Sectional sensitivity measures with artificial neural networks

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Summary:

For the design of engineering structures and the assessment of their reliability it is of main interest to appraise the importance of input quantities in view of result quantities. Sensitivity analysis provides a versatile tool to assess those importance. In the past, this was done by determining the gradients of the function of interest and deduce sensitivity statements by means of partial derivatives in a local manner. For most engineering applications those procedures are inappropriate, since it is limited to linear functions and ignores the spreading of the respective input quantities. Thus, enhanced sensitivity measures are elaborated, which assess the variances of functions in a global manner. Nevertheless, to further improve the informative value of sensitivity statements global partial derivative based sensitivity measures are introduced. However, due to the computational expense of sophisticated sensitivity analysis, efficient analysis methods are in steady advance. A main focus is thereby on the coupling of metamodeling techniques and sensitivity analysis.

Generally, sensitivity measures condense available information of global input spaces to singleton values. In consequence, the importance of local parts of the input spaces are neglected and the characteristic of the functional relationship between input and result parameters remains hidden. While this fact can be neglected in high dimensional problems, it is of main interest in low dimensional problems. This becomes obvious, considering the various software tools providing metamodel viewer. Thereby, metamodel viewer suffer the dimensionality problem; while two parameters can be visualized, the remaining parameters are fixed to discrete parameter values. Thus, modifying those parameters will alter the visualized response surface and disturb deduced information. Especially for challenging problems the evaluation of metamodel viewer results may become cumbersome. Nevertheless, for good-natured problems with few sensitive parameters those metamodel viewers are useful to derive an idea about the behavior of the function of interest.

Alternatively, in this paper the approach of sectional sensitivity measures is introduced, which does not feature the dimensionality problem. Thereby, the global sensitivity analysis is extended to provide sensitivity information in specific parts of the input space. Merging all those information together, statements about functional dependencies are obtained. Thereby, sectional sensitivity measures can be distinguished in argument based sectional sensitivity measures and sectional sensitivity measures based on the value of function. While the former is proper to deduce statements about the functional relationship between individual input and result parameters, which equals the idea of metamodel viewer, the latter is deployable for reasoning statements about influences of input parameters in specific regions of the result space. However, the generated sensitivity statements are not only useful for data mining purposes, they can be even utilized to advance optimization and reliability tasks.

While sophisticated sensitivity approaches provide worthwhile results, their computational expense hinders sometimes the applicability for industry-relevant problems. Thus, sensitivity analysis may be coupled with metamodels. Here, artificial neural networks are applied. Neural networks are capable to reason unknown dependencies between variables on the basis of a set of initial information. Thereby, the information content is stored within the neural network. Utilizing the respective properties, statements about the sensitivity may be derived. Thereby, the sensitivity is assessed by means of measures capitalizing diverse properties of the artificial neural network. Those are data handling, derivability and efficient numerical evaluation. In result, multi-faceted sensitivity measures may be defined or evaluated like weighting-based, derivative-based and even variance-based measures.

The appropriateness of the novel approaches is demonstrated by means of analytical functions and their applicability is shown by means of an industry-relevant example.

Keywords:

sensitivity analysis, sectional global sensitivity measures, neural network, data mining

1 Introduction

The simulation based design process of engineering structures is a complex and ambitious task, especially, when multiple input parameters have to be handled. Versatile tools are on hand to optimize the structure or assess the reliability by means of black-box programs. But most often, engineers long for an deepened insight into the specific problem to understand, what is going on. Therefore, so called data mining tools are available, which enable to detect structures in some predetermined point sets. These point sets can be generated from an initial random sampling or be the results of optimization or reliability runs. However, the aim is to reason dependencies between variables, mostly between input and result variables. Thereby, one big issue is to determine the influence of individual input variables in view of specific result variables. This is done by determining the sensitivity of input parameters.

Even though, first approaches of sensitivity analysis are rather old, the improvement of sensitivity measures are still of main interest in research. First sensitivity analysis were applied in experimental investigation. Thereby, individual input parameters are varied in specified ranges, one at a time, to appraise the influence on the results. This sensitivity analysis is adopted in numerical investigations and still in broad application [10]. The aim is to determine the gradient of each input parameter in a point of interest. For analytical functions this can be done in a closed form. Since those approaches focus on the influence of input parameters in specific points they are denoted as local sensitivity measures. They are proper for linear problems with non-interacted input parameters. Thus, their application for industry-relevant problems is doubtful [10].

In result, global sensitivity measures (GSM) are introduced which enable to capture even non-linear interacted characteristics in the functional relationship of input and result parameters. Global in this sense means, that opposite to local sensitivity measures the sensitivity is not assessed for specific points but rather for the input spaces. Thereby, the spreading of input parameters has to be incorporated appropriately in the sensitivity approach. This can be exemplified easily with $f(x, y) = x^2 + y$. If x varies in the range $x \in [-0.1, 0.1]$ the influence is negligible, while specifying x in a range of $x \in [-5, 5]$, the importance of x becomes superordinate. For the determination of global sensitivity measures several approaches are available. In general, two strategies can be distinguished. The first strategy assesses the structural response itself by means of evaluating the variance. Therefore, the variance decomposition is introduced. Well known approaches are, inter alia, ANOVA (analysis of variances), fast fourier transformation and Sobol indices. The latter is said to provide the best results for complex computational models [9]. The second strategy assesses the first partial derivative of the functional relationship in the integral mean and can be considered as an extension of local sensitivity measures. This approach is quite new and still under intensive research. First ideas were introduced by [8] and further improvements were presented by [1, 4, 13]

In result of a global sensitivity analysis a singleton sensitivity measure for each input dimension is obtained. All information about the nonlinear, complex functional relation of input and result parameters is condensed to a single value. This is reasonable for a high number of input parameters (e.g. more than 100). But, for low dimensional problems (e.g. up to 30) a more detailed insight is preferable. Therefore, the approach of sectional sensitivity measures is presented in this contribution. The idea is to partition the sensitivity measure per input dimension additionally and determine the global sensitivity section-wise. In result, the influence of input parameters is assessed locally. Thus, statements about the functional relationship of input and result parameters can be concluded. In consequence, the approach of sectional global sensitivity measures (SGSM) provides a reasonable alternative to visualization tools, which create scatterplots or metamodel views of extracted input dimensions in high dimensional problems. Thereby, the perturbation on account of other input dimensions is removed with SGSM.

Since the determination of SGSM may become computationally expensive, when a high accuracy is required, a combination with metamodels, here neural networks are applied, is reasonable. Thereby, the derivability of neural networks can be used to determine first partial derivatives of the function under consideration in a numerical cheap manner.

In this paper a short introduction to GSM, both variance based and derivative based, is given in Section 2. Then, the approach of sectional sensitivity is introduced in Section 3. For the purpose of numerical efficiency, sensitivity is analyzed on the basis of neural networks. An short introduction is provided in Section 4. Finally, in Section 5 the features of the presented approaches are demonstrated by means of analytical functions and the applicability is shown by means of an industry-relevant example.

2 Global sensitivity measures

The aim of sensitivity analysis is to assess the influence of individual input quantities $x_i \in \mathbb{R}$ in view of a result quantity $z \in \mathbb{R}$ in comparison to all other input parameters $x_{\sim i} = (x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_n) \in \mathbb{R}^{n-1}$.

$$f : \mathbb{R}^n \to \mathbb{R} : x = (x_i, x_{\sim i}) \mapsto f(x) =: z \tag{1}$$

A sensitivity measure S_i is defined for $i \in \{1, \dots, n\}$ as

$$S_i = \frac{\hat{S}_i}{\sum\limits_{j=1}^{n} \hat{S}_j} \quad . \tag{2}$$

In most engineering application the sensitivity measure is evaluated as given in Equation 2. Since it characterizes just the overall influence of an input quantity, it is denoted as total sensitivity measure in literature [12, 14]. A more detailed definition of sensitivity distinguishes further components $S_{i_1,\dots,i_s}$, so called partial sensitivity measures, of S_i

$$S_{i_1,\dots,i_s} = \frac{\hat{S}_{i_1,\dots,i_s}}{\sum\limits_{s=1}^{n} \sum\limits_{1 \le i_1 < \dots < i_s \le n} \hat{S}_{i_1,\dots,i_s}} \quad . \tag{3}$$

Thereby, $\sum_i^n S_i + \sum_{1 \le i \le j \le n} S_{i,j} + \dots + S_{1,2,\dots,n} = 1$ holds. On the basis of $S_{i_1,\dots,i_s}$ total sensitivity measures can be deduced

$$S_i^{tot} = \sum_{\substack{i_k = i \\ 1 \le i_k \le n}} S_{\dots,i_k,\dots} = 1 - \sum_{\substack{i_k \ne i \\ 1 \le i_k \le n}} S_{\dots,i_k,\dots} \tag{4}$$

The total sensitivity measures do not add to one, since it is not normalized to the total sum. The reason is the repeated consideration of partial sensitivity measures in Eq. (4). Applying an additional normalization, the summation to one holds again. In doing so, the sensitivity measure given in Eq. (2) is obtained

$$S_i = \frac{S_i^{tot}}{\sum\limits_{j=1}^{n} S_j^{tot}} \; . \tag{5}$$

The important task of sensitivity analysis is a proper description of $\hat{S}_i$. Commonly, $\hat{S}_i$ assesses either the function f itself or the first partial derivatives $\partial f / \partial x_i = \partial_i f$, see [1, 4, 13]. For the assessment of the respective functions the moments can be evaluated. The focus is on the expected value

$$G = \frac{1}{|H^n|} \int_{H^n} f(x)\,\mathrm{d}x \quad \text{with } H^n \subseteq \mathbb{R}^n \tag{6}$$

and the variance

$$D = \frac{1}{|H^n|} \int_{H^n} (f(x) - G)^2\,\mathrm{d}x = \frac{1}{|H^n|} \int_{H^n} f(x)^2 \mathrm{d}x - G^2 \; . \tag{7}$$

Evaluating the function f itself, the application of the expected value is unreasonable, since no useful sensitivity statements can be derived. This becomes obvious, considering the conditions for ANOVA decomposition, see Eq. (9) and (10). For the evaluation of f the consideration of the variance or higher order moments is proper. Thereby, the evaluation of partial variances, based on the ANOVA decomposition (see Section 2.1), is required to evaluate individual input quantities x_i. For the assessment of the first partial derivative $\partial_i f$, the expected value G of $\partial_i f$ for all $i = 1, 2, \dots, n$ can be determined. To additionally examine the effect of interactions, the total variance D of $\partial_i f$ can be evaluated [1].

2.1 ANOVA decomposition and Sobol indices

Consider a function f, square integrable in H^n, with the Lebesgue integral [13]. This function can be expressed with the help of the ANOVA decomposition as

$$f(x) = f_0 + \sum_{s=1}^{n} \sum_{1 \le i_1 < \cdots < i_s \le n} f_{i_1,\ldots,i_s}(x_{i_1}, \ldots, x_{i_s}) \tag{8}$$

with $s = 1, \ldots, n$ and

$$f_0 = \frac{1}{|H^n|} \int_{H^n} f(x) \mathrm{d}x = G \; . \tag{9}$$

Thereby, for $p = 1, 2, \ldots, s$ holds

$$\int_{A_{i_p}} f_{i_1,\ldots,i_s}(x_{i_1}, \ldots, x_{i_s}) \mathrm{d}x_{i_p} = 0 \; . \tag{10}$$

For the components $f_{i_1,\ldots,i_s}(x_{i_1}, \ldots, x_{i_s})$ in Eq. (8) the partial variance $D_{i_1,\ldots,i_s}$ is

$$D_{i_1,\ldots,i_s} = \int_{A_{i_1},\ldots,A_{i_s}} f_{i_1,\ldots,i_s}(x_{i_1}, \ldots, x_{i_s}) \mathrm{d}x_{i_1}, \ldots, \mathrm{d}x_{i_s} \quad . \tag{11}$$

The total variance can be detemined with the help of partial variances

$$D = \sum_{s=1}^{n} \sum_{1 \le i_1 < \cdots < i_s \le n} D_{i_1,\ldots,i_s} \quad . \tag{12}$$

On the basis of the ANOVA decomposition the sensitivity measure $\hat{S}_{i_1,\ldots,i_s}$ in Eq. (3) can be defined with

$$\hat{S}_{i_1,\ldots,i_s} = D_{i_1,\ldots,i_s} \quad \text{and} \quad \sum_{s=1}^{n} \sum_{1 \le i_1 < \cdots < i_s \le n} \hat{S}_{i_1,\ldots,i_s} = D \; . \tag{13}$$

The resulting $S_{i_1,\ldots,i_s}$ are denoted as Sobol indices. For continuous functions f condition $\hat{S}_{i_1,\ldots,i_s} = 0$ implies, that the component $f_{i_1,\ldots,i_s}$ has no importance for f. For more details about ANOVA decomposition and further explanations about the Sobol indices see [12, 14, 9]

2.2 Partial derivative based sensitivity

The sensitivity analysis on the basis of partial derivatives requires the determination of the expected values of a function g.

$$\hat{s}_i : \{[a,b]\,,\; a, b \in \mathbb{R}, a \le b\}^n \to \mathbb{R} : \; H^n \mapsto \frac{1}{|H^n|} \int_{H^n} g\,(x)\,\mathrm{d}x =: \hat{S}_i \tag{14}$$

$$\hat{S}_i = \frac{1}{|H^n|} \int_{H^n} g\,(x)\,\mathrm{d}x \tag{15}$$

Thereby, different ansatz functions are available in literature. In [8], where first ideas about derivative based sensitivity measures are presented, the function g is defined as $g = \partial f / \partial x_i$. To countervail the problem of negative signs, in [1, 4] an improved measure with $g = |\partial f / \partial x_i|$ was introduced. An alternative approach, introduced by [13], defines g with $g = (\partial f / \partial x_i)^2$. This approach enables to constitute a connection to the variance based sensitivity measure, see Section 2.1. This measure was likewise applied in [4] in a sum of a squared expected value and the variance of $\partial_i f$

$$G^2 + D = \frac{1}{|H^n|} \int_{H^n} (\partial_i f(x))^2 \, \mathrm{d}x \ , \tag{16}$$

which is identical to the approach introdcued in [13].

In this contribution g is introduced as $|\partial f / \partial x_i|$. For the numerical treatment a sequence of quasi random points $x_1, \ldots, x_j, \ldots, x_{n_{sim}}$ in H^n has to be generated. If g is Riemann integrable, the term $\int_{H^n} g(x)\mathrm{d}x$ can be evaluated, see [13], with

$$\frac{1}{|H^n|} \int_{H^n} g(x)\mathrm{d}x = \lim_{n_{sim} \to \infty} \frac{1}{n_{sim}} \sum_{j=1}^{n_{sim}} g(x_j) \ . \tag{17}$$

2.3 Remarks on global sensitivity measures

The interested reader might be confused about multiple sensitivity measures; still introduced are variance based sensitivity measures in Section 2.1, derivative based measures in Section 2.2 and anticitpating Section 4 neural network weighting based sensitivity measures. They arise due to the fact, that a mathematical definition of sensitivity is missing so far. Sensitivity can be just assessed by means of measures. Thereby, those measures appraise specific, but different, characteristic of the functional relationship f. In consequence, the announced sensitivity measures might provide diverse sensitivity evaluations. Those diverse sensitivity measures should be not rated as a discrepancy but rather as a completion.

However, the advantages of multiple sensitivity measures can be demonstrated by means of an example. Thereby, the function of interest f, see Fig. 1, is

$$f(x, y) = \sin(x) + \sin(4 \cdot y) \ . \tag{18}$$

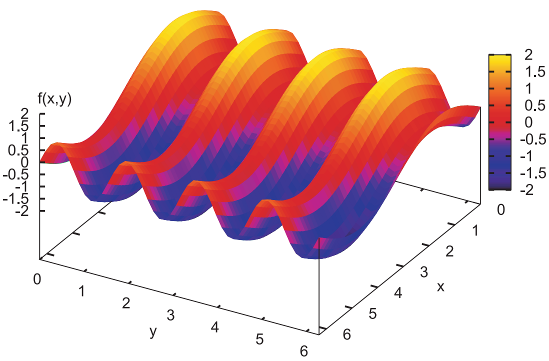

Figure 1: Function f (see Eq. (18))

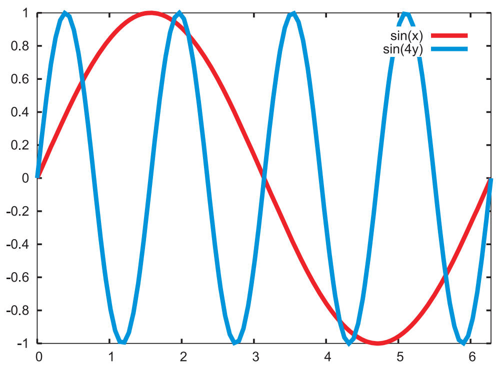

Figure 2: Individual plots of $\sin(x)$ and $\sin(4 \cdot y)$

The sensitivity S_1, S_2 is determined analytically. While the variance based sensitivity measures assess the importance of both input quantities x_1, x_2 as equal, $S_1^{Sobol} = S_2^{Sobol} = 0.5$, the derivative based sensitivity measures highlight the importance of x_2 with $S_2^{Der} = 0.80$ in comparison to x_1 with $S_2^{Der} = 0.20$. Comparing the results with Fig. 2 it becomes obvious, that the identification of differences between x_1 and x_2 is reasonable.

3 Sectional global sensitivity measure

Sensitivity measures introduced in literature have in common, that they provide for an individual input quantity x_i a deterministic value S_i. Thereby, the spreading of the respective quantity is considered in the integral mean. The aim of sectional sensitivity measures is to highlight even local effects. Since it might be of interest to capture local effects in input parameters and result parameters it has to be distinguished between argument based sectional sensitivity measures (AGSM) and sectional sensitivity measures based on the value of function (FGSM).

3.1 Argument based sectional sensitivity measures

The basic idea of AGSM is to subdivide the input space of interest $A_i = Q_i(H^n)$, with

$$\begin{aligned} Q_i: \quad \{[a,b]\,,\ a,b \in \mathbb{R}, a \le b\}^n &\to \quad \{[a,b]\,,\ a,b \in \mathbb{R}, a \le b\} \\ H^n = (A_1, \ldots, A_n) &\mapsto \quad A_i \end{aligned}$$

in a finite number N_I of subintervals $(A_i)_k^I$. For each $A_i \subseteq \mathbb{R}$, $\left((A_i)_k^I\right)_{k\in\{1,\ldots,N_I\}}$ represent a family of intervals $(A_i)_k^I \subseteq \mathbb{R}$ with

$$(A_i)_k^I \cap (A_i)_j^I = \varnothing\ , k \ne j \quad \text{and} \quad \bigcup_{k\in\{1,\ldots,N_I\}} (A_i)_k^I = A_i\ . \tag{19}$$

If this segmentation is done simultaneously for all $i = 1, \ldots, n$, note that n indicates the dimensionality of the problem, a set of subhypercuboids $(H^n)_w^{I*}$ is constituted with $w \in \{1, \ldots, (N_I)^n\}$. Thereby, for $N_I \ge 2$ holds

$$\forall\ w \in \{1, \ldots, (N_I)^n\} : (H^n)_w^{I*} \subset H^n \tag{20}$$

For each of these subhypercuboids the sensitivity in accordance to Section 2 can be determined. But, the handling of the produced data becomes a problem. Subdividing each input dimension into N_I intervals, $(N_I)^n$ combination of sensitivity values ($S_1, \ldots, S_n$) will be obtained. If the problem has a high dimensionality ($n > 3$) the evaluation of results becomes impracticable.

To countervail this problem the segmentation is just performed for an individual input quantity x_i, while all remaining input quantities $x_{\sim i}$ are considered globally. Thus, for a section k of an input quantity x_i the sensitivity term $\hat{S}^a_{i,[k]}$, in accordance to Section 2, can be specified. Since $\hat{S}_{\sim i}$ of the remaining input quantities $x_{\sim i}$ stay constant for all k, the sensitivity terms $\hat{S}^a_{i,[k]}$ can be compared among each other with

$$S^{a*}_{i,[k]} = \frac{\hat{S}^a_{i,[k]} \cdot N_I}{\sum\limits_{l=1}^{N_I} \hat{S}^a_{i,[l]}} = \frac{\hat{S}^a_{i,[k]} \cdot N_I}{\hat{S}_i} \tag{21}$$

Thereby, $S^{a*}_{i,[k]}$ enables just a qualitative sensitivity statement. Due to $\sum\limits_{l=1}^{N_I} \hat{S}^a_{i,[l]} = \hat{S}_i$ the qualitative results $S^{a*}_{i,[k]}$ can be scaled with the global sensitivity S_i

$$S^a_{i,[k]} = S^{a*}_{i,[k]} \cdot S_i = \frac{\hat{S}^a_{i,[k]} \cdot N_I}{\hat{S}_i} \cdot S_i = \frac{\hat{S}^a_{i,[k]} \cdot N_I}{\sum\limits_{j=1}^{n} \hat{S}_j} = \frac{\hat{S}^a_{i,[k]} \cdot N_I}{\sum\limits_{j=1}^{n} \sum\limits_{l=1}^{N_I} \hat{S}^a_{j,[l]}} \tag{22}$$

to deduce a quantitative statement. While S_i shows values of the interval $[0, 1]$, because it is normalized, possible values of $S^{a*}_{i,[k]}$ are in the interval $[0, N_I]$. Hence, $S^a_{i,[k]}$ provide by definition values in the interval $[0, N_I]$. Theoretically, sensitivity measures of greater than one are possible; in application this case is improbable.

The subhypercuboids $(H^n)_v^I$ with $v \in \{1, \ldots, N_I\}$, obtained by means of the discussed segmentation, have the property, that for the input quantity of interest x_i ($N_I \geq 2$)

$$\forall\, v \in \{1, \ldots, N_I\} : Q_i((H^n)_v^I) = (A_i)_v^I \subset Q_i(H^n) = A_i \tag{23}$$

and for the remaining input quantities $x_{\sim i}$

$$\forall\, j \in \{1, \ldots, i-1, i+1, \ldots, n\} \wedge v \in \{1, \ldots, N_I\} : Q_j((H^n)_v^I) = Q_j(H^n) \tag{24}$$

holds.

In this contribution the sectional sensitivity measures are evaluated with partial derivative based sensitivity measures. Thus, for the numerical realization the same point set, as introduced in Section 2.2, $x_1, \ldots, x_j, \ldots, x_{n_{sim}}$ is utilized. This point set is subdivided in accordance to the segmentation k, while $n_{sim} = \sum\limits_{k=1}^{k_{max}} n_{sim,k}$ holds. The sensitivity measure is defined, see also Eq. (17), with

$$\hat{S}^a_{i,[k]} = \frac{1}{\left|(H^n)_k^I\right|} \int_{(H^n)_k^I} g(x)dx = \frac{1}{n_{sim,k}} \sum_{j=1}^{n_{sim,k}} g(x_j) \tag{25}$$

3.2 Sectional sensitivity measures based on the value of function

The main idea of FGSM is similar to the AGSM approach. Contrarily, not the input space is segmented, but rather the result space B. Thereby, the result space is defined with

$$B = \{b; \forall x \in H^n : b = f(x)\} \quad . \tag{26}$$

Generally, B is just defined in a closed interval if f is a continuous function. For $B \subseteq \mathbb{R}$, $\left(B_m^I\right)_{m \in \{1,\ldots,N_I\}}$ is a family of intervals $B_m^I \subseteq \mathbb{R}$ with

$$B_m^I \cap B_j^I = \varnothing \; (m \neq j) \quad \text{and} \quad \bigcup_{m \in \{1,\ldots,N_I\}} B_m^I = B\ . \tag{27}$$

Due to the segmentation, for each result quantity of the subdivision $z^m \in B_m^I$ the respective input quantity $x^m \in (H^n)_m^I$ is assigned.

$$(H^n)_m^I = \left\{x^m; \forall z^m \in B_m^I : x = f^{-1}(z^m)\right\} \tag{28}$$

The obtained input quantities x^m can be described with hypercuboids just in infrequent situations. At least for linear functions f the input quantities x^m can be described with convex hulls, for nonlinear functions f this will not work anymore.

The sensitivity measures $S^f_{1,[m]}, \ldots, S^f_{n,[m]}$ for each section of the result quantities B_m^I can be determined, as described in Section 2, with

$$S^f_{i,[m]} = \frac{\hat{S}^f_{i,[m]}}{\sum\limits_{j=1}^{n} \hat{S}^f_{j,[m]}} \tag{29}$$

If f is a non-monotonic function, the input space $(H^n)_m^I$ can not be described with a continuous hull anymore. In consequence, to each subregion B_m^I in the result space multiple non-connected subregions in the input space $(A_{1,1}, \ldots, A_{n,1}), \ldots, (A_{1,c}, \ldots, A_{n,c})$ are assigned. An appropriate detection of those non-connected subregions demands the inverse solution approach [5, 6]. For a respective section $B_m^I \subset B$ not just a combination of sensitivity measures is obtained but rather a set of combinations of sensitivity measures. $\left(S^{f,1}_{1,[m]}, \ldots, S^{f,1}_{n,[m]}\right), \ldots, \left(S^{f,c}_{1,[m]}, \ldots, S^{f,c}_{n,[m]}\right)$.

It has to be noted, that it is not reasonable to compare adjacent sensitivity values $S^f_{i,[m]}$ and $S^f_{i,[p]}$, determined in adjacent sections, $B_k^I, B_p^I \subset B$, because they are scaled with $\sum_{j=1}^{n} \hat{S}_{j,[m]}^f$ and $\sum_{j=1}^{n} \hat{S}_{j,[p]}^f$ respectively. Thereby, for each non-linear function f

$$\sum_{j=1}^{n} \hat{S}_{j,[m]}^f \neq \sum_{j=1}^{n} \hat{S}_{j,[p]}^f \; . \tag{30}$$

Considering exemplarily the function $q(x_1, x_2) = x_1 + x_2^2$, even though the sensitivity of x_1 is constant in A_1, the FGSM are dissimilar in each section $(A_1)_k^I$

$$\forall\, m \in \{1, \ldots, N_I\} \wedge j \in \{1, \ldots, N_I\} \wedge m \neq j : S_{1,[m]}^f \neq S_{1,[j]}^f \; . \tag{31}$$

4 Global sensitivity measures and neural networks

As an alternative to the introduced approaches in Section 2 the sensitivity can be assessed by means of a trained neural network. Thereby, several features of the neural network can be utilized in an advantageously manner. Perceiving an artificial neural network (ANN) not only as a surrogate model to approximate a functional relationship f but rather as a versatile tool to reason the behavior of f, several characteristics of ANN can be capitalized for sensitivity analysis. Principally, these are the data storage (to memorize the characteristic of f in the weighting matrix of the ANN), derivability (to determine partial derivatives analytically) and efficient numerical evaluation. The both latter ones can be used to obtain variance based and derivative based sensitivity measures. But the utilization of the weighting matrix requires to establish a new class of sensitivity measures. These are denoted as weighting based sensitivity measures. First attempts to formulate weighting based sensitivity measures are done in literature [7]. Those ideas are further extended in this contribution.

For the formulation of weighting based sensitivity measures some basic concepts of ANNs are presented first, see also Fig. 3 and 4. ANNs save their information within the synaptic weights w_{j_k,j_k+1}^k, which connect the neurons j_k between the k-th and $k+1$-th network layer. Therefore, w_{j_k,j_k+1}^k provide all essential information about the trained input data – as expected the characteristic of f.

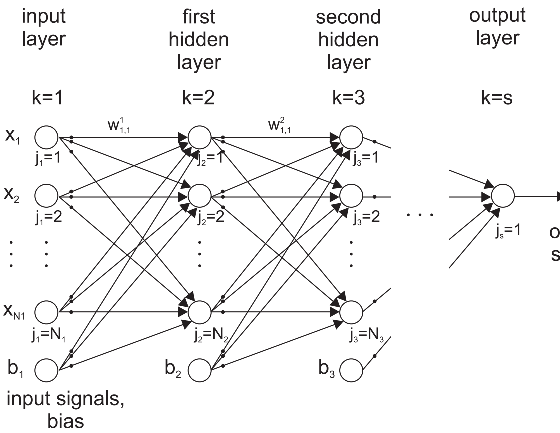

Figure 3: Scheme of artificial neural network

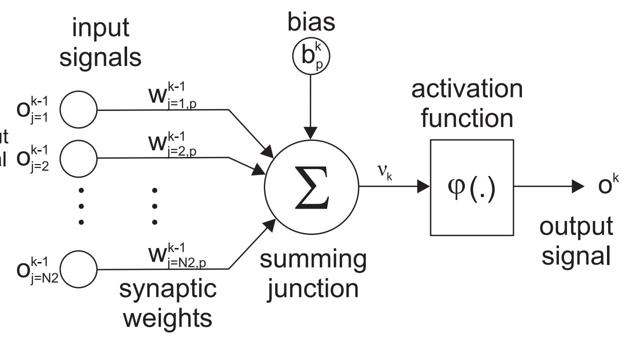

Figure 4: Scheme of p-th neuron in layer k

The sensitivity characteristic $\hat{S}_i$ can be formulated for a finite number s of neuron layers $k \in \{1, \ldots, s\}$, $j_k \in \{1, \ldots, N_k\}$ neurons per layer k respectively, with

$$\hat{S}_i = \sum_{j_{s-1}=1}^{N_{s-1}} \cdots \sum_{j_2=1}^{N_2} \left| w_{i,j_2}^1 \cdot w_{j_2,j_3}^2 \cdot \; \cdots \; \cdot w_{j_{s-1},1}^{s-1} \right| \; . \tag{32}$$

Generally, the treatment of positive and negative weights is handled controversial in the literature. In this approach, the absolute value of weights is applied, due to the fact, that the total influence should be evaluated.

As a matter of fact, the first layer of weights have the greatest influence on the output of the ANN. In consequence, concentrating on those weights offers a first good shot about the sensitivity

$$\hat{S}_i = \sum_{j=1}^{N_2} |w_{ij}| \,. \tag{33}$$

The accuracy suffers in comparison to the weight product, but the manageability is increased, especially in the presence of ANN with many hidden layers.

Formulating sensitivity measures with the pure introduction of weights approximates the mode of operation of ANN just in a rough manner. In detail, the influence of the weights behind the neurons $k \geq 2$, which accommodate activation functions, are incorporated in a crude way, due to the fact, that the weights are always multiplied with activation $y_p^k = \varphi\left(o_{j_{k-1}}^{k-1}, w_{j_{k-1},p}^{k-1}, b_p^k\right)$ of the previous neuron. To account for this fact, activation-weighting based sensitivity measures are introduced.

$$\hat{S}_i = \sum_{j_{s-1}=1}^{N_{s-1}} \cdots \sum_{j_2=1}^{N_2} \left|w_{i,j_2}^1\right| \cdot \left|y_{j_2}^2\right| \cdot \left|w_{j_2,j_3}^2\right| \cdot \left|y_{j_3}^3\right| \cdot \,\cdots\, \cdot \left|y_{j_{s-1}}^{s-1}\right| \cdot \left|w_{j_{s-1},1}^{s-1}\right| \tag{34}$$

To shorten matters, in this contribution no remarks about the efficient evaluation and derivability of neural networks are provided. The interested reader is referred to [11, 2].

5 Examples

5.1 Benchmark Polynom

In this first example the idea of AGSM and FGSM should be highlighted. Therefore, a straightforward function is considered

$$f(x_1, x_2, x_3) = 0 \cdot x_1 + 2 \cdot x_2 - x_3^2 \,, \tag{35}$$

which can be evaluated and assessed by means of visualization. Thus, the results of sensitivity analysis become comparable. In Eq. (35) the term of x_1 has no influence on f. An important feature of sensitivity measures should be in general, that insensitive parameters are assessed as such. However, the function f can be visualized in a x_2-x_3-plot.

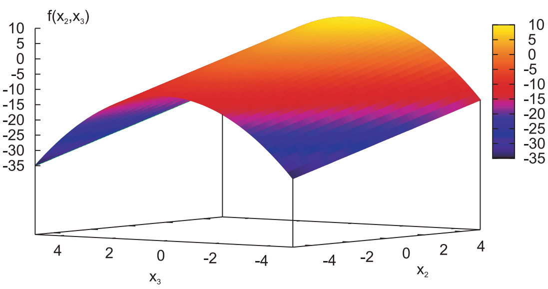

Figure 5: Function $f^*(x_2, x_3) = 2 \cdot x_2 - x_3^2$

sensitivity measure	μ		σ	
	x_2	x_3	x_2	x_3
weighting based simplified	12	88	1	1
weighting based activation-	18	82	1	2
weighting based	12	88	1	1
derivative based	27	73	0	0
variance based	38	62	0	0

Figure 6: Global sensitivity measures for f^*

First of all, global sensitivity measures on the basis of artificial neural networks are determined; the three introduced weighting based sensitivity measures, a derivative and variance based sensitive measure, see Fig. 6. In order to make sure, that the training of a neural network has no significant influence on the sensitivity results, the analysis is repeated several times. Hence, the empirical mean μ and standard deviation σ are stated. The qualitative ranking of the input quantities is the same. But the quantitative values vary between the different approaches. Thereby, the weighting based measures show similar results and highlight especially x_3. In opposite, the variance based measures emphasizes x_3 as less important. The derivative based sensitivity measure shows intermediate results.

In order to provide a better insight into this problem, sectional sensitivity measures on the basis of partial derivatives are determined. The respective results are depicted in Fig. 7 and 8. Thereby, the AGSM is potential to show the main character of the function f, separated for each dimension respectively. This feature is comparable to a metamodel viewer but advantageously the influence of other input dimensions is incorporated inherently. Additionally, the FGSM gives further information about the influence of input parameters for specific result parameter ranges. In Fig. 8 it is obvious, that the influence of x_2, x_3 is similar for large result values, while for small result values the influence of x_3 is paramount.

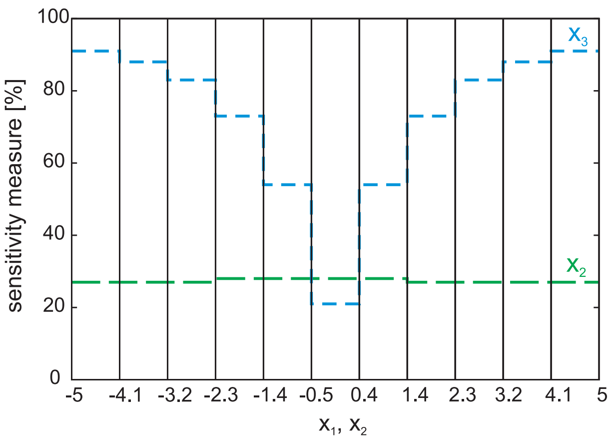

Figure 7: AGSM of polynomial function

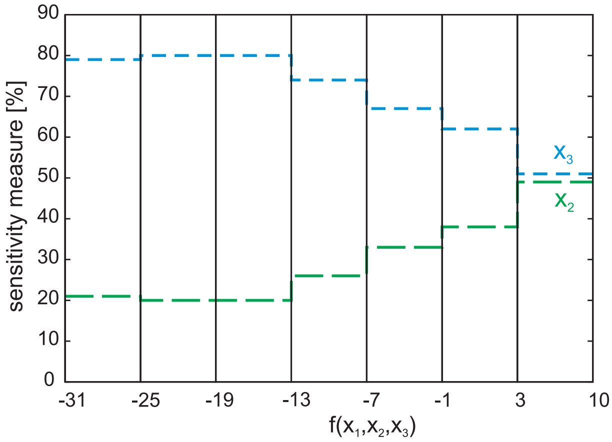

Figure 8: FGSM of polynomial function

5.2 Benchmark Ishigami

A more ambitious function is investigated in order to show the potential of the introduced approach. Therefore, the Ishigami function, see Eq. (36), is applied, since it is often used to validate sensitivity measures [14]

$$f(x_1, x_2, x_3) = \sin(x_1) + 7 \cdot \sin^2(x_2) + 0.1 \cdot x_3^4 \cdot \sin(x_1)\,. \tag{36}$$

This 3D Problem is visualized by means of the respective cross-plots in Fig. 9. Note, that the scales for the values of function vary between each plot.

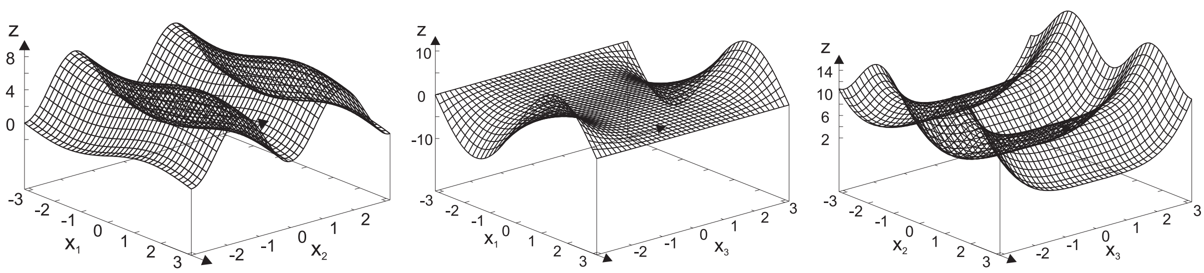

Figure 9: Cross-plots of Ishigami function

As before, the global sensitivity measures are determined with an empirical mean and standard deviation, see Fig. 10. Thereby, the concordance between weighting based and variance based sensitivity measures is high, while the derivative based measure even show another qualitative ranking. Derivative based sensitivity measures highlight the importance of x_2 and rank x_1, x_3 equally, while the other investigated GSM emphasize the importance of x_1 prior to x_2, x_3. An evaluation of those results is arguable;

a basis may provide Fig. 9. However, the higher standard deviations of the weighting based sensitivity measures show, that they are more sensitive to the training of the artificial neural network.

sensitivity measure	μ			σ		
	x_1	x_2	x_3	x_1	x_2	x_3
weighting based	48	26	26	6	4	5
simplified weighting based	42	34	24	6	4	5
activation-weighting based	45	29	26	11	9	7
derivative based	22	55	23	0	1	1
variance based	45	36	19	1	1	0

Figure 10: Sensitivity measures of Ishigami function

Furthermore, the AGSM and FGSM on the basis of derivative based sensitivity measures are determined for the Ishigami function, see Fig. 11 and 12. The results of the AGSM seems to be unusual at a first glance in comparison to the cross-plots in Fig. 9. But recalling, that the derivative based sensitivity measures assess regions with gradients of zero as non-sensitive, the appropriateness of the results becomes obvious. The results of the FGSM are intuitive and simple to interpret. If we are interested in modifying especially large or small values of the result parameters, x_3 should be altered. Comparing those predication with the results in Fig. 10 the significance of sectional global sensitivity measures is apparent. Note, that the results in Fig. 12 are simplified, since they ignore the uniqueness of the Ishigami function. Appropriate approaches to handle unique functions are on hand [5, 6], but detailed explanations are behind the scope of this approach.

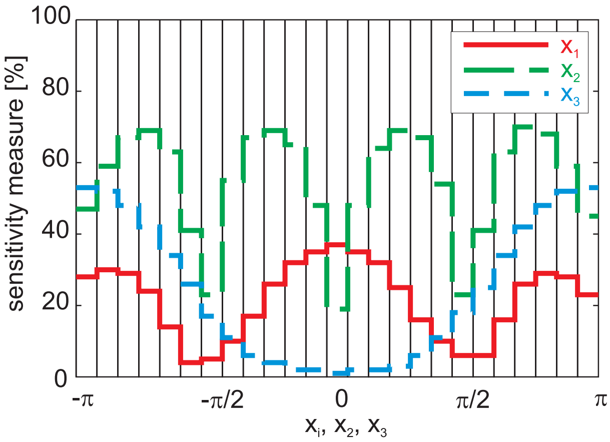

Figure 11: AGSM of Ishigami function

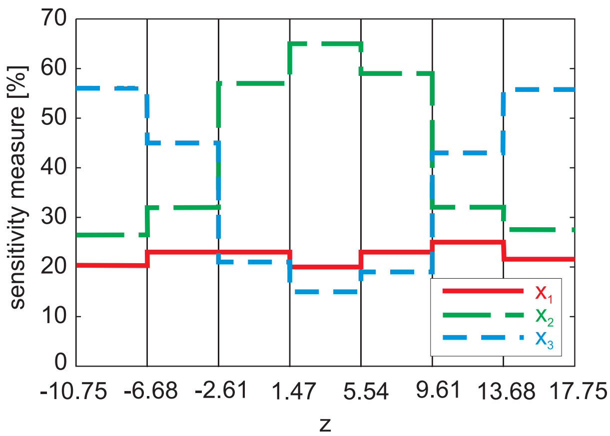

Figure 12: FGSM of Ishigami function

5.3 Radiofrequency ablation

To point out the applicability of the presented approach, the introduced methods are demonstrated for an industry-relevant example of radiofrequency ablation (RFA) for hepatic tumors, see Fig. 13. In RFA a needle shaped applicator is inserted into the tumor and by means of electric current heat is produced, which causes cell death. The introduced example is elucidated in detail in [3] to determine an optimal applicator placement under consideration of uncertain input parameters. Here, a preprocessing evaluation for this example is investigated to assess the influence of the eight input parameters in view of result parameters.

The input parameters in sequence are the electrical conductivity of the hepatic parenchyma σ_{par}, the blood vessels σ_{ves} and the tumor σ_{tum}, the position x, y, z and orientation φ, ψ of the applicator. The result of interest is the minimal temperature t_{min} within the tumor.

In Fig. 14 the values of GSM are shown. The results of derivative based and variance based GSM exhibit similar results for the qualitative assessment. The results of weighting based GSM are slightly different, because a higher priority is assigned to φ and ψ. On account of the obtained results it can be stated, that σ_{ves} and σ_{tum} are negligible for further simulations and that the positions x, y, z are most influential, since it seems to be reasonable to position the applicator in the proximity of the center of the tumor.

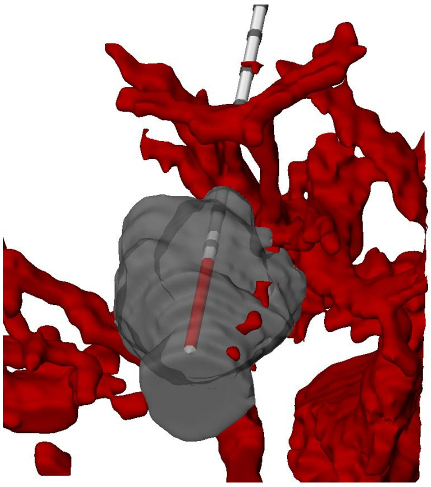

Figure 13: Visualization of RFA

input parameters	weighting	derivative based sensitivity measure	variance
σ_{par}	7	17	19
σ_{ves}	0	0	0
σ_{tum}	2	3	2
x	19	18	16
y	14	16	11
z	24	29	47
φ	19	9	4
ψ	16	8	3

Figure 14: Sensitivity measures of RFA

The AGSM and FGSM, see Fig. 15 and 16, provide a deepened insight into the problem. Thereby, AGSM highlight again the importance of the applicator positions x, y, z. Additionally, it can be reasoned that x, y, z are most sensitive in the margins of the tumor, while the remaining input parameters show similar importance when the applicator is positioned in the proximity of the center of the tumor. Supplementary, the FGSM reveal, that for small temperatures t_{min} the coordinate z is most influential, while for large temperatures t_{min} the electrical conductivity σ_{par} is most sensitive.

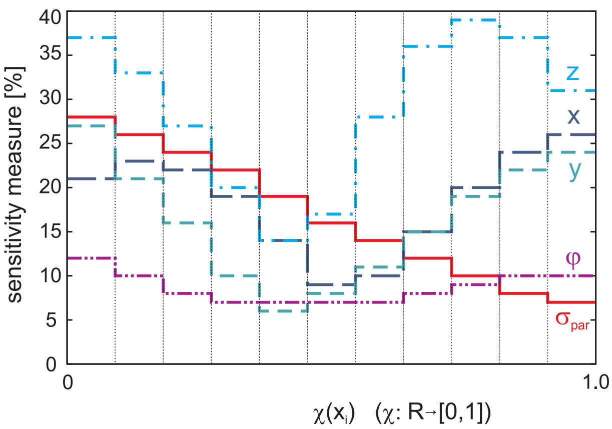

Figure 15: AGSM of RFA
(selected input parameters)

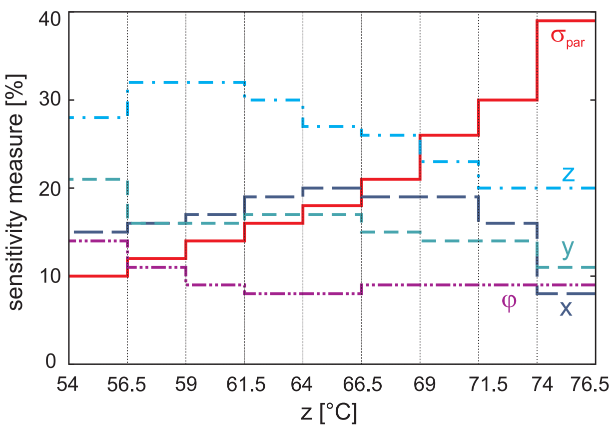

Figure 16: FGSM of RFA
(selected input parameters)

6 Conclusions

In the presented approach, a new way of investigating the functional dependency between input and result parameters is introduced. Therefore, sectional sensitivity measures are presented, both argument based sensitivity measures and sensitivity measures based on the values of function. The introduced approach may be applied in the preprocessing stage of engineering design or even utilized to steer optimization procedures and reliability analysis. The idea of argument based sensitivity measures is similar to the idea of metamodel viewer, but countervails the dimensionality problem. Hence, the influence of respective input parameters in view of result parameters is evaluated without any disturbance due to other input parameters. The approach of sensitivity measures based on the values of function focuses on the influence of input parameters on specific result parameter ranges. This is worthwhile since in many applications it is of main interest to avoid especially small or large values, e.g. in reliability assessment.

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