Higher-order approximations methods for global sensitivity analysis of nonlinear model outputs

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***Abstract*—**The article deals with the use of higher-order approximation polynomials and Latin Hypercube Sampling numerical simulation for the assessment of global sensitivity analysis of nonlinear model output. Highly effective computer evaluation of first and higher order sensitivity indices in non-additive systems is shown. The presented example of a non-additive system of a load-carrying structure was modelled using the nonlinear finite element method and assessed via variance-based sensitivity analysis. The presented sensitivity assessment allows exploration of all regions of the input space, accounting for interactions as well as nonlinear responses.

***Keywords*—**Sensitivity analysis, mathematical modelling, simulation, buckling, imperfection, reliability, stochastic.

I. Introduction

From the scientific point of view, sensitivity analysis is a set of methods that allow us understand the key findings of mathematical models [1]. Given the complexity of computer codes, it is not possible for the analyst to understand the output response of a model to changes in model inputs based on intuition. It appears that the prudent use of sensitivity analysis techniques is an integral part in the need to use well developed and often very sophisticated simulation models with maximum efficiency, see, e.g. [2, 3].

The diversity of problems that are solved through mathematical modelling has, recently, led to the development of a series of highly successful methods of sensitivity analysis, see, for e.g. [4-6]. Reviews of sensitivity methods in interdisciplinary contexts are offered in [7]. Bibliometric analysis of the trends of different sensitivity analysis practices from the last decade is published in [8].

A giant leap in studying models using computer simulations was the assigning of random variables to the model inputs [1]. Stochastic analysis is appealing, but it has a number of theoretical and practical limitations, which can lead to inaccurate or incorrect conclusions. It is worth noting in this context that scientist argue, both in favour of probabilistic methods for sensitivity analysis, as well as against their application [7, 9]. The main argument against the use of stochastic methods is that random variables are assigned also to the model inputs for which the random description is unjustified. In these situations, the analysts have two options: (i) use a method that does not require knowledge of the probability density function of the inputs variables, or (ii) create preconditions for the random variability of the input variables.

Advanced stochastic global sensitivity analysis methods are usually highly numerically intensive. Stochastic sensitivity analysis is usually evaluated using numerical simulation methods. The more complicated the computational model, the more computer time is needed to calculate a realization (one run) of the output random variable. The more complex the sensitivity analysis, the more realizations (numerical simulations) are needed to obtain statistically correct output. In all cases, the sensitivity analysis should lead to practical information on the true significance of input factors on the model output *Y*.

II. Global Sensitivity analysis

Majority of sensitivity analyses that have been published are either local or one factor-at-a-time analyses that rely on unjustified assumptions of model linearity and additivity [8]. Global approaches to sensitivity analyses, which would avert these drawbacks, are scarcely applied by a minority of researchers [8]. Variance-based global sensitivity analysis techniques are generally applicable to simulation models, but are significantly less for models used to rank alternative options, such as multi-criteria decision analysis (MCDA) methods [10-13]. In engineering fields, we try to keep up with current trends of modern research, which is focused on global sensitivity analysis of model outputs [1].

A. Sobol's sensitivity analysis

One of the most effective methods of stochastic global sensitivity analysis is Sobol's sensitivity analysis, which is based on the total decomposition of the variance of the output variable into parts with increasing dimension of input variables [14, 15].

Let Y=f(X_1,X_2,…,X_k) be a deterministic model where Y is a scalar output and X_i are k independent input factors, considered uncertain. The sensitivity of the output variable to the input variables is described by 2^n-1 sensitivity coefficients, where n is the number of input random variables. The first n main indices are first order sensitivity indices S_i. i-th index S_i (or main effect) corresponds to the fraction of variance of the

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output V(Y) that can be attributed to X_i alone. The index S_i is defined as:

$$S_i = \frac{V_{X_i}\left(E_{\mathbf{X}_{\sim i}}\left(Y|X_i\right)\right)}{V(Y)} \quad (1)$$

where X_i is the i-th factor and $X_{\sim i}$ denotes the matrix of all factors but X_i. The meaning of the inner expectation operator is that the mean of Y, the scalar output of interest, is taken over all possible values of $X_{\sim i}$ while keeping X_i fixed. The outer variance is taken over all possible values of X_i [16]. The variance V(Y) in the denominator is the total (unconditioned) variance. The main index S_i corresponds to the fraction of variance of the output V(Y) that can be attributed to X_i alone.

The remaining 2^n-n-1 sensitivity coefficients describe higher order interactions. The sensitivity index of the second order can be written as:

$$S_{ij} = \frac{V_{X_i}\left(E_{\mathbf{X}_{\sim i}}\left(Y|X_i, X_j\right)\right)}{V(Y)} - S_i - S_j \quad (2)$$

Sensitivity indices of other higher orders can be calculated analogously [16]. For a computational model with M factors, there may be interaction terms up to the order k, i.e., [16]:

$$\sum_i S_i + \sum_i \sum_{j>i} S_{ij} + \sum_i \sum_{j>i} \sum_{k>j} S_{ijk} + \ldots + S_{123\ldots M} = 1 \quad (3)$$

Equation (3) decomposes the output variance into parts attributable to individual input variables, as well as their combinations. Despite being computationally demanding, Sobol's sensitivity analysis allows the exploration of all parts of the input space taking into account interactions as well as nonlinear responses.

B. Stochastic Systems based on Nonlinear FEM

Majority of models of load bearing building structures are based on the finite element method [17]. The calculation of all sensitivity indices in (3) using the Monte Carlo (MC) method would be the universal solution, but the calculation is highly numerically demanding in most models based on the nonlinear finite element method (FEM). Using the Latin Hypercube Sampling (LHS) method [18, 19] partly reduces the demand on the high number of MC simulations, however, it does not provide such advantages that would allow us to study the nonlinear response of FEM models of real load bearing members in real time.

The objective of this article is to propose an approximation polynomial for the evaluation of Sobol's sensitivity analysis will all members in (3) in real time. Approximation is performed using numerical simulations on computers. The outputs of the nonlinear FEM model are approximated on a chosen domain.

Approximation models are an important part of optimization strategies [20, 21]. It can be noted that approximation methods are not new and have been described, for e.g., during the substitution of the function of the limit state using techniques of the Response Surface, which were developed to reduce the computational costs of structural reliability analysis [22]. However, the substitution of the real response function in Sobol's global sensitivity analysis is considerably more complicated than in the approximation of the limit states, where polynomials of the first or second order are usually sufficient.

III. COMPUTATIONAL MODEL

The influence of initial imperfections on the load carrying capacity of a compressed strut of length L=6m is studied in the article. The strut is supported in the middle by a spring with tensile stiffness K, which simulates the connection of the compressed strut to an adjacent structure, see Fig. 1. The bond partly resists buckling, however, it does not completely prevent buckling. The strut profile is HEA 200.

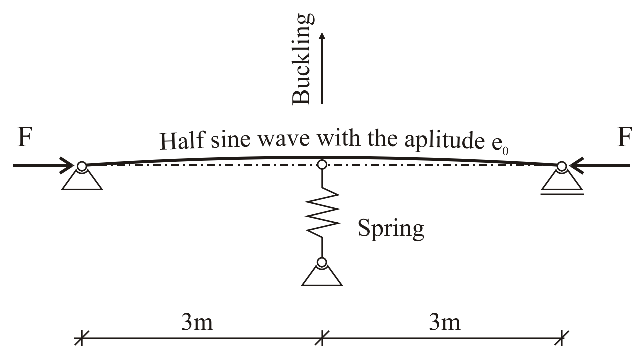

Fig. 1 Model of strut with spring

Support with stiffness K is influenced by the buckling length L_{cr}, which may lie in the interval from 0.5·L to L. If K=0 the perfectly straight strut buckles in the shape of a half sine wave, which is considered as the shape of initial imperfection of the strut axis. For K=0, L_{cr}=L=6m and slenderness λ=60. If K=∞ the perfectly straight strut buckles in the shape of a sine wave and it holds that L_{cr}=3 m and λ=30. Practically, this already occurs for K=2.051 MNm^{-1}, see Fig. 2.

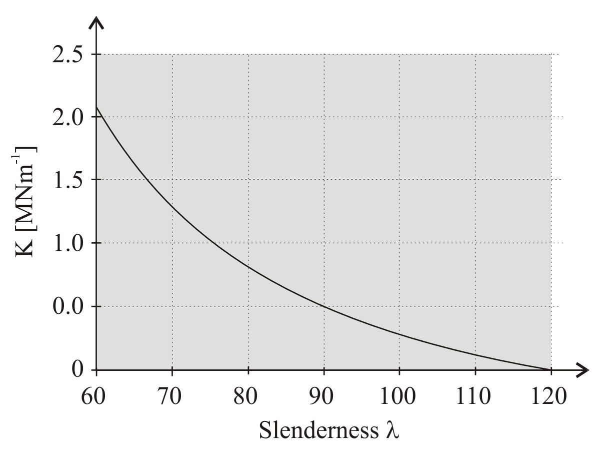

Fig. 2 Stiffness K vs. slenderness λ

IV. Initial imperfections

The initial curvature of the strut was chosen in the shape of a half-sine wave with amplitude of zero mean value and standard deviation L/1307=6m/1307=0.00459m. The standard deviation satisfies the presumption that 95 % of realizations of the random imperfections lie within the interval ± L· 0.15 % =± 6· 0.15 = ± 9 mm. This is a frequently presumed criterion in reliability analyses.

TABLE I

Initial Random Imperfections

Characteristic	Mean value	St. deviation
Cross-sectional width b	200 mm	1.9736 mm
Flange thickness t_2	10.0 mm	0.45859 mm
Yield strength f_y	297.3 MPa	16.8 mm
Young's modulus E	210 GPa	9.99 GPa
Amplitude e_0	0	4.59 mm

Gauss probability density functions were considered for all inputs listed in Table 1. Deviations of the dimensions of hot-rolled steel cross sections from its nominal values were published in [23]. In the presented study, the profile HEA 200, which is a common structural element of compressed columns, was considered. Cross-sectional height h=190mm and web thickness t_1=6.5mm were considered as deterministic variables, because their influence on the variability of the load carrying capacity is negligible. Statistical characteristics of yield strength and Young's modulus were considered analogously as in studies [24, 25].

V. Computational model

The strut was modelled using the method of beam finite elements (FEM). The resistance was calculated using the geometrically nonlinear solution, its algorithm of solution and tangential stiffness matrices were published in [26]. The resistance was calculated with an accuracy of 0.1 %, similarly as has been applied in numerous reliability studies of slender steel structures with imperfections, e.g. [27-29].

VI. Approximation function for sensitivity analysis

The evaluation of sensitivity analysis using the geometrically nonlinear FEM would require using a high number of LHS simulation runs. The numerical demand of numerical simulations on computers is the biggest limitation for calculating all members in (3). The more numerically challenging one run of the computational model is and the higher the number of input random variables in the computational model, the less the members of (3) that can be effectively calculated with reasonable costs with regard to computer time. Many analysts are thus satisfied with the calculation of first order sensitivity indices (1), the number of which equals the number of input random variables.

It is, however, desirable to calculate the other members in (3), because they could contain valuable information on the interactions among the inputs. For a high number of input factors, the number of higher order indices can be high, therefore, the evaluation of one simulation run must be sufficiently fast. This can be achieved by approximating the load carrying capacity with a polynomial, which takes into account all linear and nonlinear interactions of the input variables. The approximation polynomial satisfying the interpolation conditions was constructed for the five input random variables in Table 1 in the following non-linear form:

$$
\begin{aligned}
Y = {} & c_0 + \sum_{a=1}^{2}\sum_{i=1}^{5} c_\alpha X_i^a + \sum_{a=1}^{2}\sum_{b=1}^{2}\sum_{i=1}^{5}\sum_{j=i+1}^{5} c_\alpha \cdot X_i^a \cdot X_j^b \\
& + \sum_{a=1}^{2}\sum_{b=1}^{2}\sum_{c=1}^{2}\sum_{i=1}^{5}\sum_{j=i+1}^{5}\sum_{k=j+1}^{5} c_\alpha \cdot X_i^a \cdot X_j^b \cdot X_k^c \\
& + \sum_{a=1}^{2}\sum_{b=1}^{2}\sum_{c=1}^{2}\sum_{d=1}^{2}\sum_{i=1}^{5}\sum_{j=i+1}^{5}\sum_{k=j+1}^{5}\sum_{l=k+1}^{5} c_\alpha \cdot X_i^a \cdot X_j^b \cdot X_k^c \cdot X_l^d \\
& + \sum_{a=1}^{2}\sum_{b=1}^{2}\sum_{c=1}^{2}\sum_{d=1}^{2}\sum_{e=1}^{2} c_\alpha \cdot X_1^a \cdot X_2^b \cdot X_3^c \cdot X_4^d \cdot X_5^e
\end{aligned}
\tag{4}
$$

where c_α is 242 polynomial coefficients plus the constant member c_0, which are calculated using the method of the least squares. 400 simulation runs of Latin Hypercube Sampling method (LHS) were used to calculate the polynomial [18, 19]. The first hundred simulation runs were considered acc. to Table I. Another three hundred simulation runs were considered acc. to Table II.

TABLE II

Random Variables for Approximation

Characteristic	Min. value	Max. value
Cross-sectional width b	190.344mm	209.655 mm
Flange thickness t_2	7.75665 mm	12.2434 mm
Yield strength f_y	215.1126 MPa	379.487 MPa
Young's modulus E	161.079 GPa	258.921 GPa
Amplitude e_0	-22.4634	22.4634 mm

All variables in Table II have rectangular probability density functions. Standard deviations in Table II are enlarged so that the domain of equation (4) is set up for the evaluation of sensitivity analysis using the LHS method. Constants c_α were calculated from random simulations in which random realizations e_0 were considered with the absolute values.

VII. Sensitivity analysis results

The software to generate random realizations of LHS and to calculate Sobol's sensitivity indices in (3) was created by the author of the presented paper. The paper builds on previously published sensitivity studies [30-33]. Ten thousand LHS runs were used for the evaluation of $E_{\mathbf{X}_{\sim i}}(Y|X_i, X_j)$ in (1), and another ten thousand LHS runs were used for the evaluation of $V_{X_i}(E_{\mathbf{X}_{\sim i}}(Y|X_i, X_j))$. The variance V(Z) was evaluated with one hundred thousand LHS runs. All other twenty-six higher order sensitivity indices were evaluated analogously. Sensitivity indices were evaluated in dependence to the slenderness λ with the step 2, see Fig. 7 and Fig. 8. The pie charts in Fig. 3 to Fig. 6 show the overall pattern of decomposition (3) for selected slenderness. The nonlinear FEM solution was approximated using the least square method. The least square method yielded constants c_α in (3). All members in decomposition (3) were then evaluated using a quadratic polynomial.

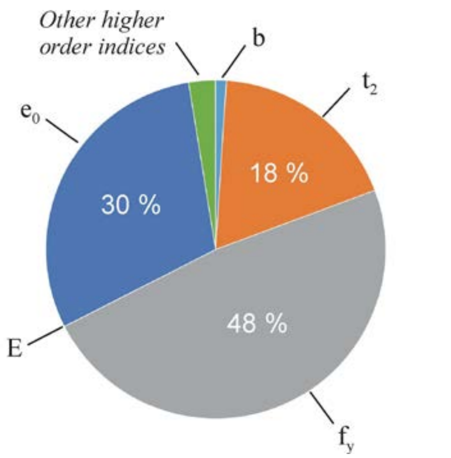

Fig. 3 Global sensitivity analysis for λ=60

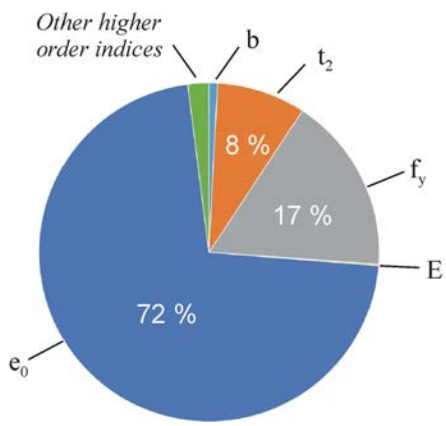

Fig. 4 Global sensitivity analysis for λ=80

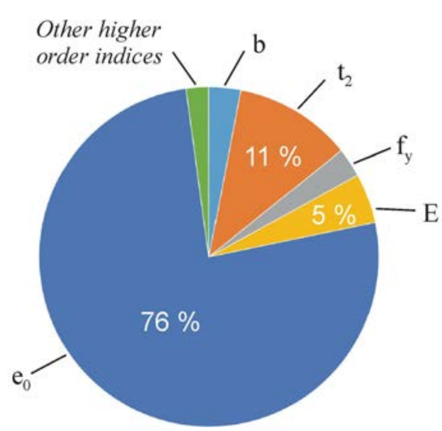

Fig. 5 Global sensitivity analysis for λ=100

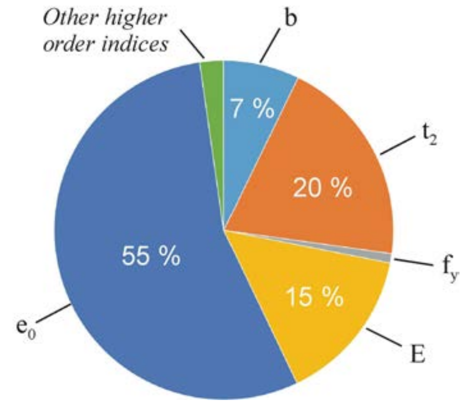

Fig. 6 Global sensitivity analysis for λ=120

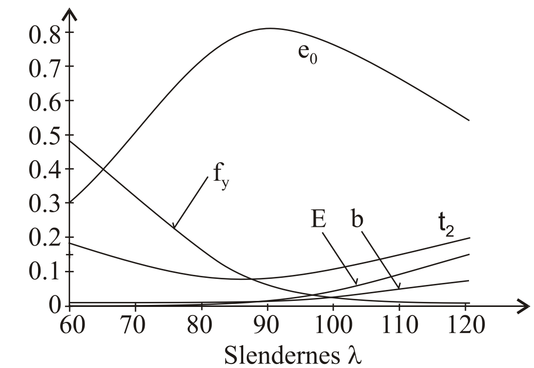

Fig. 7 Sensitivity indices S_i vs. λ

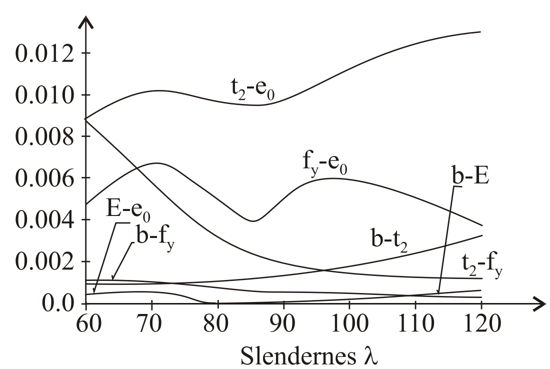

Fig. 8 Crucial higher order sensitivity indices vs λ

VIII. Conclusion

Approximation of the nonlinear FEM solution with the quadratic polynomial reduced the computational costs in global sensitivity analysis of the ultimate limit state of the steel strut. First order sensitivity indices showed that the ultimate limit state is most influenced by the variability of amplitude e_0 of the initial axial curvature of the strut for slenderness λ=90, see Fig. 7. The amplitude e_0 is also found in most stochastic interactions with other imperfections, see Fig. 8. The presented global sensitivity analysis identified all stochastic interactions present in the computational model that would have been very difficult to identify using a different approach. The most significant interaction was found between the amplitude e_0 and flange thickness t_2 in the entirety of considered slenderness, see Fig. 8. Finding these interactions, as well as the determination of their absence in the model is valuable. The results may be applicable in fuzzy probabilistic verification of procedures for safe and reliable design of structures [34, 35].

Numerous problems of computational modelling in nonlinear mechanics is either too complex for analytical solution or can not be tackled using the available analytical tools. Approximation methods and simulation techniques provide sufficiently accurate solutions while significantly reducing the complexity of the problem. The approach to the evaluation of sensitivity analysis presented here is highly effective, especially when the number of input random variables is small.

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