Polinomial chaos expansion applied to limit state functions

N Afanador García¹, G Guerrero Gómez², and C Nolasco Serna³

¹ Grupo de Investigación en Ingeniería Civil, Universidad Francisco de Paula Santander, Seccional Ocaña, Colombia
² Grupo de Investigación en Tecnología y Desarrollo en Ingeniería, Universidad Francisco de Paula Santander, Seccional Ocaña, Colombia
³ Grupo de Investigación Facultad de Educación Arte y Humanidades, Universidad Francisco de Paula Santander, Seccional Ocaña, Colombia

E-mail: nafanadorg@ufpso.edu.co, gguerrerog@ufpso.edu.co

Abstract. In structural projects, ensuring system performance within the established specifications with a maximum level of safety and taking into account the economic constraints of the project is one of the main objectives of structural design. The risks to which any physical system is subjected are called failure probability and are assessed by applying structural reliability analysis methods. The objective of the structural reliability analysis is to ensure that the strength of the elements of the structure is greater than the imposed strength demand over the service life of each of the structural elements. Structural design variables are physical quantities in structural reliability and are considered random, and can be represented in a random vector. The failure probability of a structure is obtained from the evaluation of the uncertainties inherent to the physical variables of the project, through the probability distributions of the random variables. The objective of this work was the application of polynomial chaos expansion to evaluate the failure probability in limit state functions found in the literature using numerical simulation, in order to decrease the sample size for each random variable compared to those needed using Monte Carlo simulation. This research showed that the difference between the sample size between polynomial chaos expansion and Monte Carlo simulation is 5%, saving time and computational effort.

1. Introduction

Freudenthal’s work [1] started the application of statistical concepts for the calculation of the failure probability, subsequently methodologies have been developed to deal with reliability problems at different levels; (i) level 1: partial safety coefficients are chosen for each variable (they can be: loads, resistances, etc.); (ii) level 2: Obtain the failure probability \( \rho_f \), using the joint probability density function; (iii) level 3: the overall joint density function is used to calculate the probability of failure. These methods use a linear approximation of the fault region, called first-order second-moment method (FOSM).

The first works involving the first two moments of the distributions were by [1], Mayer [2], Rzhanitzyn [3] and Basler [4], although it was not until the work of Cornell [5] who proposed the original FOSM formulation. They were later extended by the work of Hasofer and Lind [6] who based their work on the transformation/reduction of the problem to a standardized coordinate system, while Rackwitz [7] proposed the transformation of non-normal random variables to
the independent standardized normal space. Among other works are the contributions of Hohenbichler and Rackwitz [8] and Ditlevsen [9]. The second-order reliability methods (SORM) use a Taylor series development to approximate the failure regions; they are analytical methods that approximate the limit state function by means of quadratic surfaces [10–13].

Simulation techniques [14, 15] allow the solution of highly nonlinear and high dimensional problems, although with a high computational cost, especially when the failure probability is small [16–18]. With the advancement in computer technology, computational cost has decreased significantly and techniques such as Monte Carlo simulation (MCS) are computationally feasible [19]. There are other approximate methods that, with a smaller number of simulations and without loss of accuracy, allow to obtain the failure probability using polynomial chaos expansion (PCE) [20,21]. Techniques such as PCE and MCS were used in this research work to determine the failure probability of the limit state functions found in the literature.

2. Numerical simulation

The Monte Carlo method involves a significantly large number of simulations of the analytical or numerical model with combinations of random variables; taking into account the probability distribution and the distribution parameters, the random variables can be obtained by applying the inverse transformation method [14], see Equation (1).

$$\xi = \Phi^{-1}(F_i(X_i)),$$

where, $\Phi$ is the standard normal probability density function and $F_i(X_i)$, $i = 1, 2, 3, ..., n$ are the marginal probability density functions of $X_i$.

The following algorithm was used to define the values of the random variables [22]. Given the expression $Y = g(X)$ where $x$ represents the model under consideration, the symbol $X$ is a vector representing the uncertainty in the input variables and the symbol $Y$ represents an estimated output vector, thus,

(i) Define the probability distributions and distribution parameters for each input random variable.

(ii) Generate a sample value for each of the variables $j (X_j)$ by using the inverse transformation method.

(iii) Evaluate the response of the analytical or numerical model by using the values $(X_j)$.

(iv) Repeat steps (ii) and (iii) to generate a probability distribution of the response.

The number of simulations ($N$) is chosen so that the output distribution converges for a defined value.

2.1. Probability of failure

Each set generated according to its probability distribution function $f_X(x)$ is evaluated at the limit state function $(h(X))$, assuming identically and independently distributed random variables. A value of $h(X) < 0$ indicates failure, where $N_f$ is the number of simulations that would generate $h(X) < 0$. An estimate of the failure probability can be expressed by Equation (2).

$$p_f = \frac{N_f}{N}.$$  

To evaluate the reliability index of the numerical models found in the literature, the results of the MCS are used to evaluate the outcome of the PCE.
3. Polynomial chaos expansion

The function of variables that follow a normal probability distribution as a convergent series is known as polynomial chaos, see Equation (3).

\[
u (\theta) = a_0 \Gamma_0 + \sum_{i_1=1}^{\infty} a_{i_1} \Gamma_1 (\xi_{i_1} (\theta)) + \sum_{i_1=1}^{\infty} \sum_{i_2=1}^{i_1} a_{i_1 i_2} \Gamma_2 (\xi_{i_1} (\theta), \xi_{i_2} (\theta)) + \sum_{i_1=1}^{\infty} \sum_{i_2=1}^{i_1} \sum_{i_3=1}^{i_2} a_{i_1 i_2 i_3} \Gamma_3 (\xi_{i_1} (\theta), \xi_{i_2} (\theta), \xi_{i_3} (\theta)) + \cdots ,
\]

where \(a_{i_1}, a_{i_2}, \ldots, a_{i_n}\) are deterministic constants, \(\Gamma_p (\xi_{i_1}, \xi_{i_2}, \ldots, \xi_{i_p})\) denotes the \(p\)-order Hermite polynomials in terms of the independent normal multidimensional random variables \(\{\xi_{i_k}\}_{k=1}^{M}\) and \(\theta\) denotes the random character of the quantities involved. An expression to obtain a multidimensional Hermite polynomial is defined in Equation (4).

\[
\Gamma_p (\xi) = (-1)^p e^{\frac{1}{2} \xi^T \xi} \frac{\partial^p}{\partial \xi_{i_1}, \ldots, \xi_{i_n}} e^{-\frac{1}{2} \xi^T \xi}.
\]

The Hermite polynomials of order \(p\) in terms of the multidimensional independent normal random variables, are expressed in Equation (4) in vector form \(\xi = [\xi_{i_1}, \xi_{i_2}, \xi_{i_3}, \ldots, \xi_{i_p}]\).

Generally, the one-dimensional Hermite polynomials are defined in the Equation (5).

\[
\Psi_n (\xi) = (-1)^n \varphi^{(n)} (\xi) \varphi (\xi) = \frac{1}{\sqrt{2\pi}} e^{-\xi^2 / 2},
\]

where \(\varphi^{(n)} (\xi)\) is the \(n\)th derivative of the normal density. For a variable and degree \(i\), the polynomials generated can be seen in Equation (6).

\[
\{\Psi\} = \{1, \xi, \xi^2 - 1, \xi^3 - 3\xi, \xi^4 - 6\xi^2 + 3, \xi^5 - 10\xi^3 + 15\xi, \ldots\}.
\]

Equation (3) can be written in a compact form, as indicated in Equation (7).

\[
u (\theta) = \sum_{i=0}^{P} b_i \Psi_i (\xi (\theta)),
\]

where \(b_i\) and \(\Psi_i (\xi (\theta))\) are identical to \(a_{i_1}, a_{i_2}, \ldots, a_{i_P}\) and \(\Gamma_p (\xi_{i_1}, \xi_{i_2}, \ldots, \xi_{i_p})\) respectively. An example of a PCE of order 3 and dimension 2, is given in Equation (8).

\[
u (\theta) = b_0 + b_1 \xi_1 (\theta) + b_2 \xi_2 (\theta) + b_3 (\xi_1^2 (\theta) - 1) + b_4 \xi_1 (\theta) \xi_2 (\theta) + b_5 (\xi_2^2 (\theta) - 1) + b_6 (\xi_3 - 3\xi) + b_7 (\xi^3 - 3\xi) + b_8 \xi_1 (\xi_2^2 - 1) + b_9 (\xi_1^3 - 1) \xi_2,
\]

where \(\xi_1(\theta)\) and \(\xi_2(\theta)\) are independent random variables. Equation (7) can be used as a surrogate model for the limit state equations to evaluate the failure probability and the reliability index in a non-intrusive formulation.

4. Numerical experimentation

In order to validate the PCE methodology, it was implemented in the MatLab programming environment version 2017 b, on an Intel(R) core i7-5500U computer and 16 GB of RAM, in order to calculate the PCE coefficients of the equations in Table 1.
1E+06 simulations using the Monte Carlo method and 5E+04 simulations implementing PCE were performed. The limit state functions indicated in Table 1 were taken from the specialized literature and a description of the random variables together with the probability distribution, mean, and standard deviation are given in the last column. That is, \( N \) defines the normal probability distribution, and \((\mu;\sigma)\) where \(\mu\) represents the mean and \(\sigma\) corresponds to the standard deviation.

The coefficients and the dimension of the PCE representing the limit state functions defined in Table 1, are given in Table 2. The variable \( P_{CMS} \) was performed. The limit state functions indicated in Table 1 were taken from the literature. The variables \( \rho \) and finally “Order” which means: the first digit indicates the dimension of the polynomial and the second digit, the number of random variables. The results obtained indicated that the approximation using MCS is more accurate, although the estimated value of the failure probability using PCE is very good with a lower computational cost than that used in MCS.

A comparison of the results of the failure probability was performed for each equation defined in Table 1 and those estimated using PCE present in Table 2, and the results are shown in Table 3. The first column indicates the literature reference of the limit state function, the second and third columns indicate the reliability index \((\beta_{Lit.})\) and the failure probability \((\rho_{CMS})\) respectively, found in the literature. The variables \( \rho_{CMS} \) and \( \rho_{PCE} \) corresponds to the failure probability using Monte Carlo simulation, \( \rho_{PCE} \) is the failure probability using polynomial chaos expansion and finally “Order” which means: the first digit indicates the dimension of the polynomial and the second digit, the number of random variables. The results obtained indicated that the approximation using MCS is more accurate, although the estimated value of the failure probability using PCE is very good with a lower computational cost than that used in MCS.

| Problem | Performance function | Parameters |
|---------|----------------------|------------|
| 1       | \( h(\mathbf{X}) = 2.5 - 0.2357(x_1 - x_2) + 0.00463(x_1 + x_2 - 20)^4 \) | \( x_{1:2} \sim N(10;3) \) |
| 2       | \( h(\mathbf{X}) = 0.1(x_1 - x_2)^2 - \frac{x_1 + x_2}{\sqrt{2}} + 2.5 \) | \( x_{1:2} \sim N(0;1) \) |
| 3       | \( h(\mathbf{X}) = -0.5(x_1 - x_2)^2 - \frac{x_1 + x_2}{\sqrt{2}} + 3 \) | \( x_{1:2} \sim N(0;1) \) |
| 4       | \( h(\mathbf{X}) = 2 - x_2 - 0.1x_2^2 + 0.06x_1^3 \) | \( x_{1:2} \sim N(0;1) \) |
| 5       | \( h(\mathbf{X}) = 2 + 0.015(\sum_{i=1}^{9}x_i^2) - x_{10} \) | \( x_{1:2;\ldots;10} \sim N(0;1) \) |
| 6       | \( h(\mathbf{X}) = 3 - x_2 + 256x_1^4 \) | \( x_{1:2} \sim N(0;1) \) |
| 7       | \( h(\mathbf{X}) = x_1^3 + x_2^3 - 18 \) | \( x_{1:2} \sim N(10;5) \) |
| 8       | \( h(\mathbf{X}) = x_1^3 + x_2^3 - 67.5 \) | \( x_1 \sim N(10;5) \) \( x_2 \sim N(9.9;5) \) |
| 9       | \( h(\mathbf{X}) = F_Y - \frac{140}{Z} \) | \( F_Y \sim N(38;3.8) \) \( Z \sim N(54;2.7) \) |
| 10      | \( h(\mathbf{X}) = T - \frac{PL}{3W} \) | \( T \sim N(10;2) \) \( P \sim N(8;0.1) \) \( L \sim N(1E - 4; 2E - 5) \) \( W \sim N(6E + 5; 1E + 5) \) |
of E-05 or less the number of simulations using PCE increases, as well as the dispersion in the variables and the number of simulations used; for very low probability of failure of the order Limit state function expressed in polynomial chaos expansion.

Table 2.

| Problem | Limit state function with PCE |
|---------|-----------------------------|
| 1       | $h_{PEC} (\xi) = 7.004 - 0.7071\xi_1 + 0.7071\xi_2 + 4.5004 (\xi_1^2 - 1) + 9.0007\xi_1\xi_2$ +4.5004 (\xi_2^2 - 1) + 2.2502 (\xi_1^2 - 1) (\xi_2^2 - 1) +1.5001 (\xi_1^3 - 3\xi_1) \xi_2 + 1.5001 (\xi_2^3 - 3\xi_2) \xi_1$ +0.3750 (\xi_1^4 - 6\xi_1^2 + 3) + 0.3750 (\xi_2^4 - 6\xi_2^2 + 3) |
| 2       | $h_{PEC} (\xi) = 2.7 - 0.7071\xi_1 - 0.7071\xi_2 + 0.1 (\xi_1^2 - 1) - 0.2\xi_1\xi_2 + 0.1 (\xi_2^2 - 1)$ |
| 3       | $h_{PEC} (\xi) = 2 - 0.7071\xi_1 - 0.7071\xi_2 - 0.5 (\xi_1^2 - 1) + \xi_1\xi_2 - 0.5 (\xi_1^2 - 1)$ |
| 4       | $h_{PEC} (\xi) = 1.9 + 0.18\xi_1 - \xi_2 - 0.1 (\xi_1^2 - 1) + 0.06 (\xi_1^3 - 3\xi_1)$ |
| 5       | $h_{PEC} (\xi) = 2.135 - \xi_10 + 0.015 \sum_{i=1}^{9} (\xi_i - 1)^2$ |
| 6       | $h_{PEC} (\xi) = 771 - \xi_2 + 1536 (\xi_1^2 - 1) + 256 (\xi_1^4 - 6\xi_1^2 + 3)$ |
| 7       | $h_{PEC} (\xi) = 3482 + 1875\xi_1 + 1875\xi_2 + 750 (\xi_1^2 - 1) + 750 (\xi_2^2 - 1) + 125 (\xi_1^3 - 3\xi_1)$ +125 (\xi_2^3 - 3\xi_2)$ |
| 8       | $h_{PEC} (\xi) = 3395.299 + 1875\xi_1 + 1845.15\xi_2 + 750 (\xi_1^2 - 1) + 742.5 (\xi_2^2 - 1)$ +125 (\xi_1^3 - 3\xi_1) + 125 (\xi_2^3 - 3\xi_2)$ |
| 9       | $h_{PEC} (\xi) = 16.83657 + 3.8\xi_1 + 1.0635\xi_2 - 0.532 (\xi_2^2 - 1)$ |
| 10      | $h_{PEC} (\xi) = 6.4318 + 0.3409\xi_1 + 0.1\xi_2 + 0.3117\xi_3 - 0.2597\xi_4 - 0.0682 (\xi_2^2 - 1)$ +0.0682\xi_1\xi_3 + 0.0568\xi_1\xi_4 - 0.05\xi_3\xi_4$ |

Table 3. Comparison of results for different limit state functions.

| Problem | $\beta_{Lit.}$ | $p^{Lit.}$ | $p^{CMS}$ | $p^{PCE}$ | Order |
|---------|-----------------|-------------|------------|-----------|-------|
| 1       | 2.431           | 2.86E-02    | 2.83E-03   | 2.88E-03  | 42    |
| 2       | 2.481           | 4.16E-03    | 4.24E-03   | 4.21E-03  | 22    |
| 3       | 1.625           | 1.05E-01    | 1.045E-01  | 1.050E-01 | 22    |
| 4       | 1.996           | 3.47E-02    | 3.45E-02   | 3.48E-02  | 32    |
| 5       | 2.103           | 5.34E-03    | 1.645E-02  | 1.72E-02  | 210   |
| 6       | 2.925           | 1.80E-04    | 1.86E-04   | 1.83E-04  | 42    |
| 7       | 2.240           | - - -        | 5.48E-03   | 5.51E-03  | 32    |
| 8       | 1.900           | - - -        | 1.30E-02   | 1.35E-02  | 32    |
| 9       | 5.139           | - - -        | 1.14E-05   | 2.00E-06  | 22    |
| 10      | 3.480           | - - -        | 3.94E-05   | 5.00E-05  | 24    |

The precision of the results using PCE depends on the dimension, the number of random variables and the number of simulations used; for very low probability of failure of the order of E-05 or less the number of simulations using PCE increases, as well as the dispersion in the results. While the spread in the probability of failure using SMC is much higher, see Figure 1(a) and Figure 1(b).
A numerical simulation using Monte Carlo was applied to the Grootman problem, and shown in Figure 1(a), and a zoom is performed and shown in Figure 1(b). Figure 1 shows that the MCS defines the limit state function \( h = 0 \) with very few simulations, a small number of simulations defines the failure zone \( h(X) = 0 \) and a larger number of simulations the safety zone \( h(X) > 0 \).

![Figure 1](image)

**Figure 1.** Limit state function problem 6, (a) general view and (b) zoom of limit state function.

### 5. Conclusions

The results found using numerical simulation are similar to those obtained using analytical methods. This research work demonstrated that it is possible to express the limit state functions in the space of variables by means of a standard normal space transformation without loss of accuracy. The results found using numerical simulation are similar to those obtained using analytical methods. The results obtained using Monte Carlo simulation to determine the failure probability are similar to those found using polynomial chaos expansion, with no loss of accuracy and less computational effort.

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