STOCHASTIC SPECTRAL METHODS IN UNCERTAINTY QUANTIFICATION

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Abstract. *Uncertainty quantification is an important part of a probabilistic design of structures. Nonetheless, common Monte Carlo methods are highly computationally demanding or even not feasible for this task, especially in case of mathematical models of physical problems solved by finite element method. Therefore, the paper is focused on the efficient alternative approach for uncertainty quantification-stochastic spectral expansion, represented herein by Polynomial Chaos Expansion. In recent years, an application of stochastic spectral methods in uncertainty quantification is the topic of research for many scientists in various fields of science and its efficiency was shown by various studies. The paper presents basic theoretical background of polynomial chaos expansion and its connection to uncertainty quantification. The possibility of efficient statistical and sensitivity analysis is investigated and an application in analytical examples with known reference solution is presented herein. Moreover, practical implementation of methodology is discussed and developed SW tool is presented herein.*

Keywords

Polynomial chaos expansion, Sensitivity analysis, Statistical analysis, Uncertainty quantification.

1. Introduction

The mathematical model of physical problem can be represented by function M of input variables $\mathbf{X}$. Generally, the mathematical model $M(\mathbf{X})$ can be solved in implicit form by various methods e.g. finite element method, which may be highly computationally demanding. Moreover, it is necessary to assume input variables $\mathbf{X}$ as a random vector to represent natural uncertainty of real physical problems. Therefore, response of model $Y=M(\mathbf{X})$ is a random variable described by a probability distribution. This fact leads us to seek probability distribution of Y instead of deterministic result. There are several methods for this purpose (commonly called uncertainty quantification) and most of them can be generally divided to two groups of different nature: Monte Carlo simulation techniques and stochastic spectral methods.

Common method for reliability analysis and uncertainty quantification are Monte Carlo (MC) simulation techniques in various forms e.g. crude MC or Latin Hypercube Sampling (LHS). These popular methods are simple to understand and implement but their efficiency is not generally high. The core of MC methods is a pseudo-random sampling of the input random vector. To each of realizations corresponds specific solution of mathematical model. It is possible to utilize this process for estimation of the statistics of Y (typically statistical moments and probability distribution). Unfortunately, it is necessary to perform large amount of simulations uniformly covering the whole design domain for accurate estimation of statistics, which is usually not feasible in practical applications.

On the other hand, it is possible to utilize stochastic spectral expansion methods. Stochastic spectral expansion is a more recent alternative for an uncertainty propagation and it consists in representing the solution by a functional representation of the random variables expansion. The stochastic expansion methods mostly differ from each other only on the choice of the basis functions and by the calculation of the coefficients of the expansion. Typical stochastic expansion methods are Karhunen-Loéve expansion and Polynomial Chaos Expansion (PCE). These methods are typically more efficient in comparison with MC techniques but on the other hand, theory of PCE and its implementation is not straightforward. Moreover, general efficient approach for more complicated cases (correlated input variables with arbitrary probability distribution or highly non-linear complicated mathematical models) is still under development.

The paper is focused on detailed description of PCE as a highly efficient method for uncertainty quantification. First of all, basic theoretical background is briefly presented in section 2 and practical aspects of computation are discussed in section 3. Once the PCE is created, it is possible to utilize its specific form for analytical statistical and sensitivity analysis, as can be seen in section 4. The whole process is shown on simple analytical examples with known reference solution in section 5.

2. Theoretical Background

Assume a probability space $(\Omega, \mathcal{F}, \mathcal{P})$, where Ω is an event space, $\mathcal{F}$ is a σ-algebra on Ω and $\mathcal{P}$ is a probability measure on $\mathcal{F}$. If the input vector of mathematical model is random vector $\boldsymbol{X}(\omega)$, $\omega \in \Omega$, then model response $Y(\omega)$ is a random variable. A PCE is a method, originally proposed by Norbert Wiener [1], for representing variable Y as a function of an another random variable Ξ called germ with given distribution as follows:

$$Y = f(\Xi), \tag{1}$$

where the function is a polynomial expansion. A set of polynomials orthogonal with respect to the distribution of the germ are used as a polynomial basis. The orthogonality condition for all $j \neq k$ is given by inner product of any two polynomials ψ_j and ψ_k with respect to the probability measure p_ξ of the germ Ξ as follows:

$$\langle \psi_j, \psi_k \rangle = \int \psi_j(\xi)\psi_k(\xi)\, p_\xi(\xi)\, d\xi = 0. \tag{2}$$

In other words, we utilize specific orthogonal polynomials associated to the specific distribution of a germ. For example, if the germ has standard normal distribution, we get the Hermite polynomials orthogonal to the Gaussian measure:

$$\int H_j(\xi) H_k(\xi) e^{-\xi^2/2} d\xi = j!\delta_{jk}, \tag{3}$$

where δ is Kronecker delta equal to 1 if $j = k$, symbol ! represents factorial and H_j respectively H_k are Hermite polynomials of degrees j resp. k. Orthogonal polynomials associated to another distributions can be chosen according to Wiener-Askey scheme [2]. For further processing, it is beneficiary to use normalized polynomials (orthonormal), where inner product is

$$\langle \psi_j, \psi_k \rangle = \delta_{jk}, \tag{4}$$

In case of $\mathbf{X}$ and $\boldsymbol{\Xi}$ being vectors containing M random variables, the polynomial ψ_j is multivariate and it is built up as a tensor product of univariate orthogonal polynomials

$$\Psi_{\boldsymbol{\alpha}}(\xi) = \prod_{i=1}^{M} \psi_{\alpha_i}(\xi_i), \tag{5}$$

where $\boldsymbol{\alpha} \in \mathbb{N}^M$ is set of integers called multi-index. In virtue of Eq. (2) and (4), the orthonormal polynomials are defined as:

$$\langle \psi_{\boldsymbol{\alpha}}, \psi_{\boldsymbol{\beta}} \rangle = \int \psi_{\boldsymbol{\alpha}}(\xi)\psi_{\boldsymbol{\beta}}(\xi)\, p_\xi(\xi)\, d\xi = \delta_{\boldsymbol{\alpha}\boldsymbol{\beta}}. \tag{6}$$

The random variable of interest (response of mathematical model f) can be then represented according to Soize and Ghanem [3] as:

$$Y = f(\mathbf{X}) = \sum_{\boldsymbol{\alpha} \in \mathbb{N}^M} \beta_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(\xi), \tag{7}$$

where β are deterministic coefficients and ψ are orthogonal polynomials. Without loss of generality, normalized Hermite polynomials are used for construction of Wiener-Hermite PCE assuming that all input variables are transformed to uncorrelated standard normal space.

3. Practical Computation

The infinite PCE according to Eq. (7) must be truncated to final number of terms P for practical computation. Common way is to use terms whose total degree $|\boldsymbol{\alpha}|$ is equal or less than the given p. Therefore, the truncated set of PCE terms is in mathematical notation:

$$A^{M,p} = \left\{ \alpha \in \mathbb{N}^M : |\alpha| = \sum_{i=1}^{M} \alpha_i \leq p \right\}. \tag{8}$$

The cardinality of the truncated set is given by:

$$card_{A^{M,p}} \equiv P = \binom{M+p}{p} = \frac{(M+p)!}{M!\,p!}. \tag{9}$$

The deterministic coefficients β can be computed by various methods, generally divided into two groups: intrusive (constitutive equations are discretized both in the physical space and in the random space, thus it needs modified solver of this coupled system of equations) and non-intrusive (regression based on repetitive calculation of deterministic FEM for selected realizations of $\mathbf{X}$). In recent years, the special attention is given to non-intrusive approach with an emphasize on least-square minimization.

3.1. Least-Square Minimization

Assuming truncated PCE, there is an error ε due to missing terms in the definition of the truncated PCE:

$$Y = f(\mathbf{X}) = \sum_{\boldsymbol{\alpha} \in A^{M,p}} \beta_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(\xi) + \varepsilon = \tilde{f}(\mathbf{X}) + \varepsilon. \tag{10}$$

From the point of view of a regression, the PCE can be seen as a linear regression model with a constant term, thus deterministic coefficients can be simply obtained by minimization of ε by least-square regression (LSR). It is necessary to calculate sufficient number N of original model samples called experimental design with coordinates $\mathbf{x}$ and corresponding results $\mathbf{y}$ for accurate estimation of deterministic coefficients. The estimated coefficients $\tilde{\beta}$ are obtained by minimizing L_2-norm:

$$\tilde{\beta} = \left(\boldsymbol{\psi}^{\mathrm{T}}\boldsymbol{\psi}\right)^{-1} \boldsymbol{\psi}^{\mathrm{T}}\mathbf{y}, \tag{11}$$

where data matrix $\boldsymbol{\psi}$ is

$$\boldsymbol{\psi} = \left\{ \psi_{i,j} = \psi_j(\xi_i); i = 1,...,M; j = 0,...,P-1 \right\}, \tag{12}$$

The matrix $\left(\boldsymbol{\psi}^{\mathrm{T}}\boldsymbol{\psi}\right)^{-1}$ may be ill-conditioned, thus QR decomposition [4] should be employed for inversion.

3.2. Quality of Approximation

The crucial characteristic of non-intrusive LSR PCE is the accuracy of approximation. The common method for the measurement of accuracy is a coefficient of determination R^2 between the original model and its approximation via PCE:

$$R^2 = 1 - \frac{\frac{1}{N}\sum\left[f(\mathbf{x}) - \tilde{f}(\mathbf{x})\right]^2}{\sigma_Y^2}. \tag{13}$$

However, R^2 may lead to overfitting in the case of small sample size experimental designs [4]. Thus, more robust leave-one-out cross-validation Q^2 should be used. The idea of the method is to use one set of sample points to build a PCE and another set to compute the error. Q^2 sets one point apart from the full ED and builds a PCE from the remaining points. This process is repeated for every point of the experimental design. Due to the orthonormality of PCE, it is possible to analytically determinate Q^2 directly from PCE assuming full ED [5] as

$$Q^2 = 1 - \frac{\frac{1}{N}\sum\left[\frac{f(x^i) - \tilde{f}(x^i)}{1 - h_i}\right]^2}{\sigma_Y^2}, \tag{14}$$

where h_i represents the i-th diagonal term of matrix $\boldsymbol{\psi}\left(\boldsymbol{\psi}^{\mathrm{T}}\boldsymbol{\psi}\right)^{-1}\boldsymbol{\psi}^{\mathrm{T}}$.

3.3. Model Selection Algorithm

Note that, the number of terms P is highly dependent on number of input random variables M and maximal total degree of polynomials p. Therefore, in case of a large stochastic model in combination with high maximal order of polynomials, it is easy to obtain computationally highly demanding problem. The solution can be utilization of advanced model selection algorithms e.g. Least Angle Regression (LAR) [6] or least absolute shrinkage and selection operator (LASSO) to find optimal set of PCE terms as proposed by Blatman and Sudret [5].

Herein, developed SW tool [7] using automatic algorithm based on LAR was employed for numerical examples. LAR is an efficient model selection algorithm and it consists of several basic steps:

- start with empty set of predictors,
- select predictor most correlated with residual,
- increase the coefficient of selected predictor in sign of its correlation with residual until another predictor has same correlation,
- increase the coefficients of selected predictors in their joint least square direction,
- repeat the algorithm until all predictors are included in the model or given accuracy of approximation is obtained.

4. Statistical and Sensitivity Analysis

Once the approximation in form of PCE is obtained, it is possible to perform efficient statistical and sensitivity analysis due to the orthonormality among terms as will be shown in this section. First of all, the m-th statistical moment of random variable $Y = f(\mathbf{X})$ is generally according to basic theory of probability obtained as

$$\begin{aligned}\left\langle y^m\right\rangle &= \int\left[f(\mathbf{X})\right]^m p_\xi(\xi)\,d\xi = \int\left[\sum_{\boldsymbol{\alpha}\in A^{M,p}} \beta_{\boldsymbol{\alpha}}\Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi})\right]^m p_\xi(\xi)\,d\xi = \\ &= \int \sum_{\boldsymbol{\alpha}_1\in A^{M,p}} \cdots \sum_{\boldsymbol{\alpha}_m\in A^{M,p}} \beta_{\boldsymbol{\alpha}_1}\ldots\beta_{\boldsymbol{\alpha}_m}\Psi_{\boldsymbol{\alpha}_1}(\boldsymbol{\xi})\ldots\Psi_{\boldsymbol{\alpha}_m}(\boldsymbol{\xi})\,p_\xi(\xi)\,d\xi = \\ &= \sum_{\boldsymbol{\alpha}_1\in A^{M,p}} \cdots \sum_{\boldsymbol{\alpha}_m\in A^{M,p}} \beta_{\boldsymbol{\alpha}_1}\ldots\beta_{\boldsymbol{\alpha}_m}\int\Psi_{\boldsymbol{\alpha}_1}(\boldsymbol{\xi})\ldots\Psi_{\boldsymbol{\alpha}_m}(\boldsymbol{\xi})\,p_\xi(\xi)\,d\xi.\end{aligned} \tag{15}$$

This computation is not generally easy task, however in case of PCE it can be significantly simplified due to Eq. (2). Assuming orthogonality of basis functions, simplified formula for mean value is

$$\begin{aligned}\mu_Y &= \left\langle y^1\right\rangle = \int\left[\sum_{\boldsymbol{\alpha}\in A^{M,p}} \beta_{\boldsymbol{\alpha}}\Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi})\right]p_\xi(\xi)\,d\xi = \\ &= \sum_{\boldsymbol{\alpha}\in A^{M,p}} \beta_{\boldsymbol{\alpha}}\int\Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi})\,p_\xi(\xi)\,d\xi.\end{aligned} \tag{16}$$

Moreover, considering that polynomials are orthogonal to $\Psi_0 \equiv 1$ and $\int\Psi_{\boldsymbol{\alpha}}p_\xi(\xi)d\xi = 0\;\forall\boldsymbol{\alpha}\neq\mathbf{0}$. Therefore, the mean value is first term of the expansion:

$$\mu_Y = \left\langle y^1\right\rangle = \beta_0. \tag{17}$$

Similarly, an orthogonality of polynomials leads to dramatic simplification of Eq. (10) for a second statistical moment:

$$\begin{aligned}\left\langle y^2\right\rangle &= \int\left[\sum_{\boldsymbol{\alpha}\in A^{M,p}} \beta_{\boldsymbol{\alpha}}\Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi})\right]^2 p_\xi(\xi)\,d\xi = \\ &= \sum_{\boldsymbol{\alpha}_1\in A^{M,p}}\sum_{\boldsymbol{\alpha}_2\in A^{M,p}} \beta_{\boldsymbol{\alpha}_1}\beta_{\boldsymbol{\alpha}_2}\int\Psi_{\boldsymbol{\alpha}_1}(\boldsymbol{\xi})\Psi_{\boldsymbol{\alpha}_2}(\boldsymbol{\xi})\,p_\xi(\xi)\,d\xi = \\ &= \sum_{\boldsymbol{\alpha}\in A^{M,p}} \beta_{\boldsymbol{\alpha}}^2\int\Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi})^2\,p_\xi(\xi)\,d\xi = \sum_{\boldsymbol{\alpha}\in A^{M,p}} \beta_{\boldsymbol{\alpha}}^2\left\langle\Psi_{\boldsymbol{\alpha}},\Psi_{\boldsymbol{\alpha}}\right\rangle.\end{aligned} \tag{18}$$

Once we have second statistical moment, variance can be simply computed as:

$$\sigma_Y^2 = \left\langle Y^2\right\rangle - \mu_Y^2. \tag{19}$$

Assuming orthonormal polynomials, a variance can be computed using Eq. (4) simply as:

$$\sigma_Y^2 = \sum_{\substack{\boldsymbol{\alpha}\in A^{M,p}\\ \boldsymbol{\alpha}\neq\mathbf{0}}} \beta_{\boldsymbol{\alpha}}^2. \tag{20}$$

In other words, it is obtained as a sum of all squared deterministic coefficients except the first one (which is equal to mean value of mathematical model).

4.1. Analysis of Variance (ANOVA)

Characteristic form of PCE can be utilized also in global sensitivity analysis represented by Sobol' indices derived from Hoeffding-Sobol' decomposition [8]. Let $\mathbf{X}=(X_1,\ldots,X_M)$ be a random vector with independent margins and distribution denoted by $p_{\mathbf{X}}(\mathbf{x})=p_{x_1}\otimes\ldots p_{x_M}$. For any $\mathbf{x}\in\mathbb{R}^M$ and any subset $\mathbf{u}\subseteq I=\{1,\ldots,M\}$, $\mathbf{x}_\mathbf{u}$ is a subset of $\mathbf{x}$, containing variables whose indices are included in $\mathbf{u}$. According to Hoeffding-Sobol decomposition, any square integrable function $f(\mathbf{X})$ can be decomposed as:

$$f(\mathbf{x})=f_0+\sum_{i=1}^{M}f_i(x_i)+\sum_{1\le i<j\le M}^{M}f_{ij}(x_i,x_j)+\ldots+f_{1,2,\ldots M}(\mathbf{x})= \\ =f_0+\sum_{\substack{\mathbf{u}\subset\{1,\ldots,M\}\\ \mathbf{u}\neq\emptyset}}f_\mathbf{u}(\mathbf{x}_\mathbf{u}). \tag{21}$$

The Hoeffding-Sobol' decomposition is unique when there is the orthogonality between summands, i.e.:

$$\mathbb{E}\left[f_\mathbf{u}(\mathbf{x}_\mathbf{u})f_\mathbf{v}(\mathbf{x}_\mathbf{v})\right]=0\ \forall\mathbf{u},\mathbf{v}\subseteq\{1,\ldots,M\},\mathbf{u}\neq\mathbf{v}. \tag{22}$$

In consequence of the defined decomposition, the variance of Y can be decomposed as:

$$\sigma_Y^2=Var[Y]=\sum_{\substack{\mathbf{u}\subset\{1,\ldots,M\}\\ \mathbf{u}\neq\emptyset}}Var\left[f_\mathbf{u}(\mathbf{X}_\mathbf{u})\right], \tag{23}$$

where $Var\left[f_\mathbf{u}(\mathbf{x}_\mathbf{u})\right]$ are partial variances. The first Sobol' indices are obtained if $\mathbf{u}$ contains single i-th input variable:

$$S_i=\frac{Var\left[f_i(X_i)\right]}{Var[Y]}. \tag{24}$$

The second-order indices correspond to two input variables, etc. Important information about influence of input variables and all interactions can by expressed by Total Sobol' indices which includes all interactions, thus may be computed as:

$$S_i^T=\sum_{i\in\mathbf{u}}S_\mathbf{u}. \tag{25}$$

A computation of Sobol' indices by Monte Carlo is typically highly computationally demanding. Fortunately, there is a connection between PCE and Hoeffding-Sobol' decomposition as was shown in [9]. In other words, PCE can be utilized for decomposition of $Y=f(\mathbf{X})$ due to its special form (orthonormality of terms).

The PCE can be rewritten in form of Hoeffding-Sobol' decomposition by reordering of the terms:

$$f(\mathbf{x})\approx f^{PCE}(\mathbf{x})=\beta_0+\sum_{\substack{\mathbf{u}\subset\{1,\ldots,M\}\\ \mathbf{u}\neq\emptyset}}f_\mathbf{u}(\mathbf{x}_\mathbf{u})=\beta_0+\sum_{\alpha\in A_\mathbf{u}}\beta_\alpha\Psi_\alpha(\boldsymbol{\xi}), \tag{26}$$

where set of multivariate polynomials dependent on $\mathbf{u}$ is defined as:

$$A_\mathbf{u}=\left\{\boldsymbol{\alpha}\in A^{M,p}:\alpha_k\neq0\leftrightarrow k\in\mathbf{u}\right\}. \tag{27}$$

Therefore, it is possible to obtain Sobol' indices of any order by simple analytical operation (sum of selected squared deterministic coefficients divided by variance). First order indices are thus obtained as

$$S_i^{PCE}=\frac{\sum_{\alpha\in A_i}\beta_\alpha^2}{\sigma_Y^2}\quad A_i=\left\{\boldsymbol{\alpha}\in A^{M,p}:\alpha_i>0,\alpha_{j\neq i}=0\right\}, \tag{28}$$

and total Sobol' indices can be determined as

$$S_i^{T,PCE}=\frac{\sum_{\alpha\in A_i^T}\beta_\alpha^2}{\sigma_Y^2}\quad A_i^T=\left\{\boldsymbol{\alpha}\in A^{M,p}:\alpha_i>0\right\}. \tag{29}$$

Note that, these PCE based Sobol' indices are highly dependent on truncation and sparsity of PCE. Although the results are not exact, it is possible to assume their convergence dependent on the accuracy of approximation.

4.2. Analysis of Covariance (ANCOVA)

There is a strong assumption of independent random variables for derivation of Sobol' indices in section 4.1, which may be not correct in practical applications. Therefore, this section is focused on generalization of Hoeffding-Sobol decomposition considering dependent variables. Due to the statistical dependence among input random variables, it is not possible to derive a unique decomposition in terms of orthogonal summands of increasing order. However, it is possible to cast the variance of Y as a covariance decomposition. More theoretical details can be found in [10]. Estimation of covariance decomposition via PCE consists of two steps:

- building a PCE $f(\mathbf{X})$ approximation assuming uncorrelated random variables
- using the PCE as a surrogate model in order to evaluate the variance of output with the correlated input variables $f(\mathbf{X}_c)$

The variance of the model response assuming correlated input random variables is defined as

$$Var\left[f(\mathbf{X}_c)\right]=\sum_{\substack{\mathbf{u}\subset\{1,\ldots,M\}\\ \mathbf{u}\neq\emptyset}}Cov\left[f_\mathbf{u}(\mathbf{X}),f(\mathbf{X}_c)\right]. \tag{30}$$

The covariance-based total sensitivity index S_i^{cov} is then obtained as:

$$S_i^{\text{cov}}=\frac{Cov\left[f_\mathbf{u}(\mathbf{X}),f(\mathbf{X}_c)\right]}{Var\left[f(\mathbf{X}_c)\right]}, \tag{31}$$

which can be further decomposed into the sum of a structural (uncorrelated) sensitivity index S_i^u and correlative sensitivity index S_i^c defined as:

$$S_i^u=\frac{Var\left[f_\mathbf{u}(\mathbf{X})\right]}{Var\left[f(\mathbf{X}_c)\right]}, \tag{32}$$

$$S_i^c=S_i^{\text{cov}}-S_i^u. \tag{33}$$

5. Numerical Examples

Theory of PCE briefly presented in the previous sections is applied for the estimation of statistical moments, Sobol indices and failure probability in the following academic examples. The goal of this section is a presentation of PCE as a powerful efficient tool for an uncertainty quantification and a discussion of obtained results. The developed SW tool was employed for a practical computation of examples.

5.1. Deflection of Simple Beam

First academic example is the midspan deflection of a simply supported concrete beam with uniformly distributed load:

$$v_{L/2} = \frac{5qL^4}{32EbH^3}. \tag{34}$$

The stochastic model contains five random variables with lognormal distribution with parameters from Table 1, where b and H represent the width and height of the rectangular cross-section, E is the Young`s modulus of the concrete, q is the intensity of uniform load and L is the length of the beam.

Tab.1: Stochastic model of the first example-deflection of simple beam.

Variable	μ	σ	Units
$b \sim LN$	0.15	0.0075	$[\,m\,]$
$H \sim LN$	0.3	0.015	$[\,m\,]$
$E \sim LN$	30	4.5	$[\,GPa\,]$
$q \sim LN$	10	2	$[\,kN/m\,]$
$L \sim LN$	5	0.05	$[\,m\,]$

The goal of this example is an estimation of statistical moments of $v_{L/2}$ and failure probability for several given thresholds of maximal deflection. The reference solution in this simple academic example can be obtained analytically. The PCE was created using LAR in combination with experimental design containing 100 samples generated by LHS and maximal order of polynomial basis was set as $p=4$. Estimated statistical moments and reference analytical solution can be seen in the following table:

Tab.2: Statistical moments obtained by PCE and analytical solution.

Parameter	PCE (ED=100)	Analytical solution
μ	8.366	8.367
σ^2	6.429	6.443

As can be seen, an estimation of statistical moments using PCE is very close to exact values. Note that, these values are obtained directly from PCE coefficients, thus it is very efficient approach in combination with computationally demanding mathematical models, e.g. non-linear finite element models.

The second task of this example is an estimation of failure probability for several thresholds and obtained results can be seen in Tab. 3. It is obvious, that estimated failure probabilities (using PCE as a surrogate model by Monte Carlo technique) are almost exact.

Tab.3: Comparison of failure probability estimated for the original model and the PCE.

Threshold	PCE	Analytical solution
15 mm	1.716 e-2	1.721 e-2
20 mm	1.017 e-3	1.019 e-3
25 mm	6.250 e-5	6.232 e-5
30 mm	4.300 e-6	4.268 e-6

5.2. Analysis of Covariance of Simple Analytical Function

Second academic example is the polynomial analytical function with two standardized normal input random variables $X_1, X_2 \sim N(0,1)$:

$$Y = X_1 + X_2 + X_2^2 + X_1X_2 + 3. \tag{35}$$

The main task of this example is a study of ANCOVA based sensitivity indices assuming increasing correlation coefficient ρ between random variables. The PCE was created using LAR in combination with experimental design containing 20 samples generated by LHS and maximal order of polynomial basis was set as $p=2$. Due to the polynomial form of model, it was possible to reach perfect accuracy of PCE represented by $Q^2=1$. Obtained first order sensitivity indices can be seen in Tab. 4.

Tab.4: ANCOVA indices obtained by PCE for increasing correlation.

Correlation	S_1^{cov}	S_1^u	S_1^c	S_2^{cov}	S_2^u	S_2^c
$\rho=0$	0.20	0.20	0.00	0.60	0.60	0.00
$\rho=0.2$	0.19	0.17	0.02	0.59	0.51	0.08
$\rho=0.8$	0.19	0.10	0.09	0.52	0.29	0.23

As can be seen from obtained first order ANCOVA indices, the structural parts of indices S_i^u decrease with increasing correlation between X_1 and X_2 and the influence of correlative parts S_i^c is higher, as can be generally expected. Moreover, interaction between correlated variables is more important with increasing correlation, which can be recognized by decreasing of total first order sensitivity indices S_1^{cov}.

In case of uncorrelated variables, ANCOVA indices reduce to ordinary Sobol' indices. It means that, ANCOVA indices are generalization of ordinary Sobol' indices and the method works for correlated as well as uncorrelated input random variables. Nonetheless, interpretation of ANCOVA indices for more complicated models may not be so straightforward.

6. Conclusion and discussion

The paper presents polynomial chaos expansion as a powerful tool for uncertainty quantification. First of all, basic theoretical background is given and practical computation is discussed. It is also shown how to derive first statistical moments and Sobol' indices directly from explicit function in form of polynomial chaos expansion with orthonormal terms. Presented theory is applied on academic examples and obtained results are discussed. As can be seen, stochastic spectral methods are efficient and robust, thus their employment for uncertainty quantification may be beneficial, particularly for time-consuming mathematical models, whereas application of standard Monte Carlo type technique is not even feasible. Herein, in analytical examples were assumed Gaussian and Lognormal distributions, which are directly associated to Hermite polynomials, however in practical cases it is common to work with different type of distributions (e.g. Gubmbel). In such case, the convergence of PCE might be slower and additional sample points in ED might be necessary to achieve target accuracy. Therefore, Nataf transformation to standardized Gaussian space is crucial step. Note that, it is not possible to apply Nataf transformation assuming Gaussian copula for some combinations of input variables and correlation coefficients and more general approach based on copula theory should be employed. Moreover, in practical applications it is common to work with high-dimensional stochastic problems and in that case, it might be problematic for LAR to identify the best PCE basis and different model-selection algorithm might be employed. Further research work will be focused on development of general transformation technique based on copula theory and its application on more complicated examples.

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