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SURROGATE MODELLING AND SAFETY FORMATS IN PROBABILISTIC ANALYSIS OF STRUCTURES

VYUŽITI NÁHRADNÍ PLOCHY ODEZVY A FORMÁTŮ BEZPEČNOSTI V PRAVDĚPODOBNOSTNÍ ANALÝZE KONSTRUKCÍ

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Contents

1 Introduction

Uncertainties appear everywhere! When using a mathematical model, careful attention must be given to uncertainties in the model.

— Richard Feynman

The development of computational methods for civil engineering has become more important than ever, since it is often necessary to employ advanced numerical methods for the design of new structures in order to fulfil the significantly increasing economical and safety requirements in the last decades. Moreover, there are a lot of structures, especially bridges, built in the last century, which must often be enhanced for higher loads assuming actual conditions of the structures. As a result of these industrial needs, researchers and civil engineers are more interested in advanced numerical methods to solve the mathematical models of structures – typically non-linear finite element method (NLFEM). Although NLFEM is a very accurate numerical method for solving differential equations, there is still a lack of knowledge of material characteristics (e.g. fracture energy), actual geometrical properties (e.g. position of reinforcement) and even mathematical models of some physical phenomena (e.g. fracture mechanics of quasi-brittle materials) collectively called uncertainties. As can be seen from the given examples, uncertainties play an important role, especially in the case of concrete structures. This lack of knowledge may generally lead to inaccurate results and even fatal failures despite the advanced numerical analysis performed by NLFEM. In modern structural analysis, uncertainties are represented by random variables or vectors described by specific probability distribution, the structural system can then be seen as a mathematical function of a set of random parameters. Rigorously written, assuming a probability space $(\Omega, \mathcal{F}, \mathcal{P})$ where Ω is an event space, $\mathcal{F}$ is a σ-algebra on Ω (collection of subsets closed under complementation and countable unions) and $\mathcal{P}$ is a probability measure on $\mathcal{F}$. If the input variable of a computationally demanding mathematical model representing a physical system, $Y = \mathcal{M}(X)$, is a random variable $X(\omega), \omega \in \Omega$, output QoI $Y(\omega)$ is also a random variable. Therefore, the deterministic analysis of $\mathcal{M}(X)$ is extended to stochastic analysis, which typically consists of an estimation of statistical moments, estimation of a probability distribution, sensitivity analysis, and ultimately reliability analysis. Note that, the input of a mathematical model is typically represented by a random vector $\mathbf{X}$ consisting of M marginal random variables and described by a joint probability distribution function $p_{\mathbf{X}}$.

The elementary task of stochastic analysis is to propagate uncertainties through a mathematical model in order to obtain statistical and/or sensitivity information of outputs [1]. Such process is often called uncertainty quantification (UQ) and is schematically depicted in Fig. 1.1. UQ progressively grew to a mature general scientific area connecting engineers and mathematicians, since it represents a broad topic focused on practical stochastic analysis employed in almost every branch of engineering and science [2]. The necessity and popularity of UQ is clearly visible from the exponentially growing number of published journal papers in this field.

Nevertheless, the designer's greatest interest is structural reliability, which is assessed through the calculation of the probability of structural failure. The reliability analysis is focused on the estimation of the safety margin Z given as a difference between structural resistance R and action effect E. The probability of a negative safety margin – probability of failure $p_f = P(Z < 0)$, is used in reliability analysis to prove the safety of structures. Nevertheless, the direct analytical calculation of the p_f is very complicated or impossible in most cases, thus the Monte Carlo (MC) type simulation techniques should be employed. MC techniques transform the stochastic problem into a set of deterministic calculations with randomly generated input variables according to their probability

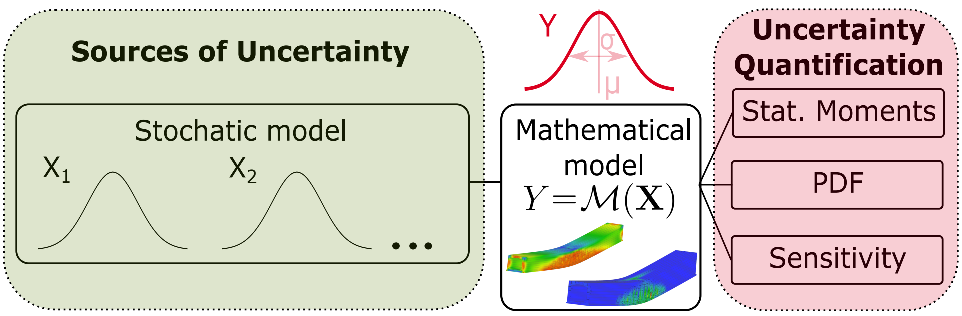

Fig. 1.1: The uncertainty quantification of a given mathematical model.

distribution law. The concept of failure probability was already implemented into the general design standards for structures, Eurocode 1990 [3], by semi-probabilistic approach. Instead of failure probability, semi-probabilistic approach is focused on the estimation of design values of load effect and structural resistance, which satisfy the given safety requirements (target failure probability) assuming that both variables are independent and separated. Design values correspond to a specific quantile of probability distribution and thus it is necessary to utilize UQ methods for its identification.

The only generally applicable method for UQ is a MC type sampling, which is based on a large number of deterministic simulations with randomly generated realizations of the input random vector according to its probability distribution. Unfortunately, it is not feasible in practical applications solved by NLFEM, since each calculation is highly computationally demanding, and MC typically works with millions of realizations. Naturally, it is possible to reduce the number of calculations by an assumption of several simplifications and the derivation of simplified formulas generally called safety formats. However, there is still a gap between a general MC analysis and significantly simplified approaches, which could lead to unrealistic results, especially in combination with NLFEM. This thesis is focused on the development of methods preserving a balance between accuracy and efficiency. Specifically, the task of the thesis is the development of methods based on surrogate models (in the context of structural reliability called response surface methods) for practical design, and the assessment of structures taking uncertainties into account.

Although there are many types of surrogate models, it is beneficial to use the techniques allowing for analytical statistical analysis of approximated quantity of interest (QoI). The obtained statistical information can be further utilized for semi-probabilistic design and the assessment of structures, or the surrogate model can be used for direct numerical integration. On the one hand, the classical technique utilized for derivation of simplifying formulas in codes is Taylor Series Expansion (TSE), which has been commonly used in engineering for decades. On the other hand, the advanced surrogate model in a form of Polynomial Chaos Expansion

(PCE) has been getting a growing attention in the recent years. Both techniques can be used for a powerful analytical analysis of QoI resulting in statistical moments and sensitivity indices. The main goal of this thesis is thus a development of theoretical methods based on the mentioned surrogate models – simplified analytical formulas derived from TSE applied in semi-probabilistic approach and efficient algorithms created specifically for PCE, which can be further used for direct MC simulation.

Aims and Objectives

The following specific aims and objectives were identified:

- Development of analytical ECoV method based on TSE:
  - review of existing methods and their comparison;
  - adaptation of TSE for civil engineering;
  - simplification of TSE in order to develop an analytical ECoV method.
- Development of efficient numerical algorithms for PCE:
  - construction of an efficient algorithm for the construction of PCE;
  - comparison with other existing surrogate models;
  - development of an innovative sampling scheme for PCE.

2 Semi-Probabilistic Approach and Safety Formats

Semi-probabilistic methods were developed as a simplification of mathematical reliability methods, where R and E are separated and design values of structural resistance R_d and action effect E_d (satisfying the given safety requirements) are determined instead of the direct calculation of the failure probability p_f. The safety check is thus reformulated to a simple form $R_d \geq E_d$. The following text is focused only on the resistance side, since it represents the main interest of this thesis. The design value of resistance R_d in Eurocode [3] is completely described by the sensitivity factor derived from First Order Reliability Method (usually simplified by the absolute value of $\alpha_R = 0.8$), the target reliability index β, and finally the first two central statistical moments together with the assumption of lognormal probability distribution of R. Obviously, for the determination of a design value by semi-probabilistic approach, it is crucial to correctly estimate the first two central statistical moments. In the context of semi-probabilistic approach, several methods were developed or adapted for this task: numerical quadrature [4], ECoV methods [5, 6] or Latin Hypercube Sampling (LHS) [7, 8]. These methods differ in sampling of random variables, i.e. the number of realizations of input random vector and their positions in a probability space. For the sake of completeness, there are also two methods implemented in Eurocode: Partial Safety Factor (PSF) method generally used for structural design, and global safety factor method for a non-linear analysis of concrete structures according to EN 1992-2 (EN 1992-2). Note that methods implemented in Eurocode need only one calculation of the mathematical model in order to obtain R_d, and thus these methods are not focused on the estimation of statistical moments, but they try to directly estimate the design quantile of resistance. Despite the success of such approach in linear calculations, its utilization in NLFEM is questionable, since calculations with extremely low material characteristics may lead to unrealistic results (PSF), or implicit assumption for the value of CoV of R in set the global safety factor could lead to a significant deviation from the real values (EN 1992-2).

The very first study conducted during the author's Ph.D. research was focused on the semi-probabilistic assessment of precast prestressed concrete roof girders using LHS, which is an MC-type method achieving generally higher accuracy in the estimation of statistical moments. The stochastic analysis consists of sensitivity analysis via Spearmann rank order correlation and statistical analysis. Since the stochastic analysis deals with a real structural element, it was also necessary to investigate the role of correlation among input random variables, which were obtained from laboratory experiments. More details can be found in ***Stochastic Modelling and Assessment of Long-Span Precast Prestressed Concrete Elements Failing in Shear*** [9]. The obtained statistical moments were utilized for the determination of R_d by semi-probabilistic approach and compared to normative methods according to Eurocode. From the obtained results, it is clear that semi-probabilistic approach in combination with LHS leads to higher R_d in comparison to the standard approach implemented in Eurocode, and thus the employment of the advanced methods is generally beneficial. Unfortunately, the whole analysis was extremely time-consuming since 100 numerical simulations of NLFEM were performed in order to obtain a reliable estimation of the first two statistical moments, which is significantly limiting for the industrial application of such approach. This complication opens up the question of possibilities for the reduction of the number of numerical simulations maintaining the accuracy of the estimated statistical moments. Although there are several existing methods for simplified estimation of coefficient of variation of structural resistance, they are typically based on a vague theoretical background and cannot incorporate information about correlation structure of input random vector.

In order to derive a simplified method for statistical analysis based on a solid theoretical background, it was necessary to review the classic method for construction of surrogate model – Taylor Series Expansion (TSE). TSE is a very efficient technique widely accepted in civil engineering, since it was used for the derivation of First Order Reliability Method (FORM). Moreover, the significant advantages of TSE are its versatility and adaptivity via arbitrary truncation of infinite series and various schemes for numerical derivation. From a practical point of view, it is worth mentioning that TSE truncated to linear terms offers a simple analytical formula for the estimation of variance based on numerical results of the mathematical model utilized for numerical derivation. One of the possible formulas for numerical derivation was proposed by Schlune et. al [5], where derivatives are approximated by a simple one-sided differencing scheme, and TSE is truncated to linear terms. Despite the simplicity of this particular form of TSE and differencing scheme, this technique achieved interesting results in several numerical studies [10, 11, 12], and thus TSE became a topic of interest for this research. In order to reduce the number of samples as much as possible while maintaining the accuracy of the approximation, several differencing schemes adapted for semi-probabilistic approach were proposed in the paper ***On Taylor Series Expansion for Statistical Moments of Functions of Correlated Random Variables*** [13]. It is shown in the paper, that the proposed differencing schemes achieve a higher accuracy, especially in the case of correlated input random variables. Moreover, the proposed methodology of three levels of increasing complexity, accuracy, and computational cost can be employed in order to progressively increase the accuracy of TSE. Although the calculations of the original mathematical model from one level of the methodology are also always used in the following level of the differencing schemes, it is still expensive for industrial applications since it represents general surrogate model without additional simplifying assumptions and thus its computational cost is highly dependent on the size of the stochastic model, i.e. number of input random variables.

The reduction of computational cost of TSE and derivation of simple analytical ECoV method was the last task of this research. The main drawback of TSE is the number of numerical simulations dependent on the size of the stochastic model, which can be circumvented by an additional strong assumption of fully correlated random variables. In this case, it was shown that TSE with simple differencing after Nataf transformation into correlated space coincides with the widely accepted and employed ECoV by Červenka in Gaussian space. Therefore, an identical process can be utilized for the transformation of the advanced differencing schemes in order to obtain analytical formulas for the estimation of mean and variance independent of the size of the stochastic model – Eigen ECoV method. Theoretical derivation and limitations of Eigen ECoV together with numerical examples are presented in ***Estimation of Coefficient of Variation for Structural Analysis: The Correlation Interval Approach*** [14]. The proposed Eigen ECoV fills the gap between the existing over-simplified methods implemented in codes commonly employed by civil engineers and the advanced techniques generally used by scientists such as LHS or TSE. It is based on the theoretical background of TSE, but its computational cost is dramatically reduced, thanks to strong assumptions, to 3 simulations (regardless of the size of the stochastic model). Naturally, it is necessary to carefully consider the applicability of these assumptions in industrial applications and their possible impact.

In order to present the synergy of TSE and the Eigen ECoV method, the correlation interval approach was proposed for industrial applications in the recent paper [14]. The estimated variance of QoI is significantly affected by the correlation among input random variables, though the definition of correlation among material characteristics is still challenging and there are no recommendations in codes. Therefore, it is beneficial to investigate two limit states: uncorrelated random variables and fully correlated random variables. Although both of the limit states are not physically acceptable, they define the interval of variance, which reflects vague or incomplete information about the correlation structure among input random variables. For practical application, it is suggested to start with the case of fully correlated random variables solved by computationally efficient Eigen ECoV, which typically leads to higher variance. If this estimation is too conservative, one should employ TSE for the estimation of variance in the case of uncorrelated random variables. Note that once the TSE is available, it is possible to analytically estimate variance for an arbitrary correlation structure, however its construction might bring high computational burden, and Eigen ECoV might then be the only feasible technique leading to a rough estimate on the safe side.

The comparison of the proposed techniques is schematically depicted in Fig.2.1 together with LHS and ECoV by Červenka. Note that the num-

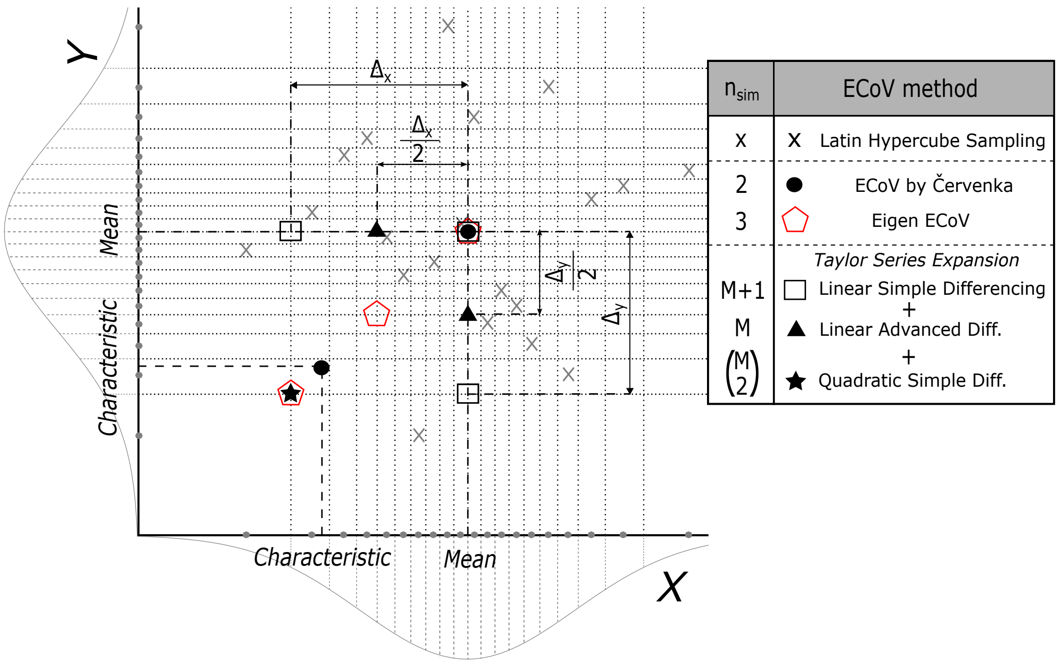

Fig. 2.1: Graphical interpretation of ECoV methods (adapted from [14])

ber of simulations for TSE is low in this 2-dimensional example, though it is highly dependent on M in contrast to Eigen ECoV. The illustration clearly presents an advantage of the proposed TSE methodology, that it is possible to progressively enrich the number of simulations in order to construct a more accurate (and expensive) form of TSE using also simulations from the previous level of approximation. Similar characteristic can be also seen in Eigen ECoV, which can be obtained directly from the simulations used by ECoV by Červenka extended by one intermediate simulation.

The significant effort was made in the development of a simple analytical ECoV method, which can be used for practical design and assessment of structures in industrial applications. The estimation of the variance interval is based on adapted TSE and novel Eigen ECoV, proposed together as the correlation interval approach. Both methods are based on several simplifications, and so there are also limitations for their employment. TSE is typically truncated only to linear terms, which might lead to an inaccurate estimation of variance in the case of non-linear functions. Additionally, there is an assumption of fully correlated input random variables in Eigen ECoV, which is not physically correct, but it leads to a dramatic reduction of the number of NLFEM calculations. The justification of both simplifying assumptions can be found in ECoV by Červenka generally accepted in the civil engineering community. As was shown in the original paper [14], ECoV by Červenka in Gaussian space corresponds to Eigen ECoV based on linear TSE with simple backward differencing, and since this technique achieves satisfactory results in many practical comparative studies [10, 11, 12] and it is already implemented in *fib* Model Code 2010 [15], it is possible to justify the assumed simplifications.

The important question arising for discussion is the ideal step-size parameter used for TSE and Eigen ECoV, since it might significantly affect the accuracy of both methods. There are generally two possibilities: a step-size parameter dependent on the target reliability index, or a fixed step-size parameter. Although a step-size parameter dependent on the target reliability index might achieve a higher accuracy [5], it is computationally inefficient for a simultaneous analysis of several structural limit states. The computational burden is caused by the fact that the original mathematical model must be calculated for each limit state (and thus different target reliability index) separately with different values of input characteristics. Fixed step-size does not bring this additional computational burden and the user can obtain the results for all limit states from a single NLFEM. Moreover, if a fixed step-size parameter is set to $c = 1.645$, it is also beneficial from a practical point of view, since Eigen ECoV is then based on three typical calculations with input characteristics easily obtained from the tables in codes: mean values, characteristic values and intermediate values.

The remaining question is whether the Eigen ECoV can be used in the case of structures with multiple failure modes. From the theoretical point of view, the Eigen ECoV should actually achieve higher accuracy in comparison to the widely employed ECoV by Červenka, since the Eigen ECoV tries to linearize the response surface using three calculations and thus it is not as sensitive to the local extrema as other existing methods (including normative methods). However, this theoretical behaviour must be also verified in numerical examples, which is a task for future research.

3 Polynomial Chaos Expansion

In the case of a comprehensive stochastic analysis or complicated examples, it is necessary to employ advanced and accurate methods for construction of the surrogate model. Naturally, it is necessary to perform a sufficiently large number of NLFEM calculations in order to obtain sufficient information about the investigated mathematical model. Moreover, a theoretical background of various types of surrogate models is usually complicated and their construction should be performed via efficient numerical algorithms. The combination of the above mentioned aspects clearly shifts the research from the field of structural safety and safety formats to computational sciences and applied mathematics, although such advanced computational methods represent a powerful tool in engineering applications. PCE as a surrogate model has got significant attention among researchers nowadays. Although a general theoretical background of this method (stochastic spectral approach) was proposed by a brilliant mathematician, Norbert Wiener, in 1938 already [16], surrogate model based on this idea was developed 60 years later [17]. Assuming that QoI has a finite variance, PCE represents the Y as a function of another random variable ξ called the germ with known probability distribution function p_ξ. The function is in the form of infinite series of the polynomial chaos expansion consisting of deterministic coefficients and basis functions orthogonal with respect to p_ξ. It is necessary to truncate the infinite series to a final number of terms for practical computation, which can be achieved by various methods. The standard approach is to select only those PCE terms whose total polynomial degree is less or equal than the given value. However, a truncated set of basis functions might be extremely high for practical computation, especially in the case of a large number of input random variables or high maximum total polynomial order, and thus there are methods for further reduction of the number of basis functions typically based on the limitation of interaction terms. This can be justified by the sparsity-of-effects principle, which states that most models describing physical phenomena are dominated by main effects and interactions of low order [18].

From the computational point of view, the calculation of PCE coefficients can be formulated in an intrusive or non-intrusive form. The intrusive approach is not widely used due to its implementation difficulties, since it reformulates the original deterministic model equations to obtain a system of equations for the PCE coefficients of the model outputs. This thesis is thus focused on a non-intrusive approach allowing for the use of third-party software as a black box within involving the calculation of PCE coefficients based on a set of model evaluations. Specifically, the regression-based non-intrusive approach is the main topic of this research, since it can be easily employed for practical UQ involving NLFEM. For the regression-based non-intrusive PCE, it is also important to employ the best model selection algorithms in order to identify the sparse set of basis functions, which is ideal for the given information matrix and leads to the best possible approximation of the original mathematical model.

As can be seen in the previous paragraphs, there are various approaches in each step of the construction process of sparse PCE, and thus the first study was focused on the comparison of methods for a construction of the truncated set of basis functions and the existing sparsity solvers. The most efficient state-of-the-art methods were utilized for the construction of an efficient and fully automatic algorithm presented in ***Polynomial Chaos Expansion for Surrogate Modelling: Theory and Software*** [19]. The proposed algorithm can be easily coupled with any third-party software for NLFEM, and it can be employed by users without deep theoretical knowledge of PCE. The combination of the Least Angle Regression for the best model selection, maximal polynomial order adaptivity, and implemented Nataf transformation lead to the best possible approximation of the original mathematical model by PCE for the given experimental design. Thanks to a combination of simplicity for the user and accuracy achieved by advanced numerical methods, the algorithm represents an ideal solution for engineers dealing with UQ of computationally demanding mathematical models. Moreover, once this algorithm was created and validated on analytical examples, it was possible to employ it for further theoretical research and comparison with novel techniques.

The developed PCE algorithm was employed for a comparison with the artificial neural network (ANN), which represents another popular regression-based non-intrusive surrogate model. Although ANN is already well known in computational science, its specific form Neural Network Ensemble (NNE) is a new and promising technique improving the accuracy of ANN by the construction of several surrogates and the combination of their estimations. NNE thus might achieve higher accuracy of an approximation thanks to statistical processing of several single ANNs. The investigation of NNE in the context of sensitivity analysis is presented in ***Neural Network Ensemble-based Sensitivity Analysis in Structural Engineering: Comparison of Selected Methods and the Influence of Statistical Correlation*** [20]. The paper is focused on several methods of sensitivity analysis of both the local and global type. The reference solution are Sobol' indices and their generalization for correlated input random variables, which are obtained by PCE, and the algorithm presented in the previous paragraph. The PCE was employed since the orthogonality of basis functions allows for powerful and efficient post-processing. Once a PCE is created, it is possible to obtain statistical moments of function and Sobol' indices without any additional computational demands. From the obtained results, it is clear that NNE achieves a high accuracy of an approximation (comparable to PCE), and it significantly outperforms a single ANN. However, NNE is still a black-box method, and thus its additional analysis during post-processing is limited, and its error estimation might be complicated.

In contrast to black-box methods, PCE is based on a strong theoretical background, which can be utilized for the derivation of interesting characteristics. Beside the error estimators, statistical moments and Sobol' indices of QoI, one might be interested in the local characteristics of the created PCE. This idea was recently presented in ***Variance-Based Adaptive Sequential Sampling for Polynomial Chaos Expansion*** [21] focused on local variance (variance density) of QoI. The idea of this approach is based on the definition of the mth statistical moment:

$$\langle y^m \rangle = \int \left[\mathcal{M}(X)\right]^m p_X(x)dx = \int \Big[\sum_{\alpha\in\mathbb{N}^M} \beta_\alpha \Psi_\alpha(\xi)\Big]^m p_\xi(\xi)d\xi =$$
$$= \sum_{\alpha_1\in\mathbb{N}^M} ... \sum_{\alpha_m\in\mathbb{N}^M} \beta_{\alpha_1}...\beta_{\alpha_m} \int \Psi_{\alpha_1}(\xi)...\Psi_{\alpha_m}(\xi)p_\xi(\xi)d\xi$$

It can be seen in the last part of this formula that in the case of PCE it is necessary to integrate over basis functions Ψ (orthonormal polynomials), which leads to a dramatic simplification in comparison to the integration of $\mathcal{M}(\mathbf{X})$. In the case of variance, one can utilize the orthogonality properties of basis functions and obtain the second raw moment of QoI directly as a sum of squared deterministic coefficients β. However, one can also see this formula as an integration of local contributions to variance, which is called variance density in the paper. Variance density is a very interesting characteristic of the PCE, since it shows the local deviations of the mathematical model from its mean value. Such information can be beneficially incorporated into the criterion defining the best possible location of samples in experimental design based on rationale of Koksma-Hlawka inequality [22].

The proposed Θ criterion for sequential sampling consists of two parts: variance density and geometrical term assuring uniform coverage of the whole design domain. Both these terms taken together lead to an ideal coverage of the design domain with respect to local variance, and thus it leads to a dense sampling in locations with functional extrema. Such approach can be easily coupled with any existing sampling scheme and it leads to a higher accuracy of PCE in comparison to the non-sequential approach. This method represents the main advantage of PCE over ANN or NNE, since the explicit form of PCE allows for analytically deriving important information about the approximation and efficiently using it for further analysis. Moreover, PCE is specifically beneficial for UQ thanks to its basis functions orthogonal with respect to a probability distribution of input random vector, which allows for a simple analytical derivation of stochastic characteristics of QoI.

Although the proposed criterion for sequential sampling can be coupled with any non-sequential sampling, it is clear from the obtained results that the final accuracy of PCE is highly dependent on the selected non-sequential technique, and thus this choice should be made carefully. Although the proposed sequential sampling leads to a significantly higher accuracy of PCE based on Latin Hypercube Sampling and Coherence D-optimal sampling, there is a potential of improvement by the employment of advanced sampling schemes generated from the target distribution that additionally avoids clustering or empty regions while maintaining true statistical homogeneity via periodic distance-based criteria [23]. The significant drawback of the proposed sampling technique is its performance based on the size of the pool of candidates generated by arbitrary non-sequential sampling. It was shown that the related aspect is a maximum polynomial order of PCE, which might be the limiting aspect of the proposed approach, and thus further studies should work with the adaptive value as was shown in the first numerical example in original article [21]. However, the adaptivity of maximum polynomial order brings additional computational burden and non-trivial techniques might be necessary for the construction of the pool of candidates in the case of coherence D-optimal sampling. Further work will thus be focused on the comparison of the proposed sequential sampling coupled with advanced sampling schemes involving adaptive techniques such as adaptive coherence D-optimal sampling and induced sampling.

The utilization of a high polynomial degree could also be circumvented by a different philosophy: the division of the design domain into small sub-spaces approximated by low-order PCEs. Such algorithm could also be based on the identical Θ criterion, though for a different purpose. In this case, the suitable criterion is used for the detection of the most important strata associated with high local variance. The identified strata are further divided into smaller parts, and local PCE approximation is created for each of them. In order to achieve an approximation with continuous derivatives on boundaries of adjoining sub-spaces, it is also necessary to use interpolating PCE instead of regression-based PCE.

4 Concluding Remarks

Obviously, the role of UQ is increasingly more important in the process of design and assessment of structures, and thus novel numerical methods for civil engineers should be created. Although the development of such techniques is a broad topic investigated by many researchers, there is still a gap between purely scientific methods and techniques for industrial applications. The results of this thesis have the potential to fill this gap, although the original task was divided into two parts and two separate techniques were investigated. Specifically, this thesis was focused on the development of novel theoretical methods for probabilistic design and assessment of structures via surrogate modeling. For the given task, the following two types of surrogate models were utilized: PCE and TSE, both employed in different contexts and for different types of applications.

The simplified safety formats can be easily used for industrial applications, although they have severe limitations. In order to develop a simple analytical theoretical method, the advanced differencing schemes adapted for civil engineering were proposed for TSE. The proposed advanced differencing schemes lead to a more accurate, but less efficient approximation of the original mathematical model in the case of functions of correlated input random variables, which is typical for NLFEM of concrete structures. Furthermore, TSE with the proposed differencing schemes was utilized for the development of a novel analytical method called Eigen ECoV, based on the theory of TSE and Nataf transformation. The Eigen ECoV represents the main result of this thesis for industrial applications, and it has the potential to significantly affect the semi-probabilistic design and assessment of structures. TSE and Eigen ECoV together form a correlation interval approach developed for industrial applications with a vague information about correlation structure among input random variables. A lack of knowledge on the joint probability distribution is typical for industrial applications, since only marginal probability distributions are usually known, although it is necessary to define a correlation structure of the input random variables in order to completely describe input random vector [24]. The correlation interval approach consequently reveals the impact of vague information about a correlation structure.

A complex stochastic analysis is typically based on an MC-type simulation and thus it is necessary to create an accurate surrogate model of the original function. The second part of the research was focused on PCE, which generally represents an efficient surrogate model for UQ. Since the construction of PCE is not simple task and there are various intrusive and non-intrusive approaches, the first step of the research was the construction of an automatic software algorithm based on the most efficient state-of-the-art methods. During the research, an efficient PCE algorithm was also implemented into a stand-alone software tool. The software is fully automatic and can be generally coupled with any third-party NLFEM software, which allows for its employment by users without deep theoretical knowledge about PCE. The developed algorithm was further employed in comparison with NNE in the context of sensitivity analysis. Although NNE has a high potential for UQ, it is a black-box method, and its post-processing is complicated. On the other hand, the theoretical characteristics of PCE were utilized in the research task focused on the adaptive sequential sampling scheme developed specifically for PCE, which significantly reduces its computational cost. The sampling technique is based on a novel philosophy, which has the potential to affect the whole scientific field of UQ.

The developed theoretical methods are based on cutting-edge techniques of UQ for civil engineering and it can be concluded that all identified aims and objectives of this thesis were met. The developed theoretical methods also represent a significant progress beyond the state-of-the-art techniques and they have the potential to become efficient tools for industrial design and the assessment of structures as well as for further theoretical research in the field of computational science and applied mechanics. However, there still remain some open questions in both research areas briefly discussed in previous text together with the directions of future research. The tasks of further work are clearly identified and ensure the continuity of this research.

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Curriculum vitæ

Personal information

Name and surname:	Ing. Lukáš Novák
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Discipline and the start date of doctoral studies

Institution: Brno University of Technology, Faculty of Civil Engineering
Field of study: Civil engineering, Structures and Traffic Constructions
Topic: Effective probabilistic design of concrete structures using safety formats and response surface
Supervisor: Prof. Ing. Drahomír Novák, DrSc.
Date of admission & inscription: 7.2.2018 & 9.2.2018

Education and qualification

Brno University of Technology, Faculty of Civil Engineering
Civil Engineering, Building Constructions, Structural mechanics

Master's thesis (supervisor prof. Ing. Drahomír Novák, DrSc.):
Probabilistic Modeling of Shear Strength of Prestressed Concrete Beams: Sensitivity Analysis and Semi-Probabilistic Design Methods (grade: A/A)

Bachelor's thesis (supervisor prof. Ing. Drahomír Novák, DrSc.):
Software of Fracture-Mechanical Parameters and Probabilistic Analysis Support Used for Statistical Analysis of Roof Prestressed Girders (grade: A/A)

Relevant courses:

Scia Engineer Certificate (FEM)	30.11.2015
Atena Červenka Consulting Advanced (NLFEM)	13-15.11.2017
JCSS: Structural reliability (South Africa)	3-12.4.2018
Reliability of structures (**organizer**, BUT)	20.6.2018
Modeling and Numerical Methods for UQ (France)	2-6.9.2019

Teaching experience:

CD004 Structural Reliability (Czech)
BD004 Structural Analysis II (Czech)

Scientific activities and academic awards

$\mathcal{H}$-index / citations: 3 (4) / 21 (34) according to WoS (Scopus)
Journal ISI papers J_{imp} / conference papers D: 6 / 11 according to Scopus

Academic awards

Medal SIGNUM PROSPERITATIS (FCE BUT)	22.11.2017
Award of dean of Faculty of Civil Engineering	19.02.2018
Czech Concrete Society award for master thesis	19.02.2018
Diploma thesis Award (BUT)	19.02.2018
Josef Hlavka Award	17.11.2018
Brno Ph.D. talent scholarship	01.01.2019

Organizations and committee memberships:

fib Task Group 3.1: Reliability of existing structures
fib Action Group 8: Non-linear finite element modelling
scientific committee of International Probabilistic Workshop 2022

Invited lectures:

Hohai University,China	29.08.2019
FCE, BUT, Brno	19.11.2019

Research positions and selected scientific projects

Brno University of Technology: Student researcher 1.1.2015- 1.1.2018
Brno University of Technology: Researcher since 1.1.2017
Advanced Materials, Technologies and Structures Center: Researcher since 1.1.2018

2020-2022 Co-Investigator	*Development of theory and advanced algorithms for UNCertainty analyses in Engineering PROblems (UNCEPRO)* INTER-Action CZ-USA project funded by Ministry of Education, Youth and Sports of Czech Republic under project No. LTAUSA19058.
2019-2021 Investigator	*Highly Efficient Reliability Analysis (HERA)* Brno Ph.D. talent project and scholarship funded by Brno City Municipality
2019 Investigator	*Moment-independent sensitivity analysis using polynomial chaos expansion* funded by Ministry of Education, Youth and Sports of Czech Republic under project No. FAST-J-19-5780
2018 Investigator	*Using polynomial chaos expansion as surrogate model* funded by Ministry of Education, Youth and Sports of Czech Republic under project No. FAST-J8-5309
2018-2020 Co-investigator	*Response surface and sensitivity analysis methods in stochastic computational mechanics (RESUS)* granted by Czech science foundation under project No. 18-13212S

Selected scientific publications

L. NOVÁK, M. VOŘECHOVSKÝ, V. SADÍLEK, M. D. SHIELDS, Variance-based Adaptive Sequential Sampling for Polynomial Chaos Expansion. Computer Methods in Applied Mechanics and Engineering, 2021, vol. 386, 114105. ISSN: 0045-7825.
DOI: 10.1016/j.cma.2021.114105 [**IF/AIS: 6.756 (D1)/1.805 (D1)**]

L. NOVÁK, D. NOVÁK, Estimation of Coefficient of Variation for Structural Analysis: The Correlation Interval Approach. Structural Safety, 2021, vol. 92, 102101. ISSN: 0167-4730.
DOI: 10.1016/j.strusafe.2021.102101 [**IF/AIS: 5.047 (Q1)/1.461 (D1)**]

L. Pan, **L. NOVÁK**, D. NOVÁK, D. LEHKÝ, M. CAO, Neural Network Ensemble-Based Sensitivity Analysis in Structural Engineering: Comparison of Selected Methods and the Influence of Statistical Correlation. Computers & Structures, 2021, vol. 242, 106376. ISSN: 0045-7949.
DOI: 10.1016/j.compstruc.2020.106376 [**IF/AIS: 4.578 (Q1)/1.131 (D1)**]

O. SLOWIK, D. NOVÁK, **L. NOVÁK**, A. STRAUSS, Stochastic Modelling and Assessment of Long-Span Precast Prestressed Concrete Elements Failing in Shear. Engineering Structures, 2021, vol. 228, 111500. ISSN: 0141-0296.
DOI: 10.1016/j.engstruct.2020.111500 [**IF/AIS: 4.471 (Q1)/0.927 (Q1)**]

L. NOVÁK, D. NOVÁK, On Taylor Series Expansion for Statistical Moments of Functions of Correlated Random Variables †. Symmetry, 2020, vol. 12, issue 8, p. 1-14. ISSN: 2073-8994.
DOI: 10.3390/sym12081379 [**IF/AIS: 2.645 (Q2)/0.304 (Q3)**]

L. NOVÁK, D. NOVÁK, Surrogate Modelling in the Stochastic Analysis of Concrete Girders Failing in Shear. In Proceedings of the fib Symposium 2019: Concrete - Innovations in Materials, Design and Structures. International Federation for Structural Concrete, 2019. p. 1741-1747. ISBN: 9782940643004.

L. NOVÁK, D. NOVÁK, R. PUKL, Probabilistic and Semi-Probabilistic Design of Large Concrete Beams Failing in Shear. In Advances in Engineering Materials, Structures and Systems: Innovations, Mechanics and Applications. London: Taylor and Francis Group CRC Press, 2019. ISBN: 9781138386969.

L. NOVÁK, D. NOVÁK, Polynomial Chaos Expansion for Surrogate Modelling: Theory and Software, Beton und Stahlbeton volume 113, ISSN:1437-1006, Austria, 2018
DOI: 10.1002/best.201800048 [**IF/AIS: 0.966 (Q3)/0.179 (Q4)**]

L. NOVÁK, D. NOVÁK; O. SLOWIK, Application of Polynomial Chaos Expansion to Reliability Analysis of Prestressed Concrete Roof Girders. In Proceedings of Engineering Mechanics 2018, ISBN 978-80-86246-88-8, Svratka, Czech Republic, 2018

L. NOVÁK, M. VOŘECHOVSKÝ, Generalization of Coloring Linear Transformation. In Proceedings of Modelování v mechanice 2018, Ostrava, Czech Republic, 2018

L. NOVÁK, L. PAN; O. SLOWIK; D. NOVÁK, Advanced Reliability and Sensitivity Analysis of Prestressed Concrete Girders Failing in Shear. In Proceedings of fib Ph.D. symposium 2018, Praha, Czech Republic, 2018

D. NOVÁK; **L. NOVÁK**, O. SLOWIK; A. STRAUSS, Prestressed Concrete Roof Girders: Part III – Semi-Probabilistic Design. In Proceedings of the Sixth International Symposium on Life-Cycle Civil Engineering (IALCCE 2018). London: CRC press, Taylor and Francis group, 2018. ISBN: 9781138626331.

Complete list of author's publications:
https://www.vutbr.cz/en/people/lukas-novak-154284/publikace

Practical research

Lukáš Novák is an active member of the practical research team cooperating with several national and international industrial partners. His task is mainly the implementation of developed advanced theoretical methods into software tools for design and the assessment of concrete structures in the following projects:

2019-2022 Co-Investigator	*Efficient semi-probabilistic methods for design and assessment of structures* funded by Technology agency of the Czech Republic under project No. TH04010138.
2019-2021 Co-Investigator	*Advanced system for monitoring, diagnosis and reliability assessment of large-scale concrete infrastructures* CZ-CHINA DELTA project funded by Technology agency of the Czech Republic under project No. TF06000016
2018-2021 Co-Investigator	*INTERREG SAFEBRIDGE project*, awarded by the European Regional Development Fund within the European Union program Interreg Austria–Czech Republic under project No. ATCZ190

Developed software tools

Theoretical methods applied during practical research were implemented into standalone software tools in order to be easily employed in future applications by industrial partners:

PCE-UQ
NOVÁK, L. and NOVÁK D.
http://www.fce.vutbr.cz/stm/novak.l/pce-uq/pce-uq.html
Comment: Lukáš Novák was the leading person in research and development of the state-of-the-art advanced software tool based on theory of Polynomial Chaos Expansion for complex reliability analysis. More details about the algorithm can be found in the following journal paper:
L. NOVÁK; D. NOVÁK, Polynomial Chaos Expansion for Surrogate Modelling: Theory and Software, Beton und Stahlbeton volume 113, ISSN:1437-1006, Austria, 2018.

SEMIP
NOVÁK, L. and NOVÁK D.
https://www.fce.vutbr.cz/STM/novak.l/semip/semip.html
Comment: Lukáš Novák was the leading person in research and development of the state-of-the-art advanced software tool focused on semi-probabilistic design and assessment of structures. More details about the implemented theoretical methods can be found in the following journal paper:
L. NOVÁK, D. NOVÁK, Estimation of Coefficient of Variation for Structural Analysis: The Correlation Interval Approach. Structural Safety, 2021, vol. 92, 102101. ISSN: 0167-4730.

Abstract

The presented doctoral thesis is focused on the development of theoretical methods for probabilistic design and assessment of structures. In order to reduce the computational burden of the probabilistic approach, the developed methods are based on surrogate models. Specifically, Taylor series expansion has been utilized for the derivation of a novel analytical method for a simplified semi-probabilistic design of structures represented by non-linear finite element models. The novel approach estimates a variance of quantity of interest and the influence of correlation among input random variables. The second part of the doctoral thesis aims at the development of efficient numerical algorithms for the construction of a surrogate model based on polynomial chaos expansion and its utilization for uncertainty quantification. Although the proposed algorithm is based on cutting edge techniques, it was beneficial to improve its accuracy and efficiency by advanced statistical sampling. Therefore, a novel technique for adaptive sequential statistical sampling, reflecting the exploration of the design domain, and exploitation of the surrogate model, is proposed specifically for polynomial chaos expansion.

Keywords

Uncertainty quantification, semi-probabilistic approach, surrogate model, polynomial chaos expansion, Taylor series expansion.