Global sensitivity analysis in view of nonlinear structural behavior

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Summary:

Global sensitivity analysis provides information about the respective significance/contribution of structural input random parameters (or combinations thereof) onto considered responses. The identification of non-relevant and relevant structural parameters for model reduction purposes is one of the major tasks. Global sensitivity analysis may also improve the understanding of the model behavior and may clarify interactions among input parameters. This paper focuses in particular on global sensitivity analysis approaches in view of nonlinearity of the underlying computational model (e. g. finite element model). Three main approaches are presented, compared and demonstrated by means of analytical and practical examples.

Keywords:

global sensitivity analysis, correlation coefficient, ANOVA, Sobol' indices, nonlinearity

1 Introduction

Structural optimization and uncertainty analysis of moderate to complex computational models is costly and often requires additionally effort due to the high number of design variables that might be considered in the design process. Responses can depend on all variables, but often the significance onto the variance of the structural responses differs greatly. In many cases a structural response is dominated by only a few variables. Objectives of a global sensitivity analysis might be [3]:

- Identification of significant and insignificant variables. Possible reduction of the dimensions (number of design variables) of the optimization problem.
- Improvement in understanding of the model behavior (highlight interactions among variables, find combinations of variables that result in high, or low, values for the model output).

In this sense, a suitable definition of global sensitivity can be found in [6]:

"Sensitivity analysis (SA) is the study of how the variation in the output of a model (numerical or otherwise) can be apportioned, qualitatively or quantitatively, to different sources of variation."

Most of the global sensitivity analysis approaches can be classified into two groups [11]:

- Regression-based methods: The standardized regression coefficients (SRC) are based on a linear regression of the output on the input vector. In a linear regression, the value of the standardized regression coefficient is exactly the same as the correlation coefficient. The Pearson correlation coefficients measure the effect of each design variable by the correlation it has with the structural response. In the case of monotone but nonlinear structural behavior rank based measures may be used, leading to the so-called SRRC (standardized rank regression coefficients). Based on these measures only limited conclusion can be drawn in the case of general nonlinear non-monotonic models. This conclusion is also appropriate for quadratic correlation approaches.
- Variance-based methods: The observed variance of the structural responses is partitioned into components induced by the respective structural variables. This decomposition of the variance is usually called ANOVA techniques for "ANalysis Of VAriance". The Fourier amplitude sensitivity test (FAST) indices [1, 7] and the Sobol' indices [8] are intended to represent the sensitivities for general (nonlinear) models.

The Sobol's variance-based approach, the Sobol' indices, has received much attention in literature in the last years since they provide accurate sensitivity information for most models [11]. The application of Sobol's approach, correlation analysis and variance-based ANOVA will lead to comparable results for the linear models. The obtained ranking of variables in terms of sensitivity will be almost equal. However, in the general nonlinear case it is assumed that Sobol's approach results in more satisfactory sensitivity measures. A brief overview about correlation analysis, ANOVA, and the decomposition of variance after Sobol is given in the following section. The (regression-based) correlation coefficient, the (variance-based) linear ANOVA, and Sobol' indices are compared at first by means of analytical examples followed by a simple crash analysis.

2 Global sensitivity analysis approaches

2.1 Correlation analysis

Correlation, (often measured as a correlation coefficient), indicates the strength and direction of a linear relationship between two random variables. A number of different coefficients are used for different situations. The best known is the Pearson product-moment correlation coefficient, which is obtained by dividing the covariance of the two variables by the product of their standard deviations. The correlation coefficient $\rho_{X,Y}$ between two random variables *X* and *Y* is defined as the Pearson correlation coefficient

$$\rho_{X,Y} = \frac{E(XY) - E(X)E(Y)}{\sqrt{E(X^2) - E^2(X)}\sqrt{E(Y^2) - E^2(Y)}}$$

(1)

where $E(\cdot)$ denotes the expected value. For a result of a numerical experiment e.g. obtained through a Monte Carlo Simulation, the Pearson product-moment correlation coefficient can be used to estimate the correlation between *X* and *Y*. The Pearson correlation coefficient is then the best estimate of the correlation of *X* and *Y*. The Pearson correlation coefficient is written:

$$r_{x,y} = \frac{\sum_{i=1}^{N} (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{N} (x_i - \bar{x})^2 \sum_{i=1}^{N} (y_i - \bar{y})^2}}$$
(2)

where \bar{x} is the mean (average) of the x_i values and \bar{y} is the mean of the y_i values. The values of the correlation coefficients from Eqs. (1) and (2) are located in the interval [-1,1], where values close to 0 indicate a weak (linear) relationship and values close to -1/1 a strong (linear) relationship between the investigated random variables *X* and *Y*.

The correlation is a very popular and powerful measure to summarize linear relationships between variables but in the case of outliers or (weak) nonlinearity it may lead to wrong conclusions. Therefore a correlation analysis does not replace the individual examination of the data (e.g. through anthill plots).

The Pearson correlation coefficient is associated with the regression coefficient obtained by linear regression analysis. Regression analysis also indicates the strength and direction of a relationship between two random variables *X* and *Y*. At this one random variable is defined to be dependent and modeled as a function of the independent variable, corresponding parameters, and a random error term. In linear regression for modeling *n* data points there is one independent variable x_i , two parameters *a* and *b*, and one error term ε_i .

$$y_i = a + bx_i + \varepsilon_i$$

The parameters *a* and *b* are estimated by using the least squares method.

$$\hat{b} = \frac{\sum_{i=1}^{N} (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{N} (x_i - \bar{x})^2}$$
(3)

$$\hat{a} = \bar{y} - \hat{b}\bar{x} \tag{4}$$

The interrelation between linear regression and the Pearson correlation coefficient is given by

$$\hat{b} = r_{x,y} \frac{s_y}{s_x} \tag{5}$$

where s_x and s_y are the standard deviations of the respective data.

The proportion of variability in the investigated data accounted for by the linear regression is defined by the coefficient of determination $R_{x,y}^2$. The variability of the data is measured through the residuals

$$\hat{u}_i = y_i - (\hat{a} + \hat{b}x_i) \tag{6}$$

The coefficient of determination $R_{x,y}^2$ is thus defined by

$$R_{x,y}^{2} = 1 - \frac{\sum_{i=1}^{N} \hat{u}_{i}^{2}}{\sum_{i=1}^{N} (y_{i} - \bar{y})^{2}}$$
(7)

In the case of linear regression, $R_{x,y}^2$ is the square of the Pearson correlation coefficient $r_{x,y}$.

2.2 ANOVA

A common ANOVA approach is presented in [10] and explained in the following. The approach is based on response surface methodology, that is, a design surface is fitted to predetermined response values

using regression analysis. Least squares approximation is used for this purpose. Consider a single response variable *Y* dependent upon a number of variables $\underline{X} = (X_1, X_2, ..., X_n)$. The exact functional relationship between these quantities is

$$\underline{Y} = f(\underline{X}) \tag{8}$$

The exact functional relationship is now approximated (e.g. polynomial approximation) as

$$f(\underline{X}) \approx f^*(\underline{X})$$
 (9)

The approximating function $f^*(\underline{X})$ is assumed to be a summation of basis functions

$$f^*(\underline{X}) = \sum_{i=1}^{L} a_i \phi_i(\underline{X})$$
(10)

where *L* is the number of basis functions $\phi_i(\cdot)$ used to approximate the model. The constants $\underline{a} = (a_1, a_2, ..., a_L)^T$ have to be determined in order to minimize the sum of square error

$$\sum_{p=1}^{P} \left\{ \left[f(\underline{X}_p) - f^*(\underline{X}_p) \right]^2 \right\} = \sum_{p=1}^{P} \left\{ \left[f(\underline{X}_p) - \sum_{i=1}^{L} a_i \phi_i(\underline{X}_p) \right]^2 \right\}$$
(11)

P is the number of experimental points and $f(\underline{X}_p)$ is the exact functional response at the experimental points \underline{X}_p .

The contribution of a single regressor variable to the model can be investigated by means of the partial F-test where F is calculated to be

$$F = \frac{\frac{a_i^2}{C_{ii}}}{\frac{\varepsilon^2}{(P-L)}}$$
(12)

The ε^2 term represents the sum of squared residuals and C_{ii} is the diagonal element of $(\underline{X}^T \underline{X})^{-1}$ corresponding to a_i , where \underline{X} is the matrix $\underline{X} = [\phi_i(\underline{X}_p)]$.

F can be compared with the *F*-statistic $F_{\alpha,1,P-L}$ so that if $F > F_{\alpha,1,P-L}$, a_i is non-zero with $(100 - \alpha)\%$ confidence. The confidence level α that a_i is not zero can also be determined by computing the α for $F = F_{\alpha,1,P-L}$. The importance of a_i is therefore estimated by both the magnitude of a_i as well as the level of confidence in a non-zero a_i .

The significance of regressor variables may be represented by a bar chart of the magnitudes of the coefficients a_i with an error bar of length $2\Delta a_i(\alpha)$ for each coefficient representing the confidence interval for a given level of confidence α . The relative bar lengths allow the analyst to estimate the importance of the variables and terms to be included in the model while the error bars represent the contribution to noise or poorness of fit by the variable.

2.3 Sobol' indices

The Sobol' indices are sensitivity measures for arbitrary complex computational models. They estimate the effect of the random input variables onto the model output [9]. This section just provides a short introduction.

The models under investigation are described by a function $\underline{Y} = f(\underline{X})$, where $\underline{X} = (X_1, X_2, ..., X_n)$ is the random input vector consisting of *n* random variables (i.e. structural parameters) and where $\underline{Y} =$

 $(Y_1, Y_2, ..., Y_m)$ denotes the random output vector consisting of random variables (i.e. structural responses). It is possible to decompose $\underline{Y} = f(\underline{X})$ into summands of increasing dimension [8].

$$f(\underline{X}) = f_0 + \sum_{i=1}^n f_i(X_i) + \sum_{1 \le i < j \le n} f_{ij}(X_i, X_j) + \dots + f_{1,2,\dots,n}(X_1, \dots, X_n)$$
(13)

Each random model response Y_j (j = 1, 2, ..., m) is characterized by its variance D^j . According to Eq. (13) it is possible to decompose each variance D^j into partial variances associated with the single random input variables $X_1, X_2, ..., X_n$ as follows:

$$D^{j} = \sum_{i=1}^{n} D_{i}^{j} + \sum_{1 \le i < k \le n} D_{i,k}^{j} + \dots + D_{1,2,\dots,n}^{j}$$
(14)

and to relate each partial variance to one Sobol' index

$$S_{i_1,...,i_s} = \frac{D_{i_1,...,i_s}^j}{D^j}$$
 with $1 \le i_1 < ..., i_s \le n, \quad s = 1, 2, ..., n$ (15)

Each of the Sobol' indices $S_{i_1,...,i_s}$ represents a sensitivity measure that describes which amount of each variance D^j is caused due to the randomness of the single random input variables and its mapping onto the output variables.

In practice, all partial sensitivity indices involving the single input variable X_i (i = 1, 2, ..., n) are summed up to the total sensitivity index S_{T_i} in order to evaluate the total effect of X_i [2]. The total Sobol' indices consider thus interaction among the input variables.

Each Sobol' index S_{T_i} represents the sensitivity of the computational model regarding its input variable X_i without any assumption of linearity or monotonicity in the model. Two essential types of problems can be studied with the aid of the Sobol' indices:

- 1. Ranking of input variables in $\underline{Y} = f(X_1, X_2, ..., X_n)$
- 2. Identification of insignificant input variables in $\underline{Y} = f(X_1, X_2, ..., X_n)$.

The approach is to estimate the Sobol' indices $S_{T_1}, S_{T_2}, ..., S_{T_n}$ and to order the variables according to these values.

In order to quantify which amount of each variance D^{j} is caused due to a single input variable X_{i} the corresponding Sobol' index $S_{T_{i}}$ may be normalized according to Eq. (16).

$$\operatorname{norm} S_{T_i} = \frac{S_{T_i}}{\sum_{k=1}^n S_{T_k}}$$
(16)

That is, input variable X_i has a share in variance D^j of norm S_{T_i} .

The Sobol' indices are practically computed using Monte Carlo simulation [11]. Using Monte Carlo simulation, the total effect of an input variable X_i may be computed as

$$\hat{S}_{T_i} = 1 - \hat{S}_{\sim i}$$
 with $\hat{S}_{\sim i} = \frac{\hat{D}_{\sim i}^j}{\hat{D}^j}$ (17)

considering the effects not containing X_i :

$$\hat{D}_{\sim i}^{j} = \frac{1}{N} \sum_{k=1}^{N} f(\underline{X}_{\sim ik}^{(1)}, X_{ik}^{(1)}) f(\underline{X}_{\sim ik}^{(1)}, X_{ik}^{(2)}) - \hat{f}_{0}^{2}$$
(18)

The superscripts (1) and (2) indicate that two different samples are generated and mixed. $\underline{X}_{\sim ik}^{(1)}$ denotes the *k*th sample point with

$$\underline{X}_{\sim ik}^{(1)} = (X_{1k}^{(1)}, ..., X_{(i-1)k}^{(1)}, X_{(i+1)k}^{(1)}, ..., X_{nk}^{(1)})$$
(19)

The mean value \hat{f}_0 may be derived by

$$\hat{f}_0 = \frac{1}{N} \sum_{k=1}^{N} f(\underline{X}_k)$$
 (20)

Monte Carlo simulation is often time-consuming and may take days to run. This means that for computationally demanding models, e.g. finite element models in engineering mechanics, efficient meta models should be applied. Besides polynomial response surface approximations, Neural and Radial Basis Function networks and Krigging approximations may also be used as response surfaces [10]. In this case, an additional amount of variance due to the approximation in dependency of the quality of the response surface appears. To take this additional variance into consideration the variance of the discrepancies between the exact functional response and the response surface at the experimental points is computed and denoted by \hat{D}_{unex}^{j} . The normalized total Sobol' index S_{T_i} is thus modified according to Eq. (21), where \hat{D}^{j} and \hat{S}_{T_i} are computed only using the response surface.

$$\operatorname{norm} \hat{S}_{T_i} = \frac{\frac{\hat{S}_{T_i}}{\sum_{k=1}^n \hat{S}_{T_k}} \hat{D}^j}{\hat{D}^j + \hat{D}_{\operatorname{unex}}^j}$$
(21)

3 Examples

3.1 Analytical Example 1

Two analytical functions

$$Y_1 = f_1(X_1, X_2) = 10X_1 + 0.5X_2^3$$

$$Y_2 = f_2(X_1, X_2) = 2X_1 - X_2^2$$
(22)
(23)

are investigated. Function Eq. (22) is nonlinear monotonic, Eq. (23) possesses a nonlinear non-monotonic behavior.

The input variables are uniformly distributed in the interval [-5,5]. The function graphs are shown in Fig. 1.



Fig. 1: Function plots of Y_1 and Y_2

In this preliminary sensitivity analysis relevant input variables should be identified and ranked for each of the functions Eqs. (22) and (23). The non-relevant variables that have none or only a small effect should be removed to reduce the model size for subsequent investigations (i.e. an optimization).

The regression-based correlation coefficient, the variance-based linear and quadratic ANOVA, and the Sobol' indices are evaluated as sensitivity measures and compared. The linear (without interaction) and quadratic ANOVA were carried out with the aid of LS-OPT [10] using 500 experimental points. It is obvious from the function plots Fig. 1 that there is no non-relevant input variable. Both variables contribute to the variance of the results Y_1 and Y_2 . The ranking of the variables can also be gained from the plots. For Y_1 the input variable X_1 and for Y_2 the input variable X_2 contribute most to the respective variances of the results Y_1 and Y_2 . The results of a numerical sensitivity analysis should support this visual interpretation. But in contrast to the Sobol' indices the correlation and ANOVA do not, see Tab. 1.

	<i>Y</i> ₁				Y ₂				
		linear	quadratic				linear	quadratic	
	r_{x_i,y_1}	ANOVA ¹	ANOVA ¹	S_{T_i}		r_{x_i,y_2}	ANOVA ¹	ANOVA ¹	S_{T_i}
X_1	0.77	0.50	0.52	0.60	(0.60	0.93	0.08	0.37
X_2	0.58	0.50	0.48	0.40	(0.00	0.07	0.92	0.63

Tab. 1: Results of the global sensitivity analysis (¹LS-OPT results, normalized)

Function Y₁

Both sensitivity measures r_{x_i,y_1} and \hat{S}_{T_i} will lead to the same ranking of the input variables X_1 and X_2 . Also the ratio of importance between X_1 and X_2 is almost comparable (0.77/0.58 vs. 0.60/0.40). The linear and quadratic ANOVA might be misleading, but also indicate the significance of both input variables.

The numerical value of the Sobol' indices $\hat{S}_{T_1} = 0.6$ and $\hat{S}_{T_2} = 0.4$ can also be expressed in terms of variance or standard deviation. The input variable X_1 is responsible for 60% and X_2 for 40% of the variance/standard deviation of the result variable Y_1 . Whereas the correlation coefficient measures the linear relation between X_1 and Y_1 . Here also X_1 has a strong (linear) effect onto the result Y_1 . As proposed in the introduction for nonlinear monotone computational models, correlation coefficients and Sobol' indices lead to the same conclusion. However, the Sobol' indices provide a clear idea of the effect of each input variable onto the variance of the result variable.

Function Y₂

Here the effect of the quadratic term X_2^2 is neglected by the correlation coefficient as well as by the linear ANOVA. That is obviously not the case. This term contributes significantly to the result Y_2 . The quadratic ANOVA as well as the Sobol' index $\hat{S}_{T_2} = 0.63$ indicate that. The input variable X_2 is responsible for the major part of the total variance, at which the quadratic ANOVA may overestimate the influence of X_2 .

3.2 Analytical Example 2

In the following the Ishigami-function [5]

$$Y_3 = f_3(X_1, X_2, X_3) = \sin X_1 + a \sin^2 X_2 + b X_3^4 \sin X_1$$
(24)

is investigated. The input variables are uniformly distributed in the interval $[-\pi,\pi]$. The example is carried out using the numerical values a = 7 and b = 0.1. The plot ($X_3 = 1.0$) of this nonlinear and non-monotonic function is shown in Fig. 2.

The results of the computation of the regression-based correlation coefficient, the variance-based linear and quadratic ANOVA, and the Sobol' indices are gathered in Tab. 2.

It is observed that the influences of X_2 and X_3 are negated by the correlation analysis as well as by the linear ANOVA. The results of the quadratic ANOVA depend on the quality of the polynomial approximation. Here the contributions of the input variable X_2 and the interacting input variables (X_1 , X_3) are detected,



Fig. 2: Function plot of the Ishigami function ($X_3 = 1.0$)

	Y_3					
					total effect	
	r_{x_i,y_3}	linear ANOVA ²	quadratic ANOVA ²	S_{i_1,\ldots,i_s}	quadratic ANOVA ²	S_{T_i}
X_1	0.44	0.69	0.11	0.314	0.29	0.45
X_2	0	0.15	0.42	0.442	0.35	0.35
X_3	0	0.16	0.19	0	0.36	0.2
X_1, X_2	-	-	0.01	0	-	-
X_1, X_3	-	-	0.25	0.244	-	-
X_2, X_3	-	-	0.03	0	-	-
X_1, X_2, X_3	-	-	-	0	-	-

	Tab. 2: Results of the global	sensitivity analysis	s (² LS-OPT	results, normalized)
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however the significance of X_1 is negated. The total effect of X_1 is thus underestimated by the quadratic ANOVA.

As a conclusion, this academic example shows the potential of the global sensitivity analysis by the Sobol' indices to investigate the dependencies of nonlinear functions with respect to the input parameters. Indeed all three input variables are important, which the common correlation analysis and the linear ANOVA are not able to detect. Due to the limited capacity of the polynomial approximation used by the quadratic ANOVA the associated ranking of the input variables is differing to the Sobol' indices.

4 Crash application

The global sensitivity analysis in view of nonlinear structural behavior is demonstrated by means of a front crash of a car model against a stonewall [4].



Fig. 3: Front crash of a car model against a stonewall

The design parameters are th_1 re, th_2 re, th_1 li, and th_2 li, that is, the sheet thickness of the cross sections according to Fig. 4.



Fig. 4: Design parameters

The considered responses are

- the chest acceleration
- the front cross section forces
- the mid cross section forces

as highlighted in Fig. 5 below.



Fig. 5: Evaluated responses of the car model

There is no information about the probability distribution functions (pdf's) of the design parameters. In that case, a straightforward approach of a normal probability distribution of the parameters is assumed. It has to be kept in mind that those possible existing probability distributions that normally differ from the normal pdf could influence the results of the sensitivity analysis significantly. The global sensitivity analysis was carried using 100 experimental points.

The results of the global sensitivity analysis are visualized with the software tool D-SPEX [12]. The correlation coefficients together with anthill plots are shown in one single plot window, Fig. 6.



Fig. 6: Correlation coefficients and anthill plots

The parameters th_1_re and th_2_re are investigated. The correlation coefficient indicates that the parameter th_1_re has a strong effect onto the front cross section forces, whereas the contribution of th_2_re with respect to the front cross section forces is insignificant. This also corresponds to the results of the linear ANOVA computed by LS-OPT, Fig. 7.



Fig. 7: Linear ANOVA results

The results of the quadratic ANOVA computed by LS-OPT are characterized by an extremely low confidence level, visualized in D-SPEX by large red error bars, Fig. 8(a). That is, the quadratic response surface used by the quadratic ANOVA is not able to represent the experimental response values. The quadratic ANOVA is thus unsuitable for global sensitivity analysis in the context of this example. In contrast to this, the LS-OPT results of the linear ANOVA suggest a comparatively high confidence level, Fig. 8(b), particularly the contribution of th_1_re with respect to the front cross section forces is characterized by short red error bars. At first sight, the linear ANOVA seems thus to be suitable for global sensitivity analysis in the context of this example.





The Sobol' indices are computed using a feedforward neural network metamodel. The results are shown in Fig. 9.



Fig. 9: Plot of normalized total Sobol' indices $norm S_{T_i}$

In the Sobol' indices plots the length of each section in one stacked bar represents the contribution of the specific parameter (th_1 re, th_2 re, th_1 li, th_2 li) to the total variance of the respective result (right chart). The left chart is an alternative depiction and illustrates the significance of the specific parameter to the single results and to all of the results.

The results of the global sensitivity analysis with respect to the parameters th_1_re and th_2_re are gathered in Tab. 3.

	\hat{r}_i	linear ANOVA	\hat{S}_{T_i}
th_1_re	0.52	1.06	0.18
th_2_re	-0.09	-0.08	0.45

Tab. 3: LS-OPT results of the global sensitivity analysis

front cross section force

In contrast to the correlation analysis and the linear ANOVA the contribution to the front cross section

forces of the variable th_2_re is most significant (45%). This discrepancy may be explained with Fig. 10.



Fig. 10: Experimental points and linear regression

Fig. 10 shows the values of the front cross section forces in dependency of the experimental values of th_2_re and the belonging linear regression used by correlation analysis and linear ANOVA. It is observable that small values of th_2_re cause a major variance of the front cross section forces. This nonlinear effect is taken into account by the Sobol' indices but can not be represented by linear regression. Recapitulatory, the suitability of correlation analysis and linear ANOVA for global sensitivity analysis (amongst others pretended by the high confidence level in Fig. 8(b)) is not objective in context of this example.

5 Conclusion

In this paper three different global sensitivity analysis approaches are presented with particular consideration of nonlinearity of the underlying computational model. The approaches are compared and demonstrated by means of analytical and practical examples. The correlation coefficient reflects the strength and direction of a linear relationship, but not any aspects of nonlinear relationships. The same applies to the linear ANOVA. The quadratic ANOVA may take nonlinearities into account, but restricted in terms of a quadratic approximation. The Sobol' indices are sensitivity measures for arbitrary (nonlinear) computational models. They quantify which amount of the variance of result variables is caused due to a single input variable or combinations thereof. Recapitulatory, correlation analysis and the linear ANOVA yield only approximate solutions for (weak) nonlinear monotonic problems, the quadratic ANOVA may take quadratic effects into account, for nonlinear non-monotonic problems relevant input variables are only identified by the Sobol' indices.

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