26th International Conference
ENGINEERING MECHANICS 2020
Brno, Czech Republic, November 24 – 25, 2020

DISTRIBUTION-BASED GLOBAL SENSITIVITY ANALYSIS BY POLYNOMIAL CHAOS EXPANSION

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Abstract: *The paper is focused on study of distribution based global sensitivity indices derived directly from polynomial chaos expansion. The significant advantage is that, once the approximation in form of polynomial chaos expansion is available it is possible to obtain first statistical moments, Sobol indices and also distribution function with proposed moment-independent sensitivity indices without additional computational demands. The key idea is to use only specific part of approximation and compare obtained conditional probability cumulative distribution function to original distribution assuming all variables free to vary. The difference between distributions is measured by Cramer-von Misses distance herein. However, it is generally possible to employ any type of measure. The method is validated by analytical example with known solution. Proposed approach is highly efficient and thus it can be recommended for practical applications, when it is not possible to perform sensitivity analysis by standard Monte Carlo approach.*

Keywords: Distribution-based sensitivity, Polynomial chaos expansion, Uncertainty quantification.

1. Introduction

The mathematical model of a physical problem can be seen as a function *f* of a set of input variables *f*(**X**). Moreover, it is assumed that *f*(**X**) is highly computationally expensive model of input random variables. The task of analysis is uncertainty quantification of mathematical model, which is not feasible and therefore, it is necessary to employ surrogate model. One of the most effective surrogate models is Polynomial Chaos Expansion (PCE) originally proposed by Norbert Wiener (1938). A PCE is a method for representing arbitrary random variables (response of mathematical model) as a function of another random variable described by distribution function. Once the PCE is available, it is feasible to perform large amount of calculations to obtain information of interest about original mathematical model, e.g. moment analysis or sensitivity analysis. There are generally two types of sensitivity analyses, on the one hand local sensitivity analysis focused on behavior of function around a point of interest (e.g. one-at-a-time and screening). On the other hand, global sensitivity analysis assuming whole design domain e.g. regression based methods and analysis of variance (ANOVA) (Sobol, 2001). A global sensitivity analysis is an area of interest for many researchers nowadays, especially ANOVA represented by Sobol' indices. Nevertheless, ANOVA methods are still highly computationally demanding. Fortunately, it was shown by Sudret (2008) how to derive Sobol' indices directly from PCE. It leads to the significant reduction of computational demands in comparison with traditional pick and freeze Monte Carlo approach.

Although ANOVA represents a strong tool for global sensitivity analysis, it takes only first two statistical moments into account. Therefore, recent theoretical research is focused on so called moment-independent sensitivity analysis. These methods generally take whole distribution of random variables into account. Herein, sensitivity measure based on Cramér-von Mises distance recently proposed by Gamboa et al. (2018) is utilized and the theory of method is briefly discussed in section 3. Unfortunately, a moment-independent sensitivity analysis is computationally even more demanding than ANOVA. Therefore, this pilot study will discuss possibility of utilizing PCE as a surrogate model for derivation of moment-independent sensitivity measures.

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doi: 10.21495/5896-3-380

2. Polynomial Chaos Expansion

Assume a probability space (Ω, $\mathcal{F}$, $\mathcal{P}$), 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 a random vector $\boldsymbol{X}(\omega)$, $\omega \in \Omega$, then the model response $Y(\omega)$ is a random variable. A PCE is a method of representing variable Y as a function of an another random variable Ξ called germ with a given distribution and representing that function as a polynomial expansion. A set of polynomials orthonormal with respect to the distribution of the germ are used as a basis of the Hilbert space $H \supset Y$ (assuming Y has a finite variance). The condition of orthogonality is given by inner product of any two functions $\psi_j$and $\psi_k$with respect to the probability density function p_ξ of Ξ as follows:

$$\langle \psi_j, \psi_k \rangle = \int \psi_j(\xi)\psi_k(\xi)p_\xi(\xi)d\xi = \delta_{jk}, \tag{1}$$

where $\delta_{jk}$is Kronecker delta. 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. The random variable of interest (response of mathematical model f) can be then represented according to Soize and Ghanem (2004) as:

$$Y = f(\mathbf{X}) = \sum_{\boldsymbol{\alpha}\in\mathbb{N}^M} \beta_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}), \tag{2}$$

where β are deterministic coefficients, ψ are multivariate orthonormal polynomials and $\boldsymbol{\alpha} \in \mathbb{N}^{\boldsymbol{M}}$ is a set of integers called multi-index. The PCE according to Eq. (2) must be truncated to finite number of terms P for practical computation. Common approach 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

$$A^{M,p} = \{\alpha \in \mathbb{N}^M : |\alpha| = \sum_{i=1}^{M} \alpha_i \leq p\} \tag{3}$$

3. Distribution-based sensitivity analysis

Let $p_Y(y)$ be the density function of model response obtained with all parameters free to vary according to their probability distribution. If we freeze one variable on x_i, we would obtain the conditional density function $p_{Y|X_1}(y)$ of model response given X_i. The shift between $p_Y(y)$ and $p_{Y|X_1}(y)$ can be measured for example as proposed by Borgonovo (2007):

$$s(X_i) = \int \left| p_Y(y) - p_{Y|X_i}(y) \right| \, dy \tag{4}$$

It is clear, that $p_{Y|X_1}(y)$ is dependent on a specific value of x_i and $s(X_i)$ is a random variable. Assuming all possible x_i, sensitivity indices based on expected shift between density functions is:

$$\delta_i = \frac{1}{2}\mathbb{E}_{X_i}[s(X_i)] \tag{5}$$

Further, following the idea of Borgonovo, Gamboa et al. (2018) recently proposed sensitivity measure based on Cramér-von Mises distance between cumulative distribution functions F (CDF), which will be utilized herein. Using Hoeffding-Sobol' decomposition of function, Gamboa et al. derived generally following Cramér-von Mises indices (CVM) for any $\boldsymbol{x} \in \mathbb{R}^{\boldsymbol{M}}$and any subset $\boldsymbol{u} \subseteq I = \{1, \dots, M\}$, $\mathbf{x}_\mathbf{u}$ concatenates the components of $\mathbf{x}$ whose indices are included in $\mathbf{u}$. The CVM for $\mathbf{x}_\mathbf{u}$ are defined as:

$$C_{\boldsymbol{u}} = \frac{\int_{\mathbb{R}} \mathbb{E}\left[\left(F^{\boldsymbol{u}}(t) - F(t)\right)^2\right] dF(t)}{\int_{\mathbb{R}} F(t)\left(1 - F(t)\right) dF(t)}, \tag{6}$$

where $\left(F^{\boldsymbol{u}}(t) - F(t)\right)^2$ is Cramér-von Mises distance between original CDF F and conditional CDF $F^{\mathbf{u}}$ given $\mathbf{X}_\mathbf{u}$, which is normalized by denominator analogously to Sobol' indices. Unfortunately, a double-loop Monte Carlo approach must be performed for practical computation of CVM and Sobol' indices, which may be computationally demanding or even not feasible for practical examples.

3.1. PCE and distribution-based sensitivity analysis

The PCE is generally a method to construct a random variable with the same distribution as a model response Y. However, it can be also utilized as a surrogate model f^{PCE}. Therefore, it is possible to utilize PCE to obtain the distribution of approximated model response Y^{PCE} using a kernel density estimator. Remember that, each term of PCE is associated to the specific random variable or combination of variables. Thus it is possible to reorder terms of PCE to obtain approximation in form of Hoeffding-Sobol' decomposition. Therefore, it is possible to express the influence of selected input random variable by evaluation of surrogate model in form of PCE reduced to selected terms. Specifically, for any $\boldsymbol{u} \subset I = \{1, \dots, M\}$let $\sim\mathbf{u}$ be the complement to $\mathbf{u}$, i.e. $\sim\mathbf{u} = I\backslash\mathbf{u}$. The reduced PCE approximation of original model $f_{\boldsymbol{u}}^{PCE}$ (neglecting the influence of selected variables $\mathbf{X_u}$ whose indices are included in **u**) has the following form:

$$f_{\boldsymbol{u}}^{PCE}(\boldsymbol{x}) = \beta_0 + \sum_{\alpha \in A_{\sim \boldsymbol{u}}} \beta_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}), \quad A_{\sim \boldsymbol{u}} = \{\boldsymbol{\alpha} \in A^{M,p} : \alpha_k \neq 0 \leftrightarrow k \in \sim \boldsymbol{u}\} \quad (7)$$

The proposed sensitivity analysis is based on difference between the cumulative distribution function $F_{Y_{PCE}}$ obtained by kernel cumulative estimation using all terms of created PCE and conditional cumulative distribution function $F_{Y_{PCE}}^{\boldsymbol{u}}$ based on results of $f_{\boldsymbol{u}}^{PCE}$. The difference can be measured by Cramér-von Mises distance $\tau_{\boldsymbol{u}}^{PCE} = \int_{\mathbb{R}} \left(F_{Y_{PCE}}^{\boldsymbol{u}}(t) - F_{Y_{PCE}}(t)\right)^2 dF(t)$. Moreover, the normalizing denominator of sensitivity measure can be simply summary of sensitivity measures for all possible conditional cumulative distribution functions derived from PCE (analogically to PCE based Sobol' indices). Therefore, the normalized sensitivity indices based on Cramér-von Mises distance derived directly from PCE are obtained as

$$C_{\boldsymbol{u}}^{PCE} = \frac{\int_{\mathbb{R}} \left(F_{Y_{PCE}}^{\boldsymbol{u}}(t) - F_{Y_{PCE}}(t)\right)^2 dF(t)}{\sum_{\substack{\Delta = \mathbb{P}(I) \\ \Delta \neq I}} \tau_{\Delta}^{PCE}}, \quad (8)$$

where $\Delta = \mathbb{P}(I)$is power set of *I*, i.e. Δ contains all possible subsets of *I*. Obviously, it is possible to get $C_{\boldsymbol{u}}^{PCE}$ of any order as in case of Sobol' indices if and only if the PCE contains terms of desired order.

4. Numerical example

Several test functions with known analytical solution for moment independent importance measure were published by Borgonovo el al. (2011). The multiplicative model with lognormal input random variables was selected as a benchmark:

$$Y = \prod_{i=1}^{n} X_i^{a_i}, \quad (9)$$

where X_i are independent random variables with lognormal distribution $LN(\eta\,; \xi)$, where η and ξ are the mean value and standard deviation of $\ln(X_i)$. The reference value is given for the mathematical model containing 3 input random variables (n = 3), with equal weights (**a** = **1**) and parameters of the lognormal distribution $\boldsymbol{\eta} = \mathbf{1}$ and $\boldsymbol{\xi}^T = [16,\ 4,\ 1]$.

Surrogate model represented by PCE was created by developed software tool (Novák and Novák, 2018) with maximal polynomial degree $p = 10$ and experimental design contained 1000 samples generated by Latin Hypercube Sampling implemented in software FReeT (Novák et al., 2014). The cardinality of truncated set of PCE multivariate polynomials is $P = 286$. The sparse PCE build up by Least Angle Regression (Efron et al., 2004) contained 40 terms. The accuracy of PCE measured by coefficient of determination is $R^2 = 0.98$. Once the PCE was available, it was utilized as a surrogate model for same samples as used for experimental design ($n_{sample} = 10^3$). The results were analysed using kernel cumulative estimation and sensitivity indices $C_{\mathbf{u}}^{PCE}$ were computed. Obtained results, reference values obtained analytically (Borgonovo et al., 2011) and normalized reference values by their sum (relative values) are compared in Tab. 1. As can be seen, proposed indices lead to well estimation of relative probability-based sensitivity indices as expected.

Tab. 1: Reference solution and estimated sensitivity indices by proposed method.

Random var.	Reference δ	Normalized δ (relative)	Proposed indices (relative)
X_1	0.472	0.68	0.68
X_2	0.155	0.22	0.24
X_3	0.071	0.10	0.08

5. Conclusions

The paper represents a study discussing the possibility of utilizing the polynomial chaos expansion for a distribution-based global sensitivity analysis. A practical computation of such sensitivity indices is typically carried out by double loop Monte Carlo approach, which is highly time consuming and in practical applications usually not feasible. Therefore, authors proposed herein a novel method for the estimation of sensitivity indices based on Cramér-von Mises distance derived directly from surrogate model in form of PCE. The simple analytical example was utilized for a validation of proposed method. Obtained results summarized in Tab. 1 show high accuracy of proposed sensitivity indices in comparison with normalized reference solution. The normalization is necessary due to different normalizing denominator, which is simplified to sum of CVM distances between original CDF and all possible conditional CDFs. Therefore, obtained results are relative and dependent on structure of PCE, therefore they converge to exact values with increasing number of PCE terms. As can be seen, the proposed methodology is able to crucially reduce computational demands of a moment-independent sensitivity analysis. Although, the proposed method works very efficiently in presented simple example, it is necessary to explore the behaviour of the method in more complex examples with different probability distributions. Moreover, presented approach will be further investigated in context of reliability-oriented sensitivity analysis (Kala, 2020), which is highly computationally demanding as well as distribution-based global sensitivity analysis.

Acknowledgement

The authors would like to express their thanks for the support provided by the Czech Science Foundation Project No. 20-01734S and the support provided by the Czech Ministry of Education, Youth and Sports under project No. FAST-J-20-6417. The first author is Brno PhD. Talent Scholarship Holder - Funded by the Brno City Municipality.

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