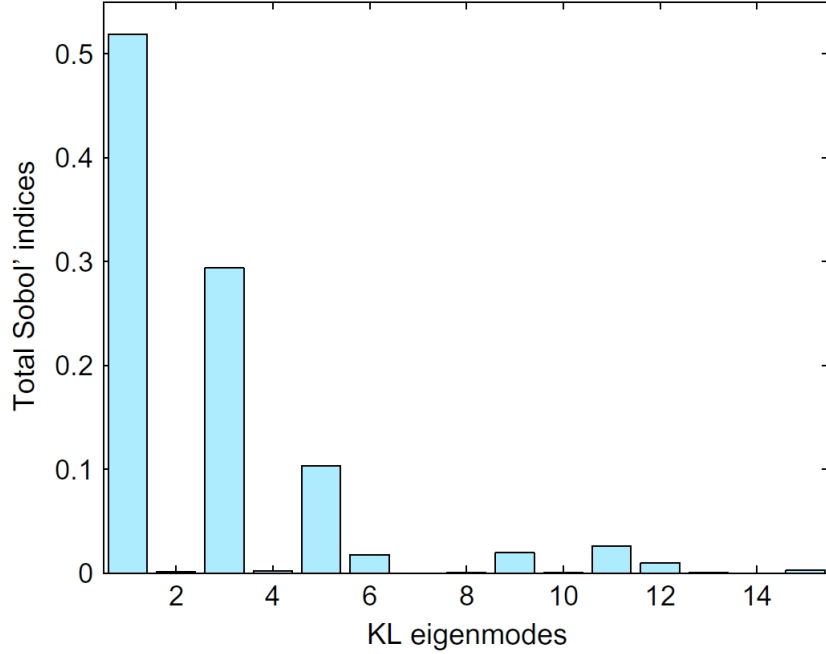


Figure 10: Example #3 : Foundation on a soil mass with spatially varying Young's modulus – Total Sobol' indices (after Blatman and Sudret (2011a))

## 6 Conclusions

Accounting for uncertainties has become a crucial issue in modern geotechnical engineering due to the large variability of soil properties as well as the associated limited information. The uncertainty analysis framework that is nowadays widely used in many fields applies equally to geotechnics. Starting from a computational model used for assessing the system performance, the input parameters are represented by random variables or fields. The effect of the input uncertainty onto the model response (*i.e.* the system performance) can be assessed by a number of numerical methods.

Monte Carlo simulation (MCS) offers a sound framework for uncertainty propagation, however its low efficiency precludes its use for analyses involving finite element models. Classical structural reliability methods such as FORM and SORM may be used, at the price of some linearizations and approximations. In contrast, the so-called polynomial chaos expansions allow for an accurate, intrinsic representation of the model output. The series expansion coefficients may be computed using non intrusive schemes which are similar in essence to MCS: a sample set of input vectors is simulated and the corresponding model output evaluated. From this data, algorithms such as least-square minimization or least-angle regression may be used.

The resulting series expansion can be post-processed in order to compute the statistical moments of the model response (mean value, standard deviation, etc.), quantiles and confidence intervals or even the probability density function. In the latter case, the PC expansion is used as a surrogate to the original computational model. Due to its polynomial expression it can be used together with Monte Carlo simulation and kernel

smoothing techniques.

PC expansions appear also extremely efficient in the context of sensitivity analysis. The Sobol' indices, which are considered as the most accurate sensitivity measures, may be computed analytically from PC expansions coefficients by simple algebra. The PC expansion itself may be reordered so as to exhibit the so-called Sobol' decomposition, which allows for detecting the linear and non linear effects of the input variables as well as their interaction.

Problems involving spatial variability of the material properties may be efficiently addressed by introducing random fields and using discretization techniques. The discretized field is represented by a vector of (usually) standard normal variables, whose size may be large (*e.g.* 20-100) especially when the correlation length of the field is small. However, the so-called sparse PC expansion technique may be used so that the full analysis can be carried out using a few hundred to a thousand model runs.

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## Appendix A: List of symbols

$\alpha$	Multi-index of $\Psi_\alpha$
$\delta_Y^2$	PC-based response skewness
$D_i, D_{\mathbf{u}}$	Partial variance
$\widehat{Err}_E$	Empirical error
$\widehat{Err}_{LOO}$	Leave-one-out error
$f_{\mathbf{X}}$	Probability density function of the input vector
$f_{X_i}$	Marginal distribution of $X_i$
$g(\cdot)$	Limit state function
$h$	Kernel bandwidth
$H_{e_j}$	Hermite polynomial
$\kappa_Y^2$	PC-based response kurtosis
$K(\cdot)$	Kernel function
$M$	Dimension of the input random vector $\mathbf{X}$
MCS	Abbreviation of ‘‘Monte Carlo simulation’’
$P_j$	Legendre polynomials
$P_f$	Probability of failure
PC	Abbreviation of ‘‘polynomial chaos’’
$\pi_j^{(i)}, \psi_j^{(i)}$	Univariate orthogonal (resp. orthonormal) polynomials
$Q_{p\%}$	$p\%$ -quantile
$\sigma_Y^2$	PC-based response variance
$S_i, S_{ij}$	Sobol’ index
$S_i^T$	Total Sobol’ index
$\mathbf{X}$	Input random vector
$y = \mathcal{M}(\mathbf{x})$	Model response (quantity of interest)
$y_\alpha$	Coefficient of the polynomial chaos expansion
$\Psi_\alpha(\mathbf{x})$	Multivariate orthonormal polynomials
$\mathcal{A}, \mathcal{A}^{M,p}$	Truncation set
$\mathcal{A}^{M,p,q}$	Hyperbolic truncation set
$\mathcal{D}_s, \mathcal{D}_f$	Safe (resp. failure) domain
$\mathcal{LN}(\lambda, \zeta)$	Lognormal distribution
$\mathcal{M}$	computational model
$\mathcal{M}_i(x_i), \mathcal{M}_{ij}(x_i, x_j), \mathcal{M}_{\mathbf{u}}(x_{\mathbf{u}})$	Terms in the Sobol’-Hoeffding decomposition
$\mathcal{T}$	Isoprobabilistic transform
$\mathcal{U}(a, b)$	Uniform distribution on $[a, b]$
$\mathcal{X}$	Experimental design of computer simulations

## Appendix B: Hermite polynomials

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

$$y'' - x y' + n y = 0 \quad n \in \mathbb{N} \quad (\text{A.1})$$

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

$$He_0(x) = 1 \quad (\text{A.2})$$

$$He_{n+1}(x) = x He_n(x) - n He_{n-1}(x) \quad (\text{A.3})$$

They are orthogonal with respect to the Gaussian probability measure:

$$\int_{-\infty}^{\infty} He_m(x) He_n(x) \varphi(x) dx = n! \delta_{mn} \quad (\text{A.4})$$

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

$$\mathbb{E}[He_m(U) He_n(U)] = n! \delta_{mn} \quad (\text{A.5})$$

The first four Hermite polynomials are:

$$He_0(x) = 1 \quad He_1(x) = x \quad He_2(x) = x^2 - 1 \quad He_3(x) = x^3 - 3x \quad (\text{A.6})$$

Due to (A.5) the orthonormal polynomials read:

$$\psi_0(x) = 1 \quad \psi_1(x) = x \quad \psi_2(x) = (x^2 - 1)/\sqrt{2} \quad \psi_3(x) = (x^3 - 3x)/\sqrt{6} \quad (\text{A.7})$$

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