Chapter 8

Response surfaces based on polynomial chaos expansions

8.1. Introduction

8.1.1. *Statement of the reliability problem*

Let us recall the problem stated in the introduction of Chapter 1. Of interest is a building or a part of a building reduced to a mechanical structure, whose behaviour may be represented by a *mechanical model*. The latter is described by a transfer function $\mathcal{M}$ (often known implicitly, *e.g.* under the form of a finite element code) that allows one to evaluate the effects of the loading (*e.g.* displacements, strains, stresses) depending on input parameters which describe the structure and its environment, that is the geometrical properties (*e.g.* dimensions, cross-section areas and moments of inertia of the beam elements), the material properties (*e.g.* Young's modulus, Poisson's coefficient) and the loading (*e.g.* applied loads, thermal loading). All these input parameters are gathered in a vector $\boldsymbol{x}$. The model response is denoted by $\boldsymbol{y} = \mathcal{M}(\boldsymbol{x})$.

Then, a *probabilistic model* is defined for the input parameters. In this context, the latter are described by a *random* vector $\boldsymbol{X}$ (of size M) with prescribed joint probability density function (PDF) $f_{\boldsymbol{X}}(\boldsymbol{x})$.

Lastly, a *limit state function* is defined that mathematically represents the failure criterion with respect to which the structure has to be justified. This function writes $g(\mathcal{M}(\boldsymbol{X}), \boldsymbol{X}')$ and accounts for the effects of the loading (*e.g.* displacements,

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stresses) to which (probabilistic or deterministic) limits – gathered in a vector $\boldsymbol{X}'$ – are assigned. It is conventionally defined in such a way that its negative values correspond to realizations $\boldsymbol{x}$ of the input parameters which lead to failure.

Denoting by $f_{\boldsymbol{X},\boldsymbol{X}'}$ the joint PDF of $\boldsymbol{X}$ and $\boldsymbol{X}'$, the reliability analysis is aimed at evaluating the probablity of failure P_f of the structure under consideration that reads:

$$P_f = \int_{\{\boldsymbol{x}: g(\mathcal{M}(\boldsymbol{x}),\boldsymbol{x}')\leq 0\}} f_{\boldsymbol{X},\boldsymbol{X}'}(\boldsymbol{x},\boldsymbol{x}')\,d\boldsymbol{x} \qquad [8.1]$$

Many methods many used to solve this problem, such as Monte Carlo simulation, FORM/SORM methods, directional simulation, subset simulation, see *e.g.* the references Ditlevsen and Madsen [DIT 96], and Lemaire [LEM 05].

8.1.2. *From Monte-Carlo simulation to polynomial chaos expansions*

The Monte Carlo method is well known in structural reliability and more generally in probabilistic mechanics. It relies upon the generation of a random sample of the input variables, denoted by $\mathcal{X} = \{\boldsymbol{x}_i, i = 1,...,N\}$. Then the number of simulated failures N_f (*i.e.* the number of realizations $\boldsymbol{x}_i$ that lead to a negative value of the limit state function, the evaluation of which requiring a mechanical calculation $\boldsymbol{y}_i = \mathcal{M}(\boldsymbol{x}_i)$). Then the probability of failure is estimated by $\hat{P}_f = N_f / N$. The Monte Carlo method is simple to carry out and also robust since it provides confidence intervals for the estimate $\hat{P}_f$. However it is computationally very expensive, especially when low probabilities of failure are sought (with orders of magnitude ranging from 10^{-3} to 10^{-6} in practice). Indeed, it is shown that an accurate estimation (say with a relative accuracy of 5%) of a probability of magnitude 10^{-k} requires about $N = 4.10^{k+2}$ points in the sample.

From another point of view, the Monte Carlo method consists in characterizing the random response of the structure $Y = \mathcal{M}(\boldsymbol{X})$ *pointwise* in its domain of variation. Thus a large number of simulations is expected in order to accurately estimate the probabilistic feature of Y, *e.g.* through its PDF $f_Y(y)$ that is estimated by the histogram of the sample $\mathcal{Y} = \{\mathcal{M}(\boldsymbol{x}_i), i = 1,...,N\}$. In the industrial context, most of models are of finite element type and necessitate a significant CPU time (say from a few minutes to a few hours), hence this approach cannot be applied.

As an alternative, Y can be considered intrinsically as a random variable belonging to a specific space (such as the space of random variables with a finite

variance), and can be represented in a *suitable basis* of this space. Thus the response will be cast as a converging series as follows:

$$Y \approx \sum_{j=0}^{+\infty} a_j \Psi_j \qquad [8.2]$$

where $\{\Psi_j, j \in \mathbb{N}\}$ is a set of random variables that form the basis and where $\{a_j, j \in \mathbb{N}\}$ is the set of the "coordinates" of Y in this basis. In particular, a special focus is given to bases made of *orthonormal polynomials* of random variables. The series in [8.2] is then referred to as *polynomial chaos* (PC) *expansion*.

In the remainder of this chapter, one successively describes the building of the PC basis (section 8.2), then the computation of the PC coefficients and their post-processing dedicated to reliability analysis (section 8.3). Lastly, two application examples are addressed in section 8.4.

8.2. Building of the polynomial chaos basis

8.2.1. Orthogonal polynomials

For the sake of simplicity, the input random variables are assumed to be independent. Their marginal PDF is denoted by $f_i(x_i)$, thus their joint PDF reads $f_{\boldsymbol{X}}(\boldsymbol{x}) = \prod_{i=1}^{M} f_i(x_i)$. For each input random variable X_i, a family of orthonormal polynomials $\{P_j^i, j \in \mathbb{N}\}$ can be defined, such that $P_0^i \equiv 1$ and the degree of each polynomial P_j^i is j, $j > 0$. The orthonormality property is defined by:

$$< P_j^i , P_k^i > \equiv \int_{D_i} P_j^i(x)\, P_k^i(x)\, f_i(x)\, dx = \delta_{j,k} \qquad [8.3]$$

where $\delta_{j,k} = 1$ if $j = k$ and 0 otherwise, and D_i is the support of the random variable X_i. In practice, classical families of orthonormal polynomials can be associated with usual continous random variables. If X_i is Gaussian (resp. uniform), the corresponding family is the one made of the Hermite (resp. Legendre) polynomials [ABR 70, SCH 00].

Then a basis made of *multivariate* polynomials $\left\{\Psi_j, j \in \mathbb{N}\right\}$ can be easily built up by *tensorization*, that is by multiplying the univariate polynomials as follows:

$$\psi_\alpha(\boldsymbol{x}) \equiv \psi_{\alpha_1,..,\alpha_M}(\boldsymbol{x}) = P^1_{\alpha_1}(x_1) \times \cdots \times P^M_{\alpha_M}(x_M) \qquad [8.4]$$

It is shown by Soize et Ghanem [SOI 04] that the family $\left\{\Psi_\alpha \equiv \psi_\alpha(\boldsymbol{X}), \alpha \in \mathbb{N}^M\right\}$ form an appropriate countable basis to represent the random response $Y = \mathcal{M}(\boldsymbol{X})$ of a mechanical model. In addition, this basis is *orthonormal* with respect to the inner product in the space of random variables with a finite variance defined by the mathematical expectation $< Y_1, Y_2 >= \mathbb{E}\left[Y_1 Y_2\right]$. Indeed, due to Eqs.[8.3],[8.4], one gets::

$$< \Psi_\alpha, \Psi_\beta >= \mathbb{E}\left[\psi_\alpha(\boldsymbol{X})\psi_\beta(\boldsymbol{X})\right] = \delta_{\alpha\beta} \qquad [8.5]$$

The elements of the basis (indexed by their multi-index α) are classically ordered according to their increasing total degree $p = |\alpha| = \sum_{i=1}^{M} \alpha_i$, and are enumerated from $j = 0$ to infinity as in Eq.[8.2] (an algorithm allowing a systematical building of the basis may be found in [SUD 06]).

In practice, it is necessary to only retain a finite number of terms in the PC basis. Then the series is generally truncated in such a way that only those basis polynomials ψ_j with total degree not greater than a given p are retained. Hence a truncated series containing P terms:

$$Y \approx \mathcal{M}^{PC}(\boldsymbol{X}) \equiv \sum_{j=0}^{P-1} a_j \, \psi_j(\boldsymbol{X}) \qquad [8.6]$$

where it is shown that $P = \binom{M+p}{p}$.

8.2.2. Example

Let us consider the random response Y of a mechanical model $Y = \mathcal{M}(X_1, X_2)$ depending on two Gaussian random variables X_1 and X_2, with mean μ_i (resp. standard deviation σ_i), $i = 1,2$. Upon applying the linear mapping $X_i = \mu_i + \sigma_i \xi_i$, the response can be recast in terms of standard Gaussian random variables, that is $Y = \tilde{\mathcal{M}}(\xi_1, \xi_2)$.

The family of orthogonal polynomials with respect to the standard Gaussian PDF $\varphi(x) = 1/\sqrt{2\pi}e^{-x^2/2}$ is the family of Hermite polynomials $\left\{He_j(x), j \in \mathbb{N}\right\}$. They are defined by the following recurrence relationship:

$$\begin{aligned} He_{-1}(x) \equiv He_0(x) &= 1 \\ He_{n+1}(x) &= x\,He_n(x) - n\,He_{n-1}(x) \end{aligned} \qquad [8.7]$$

The resulting polynomials are orthogonal but not orthonormal. They have various specific properties as shown in [BAR 05]. In particular, it is shown that $< He_n, He_n >= n!$. Therefore the family $\left\{He_j(x)/\sqrt{n!}, j \in \mathbb{N}\right\}$ is orthonormal. The four first normalized Hermite polynomials are thus $\left\{1, x, (x^2-1)/\sqrt{2}, (x^3-3x)/\sqrt{6}\right\}$.

Assume that the expansion of the random response Y onto a PC basis of maximal degree $p = 3$ is of interest. The retained polynomials are built from products of Hermite polynomials in ξ_1 and ξ_2 (table 8.1). Hence an approximation of the model response (*stochastic response surface*) is sought under the form:

$$\begin{aligned} Y \equiv \mathcal{M}^{PC}(\xi_1,\xi_2) &= a_0 + a_1\xi_1 + a_2\xi_2 + a_3(\xi_1^2-1)/\sqrt{2} + a_4\xi_1\xi_2 \\ &+ a_5(\xi_2^2-1)/\sqrt{2} + a_6(\xi_1^3-3\xi_1)/\sqrt{6} + a_7(\xi_1^2-1)\xi_2/\sqrt{2} \\ &+ a_8(\xi_2^2-1)\xi_1/\sqrt{2} + a_9(\xi_2^3-3\xi_2)/\sqrt{6} \end{aligned} \qquad [8.8]$$

where the coefficients $\{a_j, j = 0,\ldots,9\}$ must be determined.

j	$\boldsymbol{\alpha}$	$\Psi_{\alpha} \equiv \Psi_j$
0	[0,0]	$\Psi_0 = 1$
1	[1,0]	$\Psi_1 = \xi_1$
2	[0,1]	$\Psi_2 = \xi_2$
3	[2,0]	$\Psi_3 = \left(\xi_1^2-1\right)/\sqrt{2}$
4	[1,1]	$\Psi_4 = \xi_1\xi_2$
5	[0,2]	$\Psi_5 = \left(\xi_2^2-1\right)/\sqrt{2}$
6	[3,0]	$\Psi_6 = \left(\xi_1^3-3\xi_1\right)/\sqrt{6}$
7	[2,1]	$\Psi_7 = \left(\xi_1^2-1\right)\xi_2/\sqrt{2}$
8	[1,2]	$\Psi_8 = \left(\xi_2^2-1\right)\xi_1/\sqrt{2}$
9	[0,3]	$\Psi_9 = \left(\xi_2^3-3\xi_2\right)/\sqrt{6}$

Table 8.1. *Example of building of a polynomial chaos of degree 3 with 2 variables*

8.3. Computation of the coefficients of the expansion

8.3.1. Introduction

Polynomial chaos expansions have been originally introduced to represent random fields [WIE 38]. They have been used more recently for solving stochastic partial differential equations (SPDE) [GHA 91]. In this setup, investigations have been conducted in many fields such as biology, mechanics, fluid mechanics and thermal physics [WIN 85, ISU 98, SUD 04, GHA 98, XIU 03, KNI 06]. The weak formulation of these SPDE's is discretized both in the physical space (*e.g.* by finite elements) and in the probabilistic space (*e.g.* onto the PC basis). The coefficients arising from Eq.[8.6] are obtained by a Galerkin method [GHA 91], and are obtained by solving a large system of coupled linear equations, which may reveal time and memory consuming [PEL 00]. This method is referred to as *intrusive* due to the coupled nature of the system. The application of intrusive spectral methods have been initially proposed in [SUD 00, SUD 02].

On the other hand, *non intrusive* methods have received an increasing interest for a few years. They allow one to compute the coefficients in Eq.[8.6] by means of a set of *deterministic* calculations, *i.e.* a set $\mathcal{Y} = \{\mathcal{M}(\boldsymbol{x}_i), i = 1, \ldots, N\}$ of evaluations of the model response at suitably chosen values of the input variables. The label *non intrusive* indicates that these methods can be applied using the deterministic code associated with the model $\mathcal{M}$ without modification.

Two classes of approaches may be distinguished among the non intrusive methods, namely the *projection* approach [LEM 01, BAR 05, BAR 06, BLA 07] and the *regression* approach [BER 05, BER 06]. They are detailed in the sequel.

8.3.2. Projection methods

The so-called *projection methods* take benefit of the orthonormality of the PC basis. Indeed, by multiplying the expansion [8.2] by $\psi_j(\boldsymbol{X})$ and by integrating with respect to the joint PDF $f_{\boldsymbol{X}}(\boldsymbol{x})$ of $\boldsymbol{X}$, one gets:

$$a_j = \mathbb{E}\left[\mathcal{M}(\boldsymbol{X})\,\psi_j(\boldsymbol{X})\right] \equiv \int_{D_{\boldsymbol{X}}} \mathcal{M}(\boldsymbol{x})\psi_j(\boldsymbol{x})\, f_{\boldsymbol{X}}(\boldsymbol{x})\, d\boldsymbol{x} \qquad [8.9]$$

In practice, the above expression is estimated using classical methods for numerical integration, which consist in approximating the multi-dimensional integral by a weighted sum as follows:

$$\hat{a}_j \approx \sum_{i=1}^{N} w_i\, \mathcal{M}(\boldsymbol{x}^{(i)})\, \psi_j(\boldsymbol{x}^{(i)}) \qquad [8.10]$$

Several techniques can be considered which differ from the choice of the integration *points* $\boldsymbol{x}^{(i)}$ and *weights* w_i.

The so-called *simulation* method relies upon the choice of N *random* integration points and integration weights equal to $1/N$, which leads to:

$$\hat{a}_j \approx \frac{1}{N} \sum_{i=1}^{N} \mathcal{M}(\boldsymbol{x}^{(i)})\, \psi_j(\boldsymbol{x}^{(i)}) \qquad [8.11]$$

This corresponds to the application of Monte Carlo simulation to the estimation of the expectation in [8.9]. The accuracy of the coefficients estimators depends on the adopted sampling strategy. In case of a standard random sample (classical Monte Carlo simulation), a relatively low convergence rate in $N^{-1/2}$ is obtained. The convergence speed may be increased using stratified sampling techniques, such as *latin hypercube sampling* [MCK 79]. Moreover, it is shown that the use of *quasi-random numbers* [NIE 92], which are generated from deterministic *low discrepancy sequences*, guarantees a better filling of the domain of variation of the parameters and lead to faster convergences [BLA 07].

As an alternative, the integral in Eq.[8.9] can be approximated by a *Gauss quadrature* scheme. Its principle is well known in the unidimensional case: the integral of a function $h(x)$ (weighted by a function $w(x)$) is estimated by a sum of evaluations of h in a set of *quadrature points*:

$$I = \int_D h(x)\, w(x)\, dx \approx \sum_{k=1}^{n} w_i\, h(x_i) \qquad [8.12]$$

The Gauss method allows one to integrate exactly any polynomial function of degree not greater than $2n-1$ with n suitable integration points, namely the roots of the orthogonal polynomials with respect to the weight function $w(x)$ in the sense of Eq.[8.3]. The extension to the multi-dimensional case (integral [8.9]) is obtained by *tensorizing* the univariate quadrate rules:

$$a_j \approx \sum_{i_1=1}^{n_1} \cdots \sum_{i_M=1}^{n_M} w_{i_1}^1 \cdots w_{i_M}^M\, \psi_j\left(x_{i_1}^1, \ldots, x_{i_M}^M\right) \mathcal{M}\left(x_{i_1}^1, \ldots, x_{i_M}^M\right) \qquad [8.13]$$

Isotropic formulae are commonly used, that is formulae which satisfy $n_1 = \ldots = n_M = n$. It is shown that this scheme allows one to integrate exactly any multivariate polynomial of partial degree not greater than $2n-1$. Now, if the model

response is approximated by a PC expansion of degree p, then the integrand in [8.9] is a polynomial of total degree $2p$. Therefore a tensorized quadrature rule with $n = p+1$ points is used in order to estimate the coefficients. Such a strategy leads to perform $N = (p+1)^M$ model evaluations, which may reveal cumbersome in presence of a large number of input parameters (say $M \geq 5$).

The computational effort may be dramatically reduced by replacing the full tensor-product [8.13] with the so-called Smolyak scheme [SMO 63], also known as sparse quadrature. This technique has been applied in relation to PC expansions in [KEE 03, SUD 07].

8.3.3. Regression methods

8.3.3.1. *Direct approach*

An alternative method to projection consists in computing the coefficients which provide the best approximation of $Y = \mathcal{M}(\boldsymbol{X})$ in the least squares sense by a truncated PC expansion containing a fixed number P of terms. Using the following vector notation:

$$\boldsymbol{a} = \left\{a_0, ..., a_{P-1}\right\}^{\mathrm{T}} \qquad [8.14]$$

$$\boldsymbol{\psi}(\boldsymbol{X}) = \left\{\psi_0(\boldsymbol{X}), ..., \psi_{P-1}(\boldsymbol{X})\right\}^{\mathrm{T}} \qquad [8.15]$$

equation [8.6] rewrites:

$$\mathcal{M}^{PC} = \boldsymbol{a}^{\mathrm{T}}\, \boldsymbol{\psi}(\boldsymbol{X}) \qquad [8.16]$$

Let us consider a set $\mathcal{X} \equiv \{\boldsymbol{x}^{(1)}, ..., \boldsymbol{x}^{(N)}\}^{\mathrm{T}}$ of realizations of the input random vector, that is an *experimental design*. Let us denote by $\mathcal{Y}$ the set of corresponding model evaluations. The experimental design may be built either from a random or a quasi-random sample (see Section 8.3.2), or from the roots of the orthogonal polynomials that are used to build the basis [BER 05].

The problem consists in finding the vector of coefficients $\hat{\boldsymbol{a}}$ that minimize the sum of squared errors (cf. chapter 1, [1.6-7]), that is:

$$\hat{\boldsymbol{a}} = \arg\min_{\boldsymbol{a}} \sum_{i=1}^{N} \left(\boldsymbol{a}^{\mathrm{T}} \psi(\boldsymbol{x}^{(i)}) - \mathcal{M}(\boldsymbol{x}^{(i)}) \right)^2 \qquad [8.17]$$

It is shown that the solution can be obtained in closed form as follows:

$$\hat{\boldsymbol{a}} = \left(\boldsymbol{\Psi}^{\mathrm{T}} \boldsymbol{\Psi} \right)^{-1} \boldsymbol{\Psi}^{\mathrm{T}} \mathcal{Y} \qquad [8.18]$$

where the generic entry of matrix $\boldsymbol{\Psi}$ is given by:

$$\boldsymbol{\Psi}_{ij} = \psi_j(\boldsymbol{x}^{(i)}) \quad i = 1,\ldots,N \quad j = 0,\ldots,P-1 \qquad [8.19]$$

It is necessary that the number N of model evaluations be greater than the number P of unknown coefficients in order to make the problem well-posed. In the case of a random or a latin hypercube [MCK 79] experimental design, the rule-of-thumb $N = 2P$ generally leads to satisfactory results. As shown in [BER 05, BER 06], the regression methods reveals particularly efficient to compute the PC coefficients. It also allows one to define *a posteriori* error estimates as well as an adaptive strategy for building the PC basis, which is outlined in the sequel [BLA 09].

8.3.3.2. *Error estimation*

The approximation error of a PC expansion can be quantified by the *coefficient of determination* R^2, which is currently used in regression analysis. This coefficient depends on the sum of squared deviations between the "true" model response and the PC representation:

$$R^2 \equiv 1 - \frac{1/N \sum_{i=1}^{N} \left(\mathcal{M}(\boldsymbol{x}^{(i)}) - \mathcal{M}^{PC}(\boldsymbol{x}^{(i)}) \right)^2}{\hat{V}[Y]} \qquad [8.20]$$

where $\hat{V}[Y]$ is the empirical variance of the model evaluations:

$$\hat{V}[Y] \equiv \frac{1}{N-1} \sum_{i=1}^{N} \left(y^{(i)} - \bar{y} \right)^2 \qquad \bar{y} = \frac{1}{N} \sum_{i=1}^{N} y^{(i)} \qquad [8.21]$$

Thus, $R^2 = 1$ corresponds to a perfect adequation whereas $R^2 = 0$ indicates a very poor approximation. However, the R^2 coefficient should be used with caution, as it tends to underpredict the genuine approximation error. In the extreme case $N = P$, the PC approximation interpolates the model realizations, which leads to $R^2 = 1$ even if the error may reveal significant for points that do not belong to the experimental design. This phenomenon is known as *overfitting*.

As a consequence, a more robust error estimate is used, which is based on cross validation technique named *leave-one-out* [ALL 71, SAP 06]. In this setup, for any point in the experimental design $\boldsymbol{x}^{(i)}$, one computes the deviation $\Delta^{(i)}$ between the observation $y^{(i)} = \mathcal{M}(\boldsymbol{x}^{(i)})$ and the evaluation in $\boldsymbol{x}^{(i)}$ of a PC expansion denoted by $\mathcal{M}^{PC}_{\mathcal{X}\setminus\boldsymbol{x}^{(i)}}$, whose coefficients are computed from the experimental design $\mathcal{X}\setminus\{\boldsymbol{x}^{(i)}\}$ obtained by removing the point $\boldsymbol{x}^{(i)}$ from $\mathcal{X}$. By analogy with the R^2 coefficient, one defines the Q^2 coefficient as follows:

$$Q^2 \equiv 1 - \frac{1/N \sum_{i=1}^{N} \Delta^{(i)\,2}}{\hat{V}[Y]} \qquad \Delta^{(i)} = \mathcal{M}(\boldsymbol{x}^{(i)}) - \mathcal{M}^{PC}_{\mathcal{X}\setminus\boldsymbol{x}^{(i)}}(\boldsymbol{x}^{(i)}) \qquad [8.22]$$

8.3.3.3. *Adaptative approach*

It has been shown in paragraph 8.3.3.1 that the size N of the experimental design has to be greater than the number P of terms in the truncated PC series in order to solve the regression problem. Now, P strongly increases with both the maximal degree p of the PC expansion and the number M of input random variables, according to the formula $P = \binom{M+p}{p} = \frac{(M+p)!}{M!\,p!}$. Thus the regression method may lead to intractable calculations in high dimension (say $M \geq 10$). In order to reduce the number of model evaluations, a *sparse* PC approximation of the response *Y* is sought, that is a PC representation which only contains a small number of nonzero coefficients. Of course it is not possible to determine *a priori* the significant terms. Hence an iterative procedure has been proposed in [BLA 08, BLA 09, BLA 10b] to build up step-by-step a sparse PC expansion. The algorithm is sketched in Figure 8.1.

First, an initial experimental design $\mathcal{X}$ is considered and the associated model evaluations are gathered in $\mathcal{Y}$. The model response is approximated by a PC expansion of degree $p = 0$ (*i.e.* the current basis is a constant term). Then, terms corresponding to polynomials with increasing degree p and interaction order j are proposed. Two steps can be distinguished:

- a *forward* step: all the candidate terms are added in turn to the current basis. The changes in R^2 due to the addition of each term are evaluated. Eventually all those terms which lead to a significant increase of R^2 are retained;

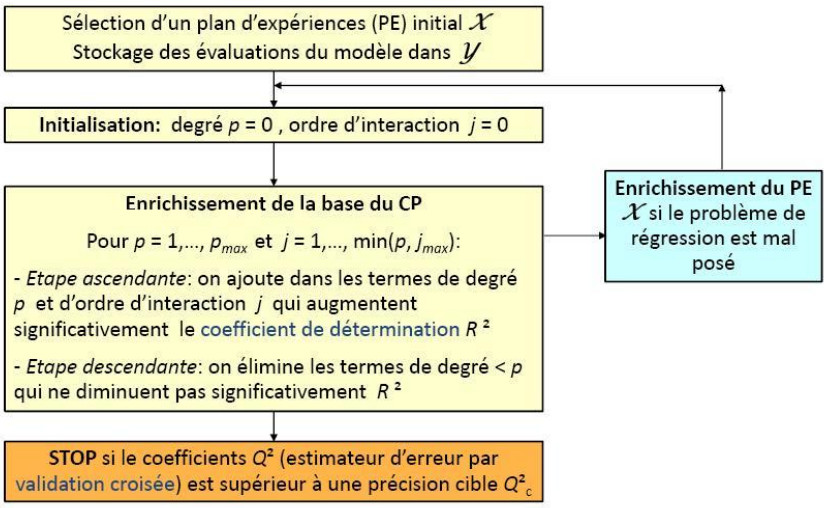

Figure 8.1. *Schéma de l'algorithme pour la construction pas-à-pas d'un chaos polynomial creux*

– a *backward* step: all the terms in the current basis are removed in turn, and the associated changes in R^2 are computed. Eventually all those terms which lead to an insignificant decrease of are R^2 discarded.

Besides this adaptivity of the PC basis, the experimental design is systematically enriched in such a way that the various regression problems be always well-posed. In this purpose, sequential sampling strategies are adopted, which are based either on quasi-random numbers or *nested* LHS [WAN 03, BLA 10b]. The algorithm stops when the Q^2 coefficient related to the current PC approximation has reached a target accuracy Q^2_{tgt} .

8.3.4. Post-processing of the coefficients

As mentioned previously, the random variable $Y = \mathcal{M}(\boldsymbol{X})$ is thoroughly defined by its coefficients a_j which can be estimated by means of several non intrusive methods. In particular, the mean and the variance Y can be derived analytically from these coefficients due to the orthonormality of the basis:

$$E[Y] = a_0 \qquad V[Y] = \sum_{j=1}^{P-1} a_j^2 \qquad [8.23]$$

For reliability analyses, one substitutes the model response by a PC decomposition into the limit state function that describes the system failure. Considering for simplicity a failure criterion associated with a deterministic maximum admissible threshold $y_{\max}$, the limit state function reads:

$$g(\boldsymbol{X}) = y_{\max} - \mathcal{M}(\boldsymbol{X}) \qquad [8.24]$$

Substituting the model response $\mathcal{M}(\boldsymbol{X})$ by a PC expansion $\mathcal{M}^{PC}(\boldsymbol{X})$ into Eq. [8.24], one gets the *analytical* limit state function:

$$g^{PC}(\boldsymbol{X}) = y_{\max} - \sum_{j=0}^{P-1} a_j \psi_j(\boldsymbol{X}) \qquad [8.25]$$

This quantity corresponds to a *stochastic response surface* which repaces the original limit state function, that is an analytical (polynomial) expression whose evaluation cost is negligible. Thus the probability of failure may be estimated inexpensively by applying the classical reliability methods (*e.g.* direct Monte Carlo simulation, FORM and importance sampling).

It has to be noticed that the PC-based approximation [8.25] differ from the quadratic response surfaces used in reliability analysis, which are *local* approximations (at the vicinity of the design point when using FORM). In this context, a parametric study leads to build a new response surface for each value of the parameter, in contrast to the PC approach.

8.4. Applications in structural reliability

8.4.1. *Elastic truss*

8.4.1.1. *Problem statement*

One considers the elastic truss represented in figure 8.2 [BLA 07, SUD 07]. Ten input random variables are assumed, whose distributions, means and standard deviations are reported in table 8.2. The quantity of interest is the (random) maximum vertical displacement of the structure denoted by $V_1 = \mathcal{M}(\boldsymbol{X})$.

8.4.1.2. *Reliability analysis*

Of interest is the reliability of the truss structure with repect to an admissible maximal displacement. The associated limit state function reads:

$$g(\boldsymbol{X}) = v_{\max} - |\mathcal{M}(\boldsymbol{X})| \leq 0,\ v_{\max} = 11\,\text{cm} \qquad [8.26]$$

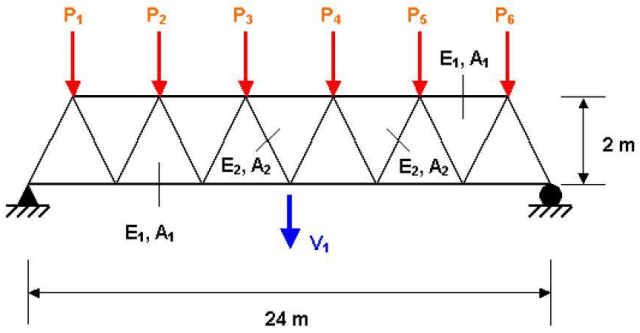

Figure 8.2. *Truss structure with 23 bar elements*

Variable	Distribution	Mean	Standard Deviation
E_1, E_2 (MPa)	Lognormale	210 000	21 000
A_1 (cm²)	Lognormal	20	2
A_2 (cm²)	Lognormal	10	1
P_1- P_6 (kN)	Gumbel	50	7,5

Table 8.2. *Elastic truss – input random variables*

The reference value of the probability of failure is obtained by direct Monte Carlo simulation using $N = 10^6$ samples. The reliability analysis is carried out from various PC approximations of the response (denoted by $\mathcal{M}^{PC}(\boldsymbol{X})$) made of normalized Hermite polynomials. To this end, the input random vector $\boldsymbol{X}$= $\{E_1,E_2,A_1,A_2,P_1,\ldots,P_6\}^T$ is transformed into a random vector containing independent standard Gaussian variables.

A PC expansion of degree 3 is considered. The PC coefficients are computed by Smolyak sparse quadrature ($1,771$ calculations have been performed). The reference results are obtained by applying an importance sampling strategy (the importance PDF is centered on the design point determined by FORM), from which one gets a generalized reliability index. The results are gathered in table 8.3. A 2% accuracy on the reliability index is obtained for all the admissible thresholds in the interval [10-16] cm.

The results obtained from a PC expansion whose coefficients have been estimated by regression are reported in table 8.4. Precisely, the reliability indices are alternatively computed from a full PC expansion of degree $p = 3$ and from a sparse

PC representation. Whatever the approach, the coefficients have been calculated from an experimental design made of quasi-random numbers. It appears that both the full and the sparse PC approximation yield accurate estimates of β, with a relative error less than $3,5\%$.

Threshold (cm)	**Reference**		**Smolyak Projection**	
	P_f	β	P_f	β
10	$4.31\text{x}10^{-2}$	1.715	$4.29\text{x}10^{-2}$	1.718
11	$8.70\text{x}10^{-3}$	2.378	$8.73\text{x}10^{-3}$	2.377
12	$1.50\text{x}10^{-3}$	2.967	$1.47\text{x}10^{-3}$	2.974
14	$3.49\text{x}10^{-5}$	3.977	$2.83\text{x}10^{-5}$	4.026
16	$6.03\text{x}10^{-7}$	4.855	$4.01\text{x}10^{-7}$	4.935

Table 8.3. *Elastic truss – Reliability results obtained using a third order polynomial chaos expansion based on Smolyak projection*

It is observed though that the sparse PC approach only requires about half (resp. one eighth) as many calculations as the full PC approach based on regression (resp. based on Smolyak quadrature).

Threshold (cm)	**Reference**	**Full PC**		**Sparse PC**	
	β^{REF}	$\hat{\beta}$	ε (%)	$\hat{\beta}$	ε (%)
10	1.715	1.71	0.6	1.72	0.0
11	2.378	2.38	0.0	2.38	0.0
12	2.967	2.98	0.3	2.99	0.7
14	3.977	4.04	1.5	4.07	2.3
16	4.855	4.95	2.1	5.02	3.5
Error $1 - Q^2$		$1\text{x}10^{-6}$		$9\text{x}10^{-5}$	
Number of terms		286		114	
Number of model evaluations		443		207	

Table 8.4. *Elastic truss – Reliability results obtained using a full (with p=2) and a sparse PC expansion based on regresion*

8.4.2. Frame structure

The frame structure represented in figure 8.3 is now considered [LIU 91, BLA 10b]. The frame beam elements are made of 8 different materials, whose properties are gathered in table 8.5.

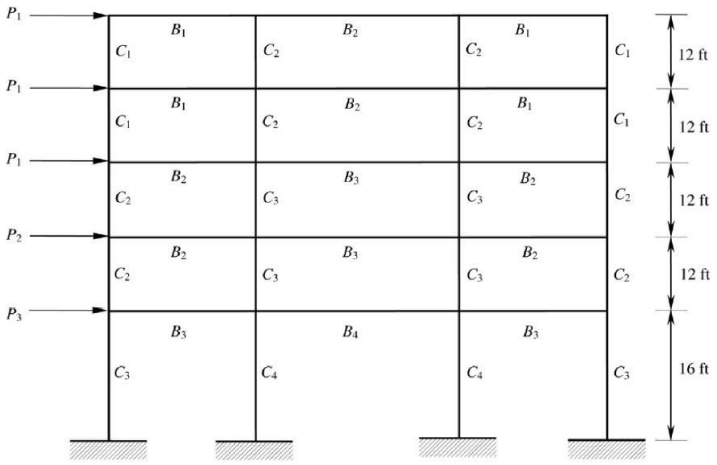

Figure 8.3. *Example of a frame structure subjected to lateral loads*

Element	Young's modulus	Moment of inertia	Cross-sectional area
B_1	E_4	I_{10}	A_{18}
B_2	E_4	I_{11}	A_{19}
B_3	E_4	I_{12}	A_{20}
B_4	E_4	I_{13}	A_{21}
C_1	E_5	I_6	A_{14}
C_2	E_5	I_7	A_{15}
C_3	E_5	I_8	A_{16}
C_4	E_5	I_9	A_{17}

Table 8.5. *Frame structure – Element properties*

The response of interest is the horizontal component u of the top-floor displacement at the top right corner. The 3 applied loads, the 2 Young's moduli, the 8 moments of inertia and the 8 cross-section areas of the frame components are assumed to be random. They are collected in the random vector

$\boldsymbol{X} = \{P_1, P_2, P_3, ..., I_6, ..., I_{13}, A_{14}, ..., A_{21}\}^T$ of size $M = 21$. The properties of the random variables are reported in table 8.6.

Variable	Distribution	Mean †	Standard Deviation †
P_1 (kN)		133.454	40.04
P_2 (kN)	Lognormal	88.970	35.59
P_3 (kN)		71.175	28.47
E_1 (kN/m²)	Truncated normal over	2.17375x10^7	1.9152x10^6
E_2 (kN/m²)	$[0, +\infty[$	2.37964x10^7	1.9152x10^6
I_6 (m^4)		8.13443x10^{-3}	1.08344x10^{-3}
I_7 (m^4)		2.13745x10^{-2}	2.59609x10^{-3}
I_8 (m^4)		2.59610x10^{-2}	3.02878x10^{-3}
I_9 (m^4)	Truncated normal over	1.08108x10^{-2}	2.59610x10^{-3}
I_{10} (m^4)	$[0, +\infty[$	1.41055x10^{-2}	3.46146x10^{-3}
I_{11} (m^4)		2.32785x10^{-2}	5.62487x10^{-3}
I_{12} (m^4)		2.59610x10^{-2}	6.49024x10^{-3}
I_{13} (m^4)		2.13745x10^{-2}	2.59609x10^{-3}
A_{14} (m²)		3.12564x10^{-1}	5.58150x10^{-2}
A_{15} (m²)		3.72100x10^{-1}	7.44200x10^{-2}
A_{16} (m²)		5.06060x10^{-1}	9.30250x10^{-2}
A_{17} (m²)	Truncated normal over	5.58150x10^{-1}	1.11630x10^{-1}
A_{18} (m²)	$[0, +\infty[$	2.53020x10^{-1}	9.30250x10^{-2}
A_{19} (m²)		2.91168x10^{-1}	1.02323x10^{-1}
A_{20} (m²)		3.73030x10^{-1}	1.20933x10^{-1}
A_{21} (m²)		4.18600x10^{-1}	1.95375x10^{-1}

† The mean value and the standard deviation of the cross-sections, moments of inertia and Young's moduli are those of the untruncated Gaussian

Table 8.6. *Frame structure – input random variables*

Moreover, the input random variables are correlated as follows: the correlation coefficients between the cross-section areas and the moments of inertia of a given element are equal to $\rho_{A_i I_i} = 0{,}95$, the correlation coefficients related to the other geometrical properties are equal to $\rho_{A_i I_j} = \rho_{I_i I_j} = \rho_{A_i A_j} = 0{,}13$, the correlation coefficient between the two Young's moduli is equal to $\rho_{E_4 E_5} = 0{,}9$. The random

vector $\boldsymbol{X}$ is transformed into a vector of independent standard Gaussian random variables by means of a *Nataf transform* $\boldsymbol{X} = T(\xi)$ [NAT 62] prior to building the PC expansion.

Let us study the serviceability of the frame structure with respect to the limit state function:

$$g(\boldsymbol{X}) = u_{\max} - \mathcal{M}(T(\xi)) \qquad [8.27]$$

where $u_{\max}$ is a maximal admissible horizontal displacement. It is approximated by an analytical function by replacing the model $\mathcal{M}(T(\xi))$ with its PC representation made of Hermite polynomials, denoted by $\mathcal{M}^{PC}(\xi)$. One carries out a parametric study varying the threshold u_{max} from 4 to 8 cm. The generalized reliability indices are estimated b post-processing a full third-order PC as well as a sparse PC. The results are reported in table 8.7.

As observed in the truss example, the estimation error of the reliability index slightly increases with the threshold value. Both types of PC approximation yield relative errors on β less than 5% when the threshold ranges from 4 to 8 cm. The sparse PC approach reveals much more efficient than the full PC approach, with a gain factor of 8 in terms of number of model evaluations (only 450 finite element runs instead of 3,724).

Threshold (cm)	**Reference**	**Full PC**		**Sparse PC**	
	β^{REF}	$\hat{\beta}$	ε (%)	$\hat{\beta}$	ε (%)
4	2.27	2.26	0.4	2.29	0.9
5	2.96	3.00	1.4	3.01	1.7
6	3.51	3.60	2.6	3.61	2.8
7	3.96	4.12	4.0	4.11	3.8
8	4.33	4.58	5.8	4.56	5.3
Error $1 - Q^2$		$1x10^{-3}$		$1x10^{-3}$	
Number of terms		2,024		138	
Number of model evaluations		3,724		450	

Table 8.7. *Frame structure – Estimates of the generalized reliability index* $\beta = -\Phi^{-1}(P_f)$ *for various values of the threshold displacement*

8.5. Conclusion

The methods based on polynomial chaos expansions have motivated many investigations over the last few years. Their application to structural reliability is quite novel and can be viewed as a particular type of *stochastic response surface*. This chapter has shown the principles of these methods with respect to the simulation techniques classically used in reliability analysis, and has introduced their formalism.

The two application examples have shown the interest in using PC-based response surfaces for reliability analysis. Indeed, at the computational cost of the order of 200 calls to the finite element model for the elastic truss (resp. 450 calls for the frame structure), one obtained the probabilities of failure related to various thresholds, for a problem involving 10 (resp. 21) input random variables. In practice, the parametric study is carried out at a negligible cost with respect to a single reliability analysis, as the polynomial chaos expansion is built once and for all, and is then post-processed for the various threshold values.

In addition to probabilities of failure, the polynomial chaos expansion can be also used in order to study the sensitivity of the response, by evaluating its probability density function, its statistical moments and the sensitivity indices to the input variables, still without requiring any additional model evaluation [SUD 07, BAR 07]. The latter reference [BAR07] has shown though that the use of a basis made of Lagrange polynomials is a relevant alternative to Hermite polynomials when the number of input parameters remains low (say $M < 4$-5).

Lastly, the building of adaptive sparse polynomial bases paves the way to the solving of high-dimensional problems (M~50-100) at a reasonable computational cost (N<1000), in particular thanks to the introduction in probabilistic mechanics of advanced statistical regression methods such as LAR (*Least Angle Regression*) [BLA 10a].

8.6. Bibliography

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