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Sensitivity method for extreme-based engineering problems

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ABSTRACT

Engineering models are becoming increasingly complex, involving a larger number of variables. As a result, engineers struggle to deeply understand the models and therefore validate and properly use them. Sensitivity analyses (SA) are usually conducted to help with this task. Nonetheless, the knowledge and computational efforts required to conduct SA increases with the complexity of the model. This paper presents a conceptually simple method to conduct the SA of extreme-based engineering problems, that is, those problems whose outcome of interest is their maximum or minimum values. This type of problems is of relevance for reliability-based design. The method requires to iteratively maximize or minimize the model by fixing one input factor at each time. Then, the variation of the optimal surface is evaluated. The method permits the visualization and measure of the input factors' influence on the extreme model response, with no need of defining the probability distribution of the input factors. Both the easiness of application and interpretation, along with a low computational cost for problems dealing with extreme values, make the proposed method very convenient to practitioners.

1. Introduction

With the advances in computational tools and the availability of Big Data, models (both, law-driven and data-driven) are becoming increasingly more complex. The main issue related to the high-dimensional models used in Engineering is that engineers can hardly identify the input factors (i.e., variables and parameters) whose accuracy is of primary relevance for the quality of the output, and the input factors whose less accurate estimation can be used without a significant loss of credibility of the model response. It may be also of interest to identify for a given factor, which range of values has an innocuous model response (e.g., not affecting the failure surface), and which values trigger a sudden change in this response. These questions should be answered to deeply understand an engineering model and therefore be able to validate and properly use it. Sensitivity analyses are performed to this aim.

Sensitivity methods can be broadly classified as local and global methods. Very roughly, the former are useful to understand the direct relationship between input factor and model response at a point (or set of points) of the input variability space, whereas the latter provides the global relationship between factor and model response generalized over the complete domain of definition of the factors. Giving the limitation of the local methods when dealing with the high-dimensional problems of real life, most of the recent works focus on the global methods (e.g., [1,2]), with a particular interest in reducing their computational

load (e.g., [3]). Global approaches fail to answer which part of the input space results in the largest change of the response surface. To address this problem, authors such as [4,5] and [6] present several techniques combining both approaches.

In the case of the reliability field, the part of the response surface that yields failure is of interest. Thus, the sensitivity analysis (SA) can be efficiently simplified by focusing on this part of the response, that is, the extreme response. In this line, failure probability-based approaches (e.g., [7,8]) aim to identify the input factors with more potential to reduce the probability of failure.

SA of high-dimensional problems is usually addressed numerically. This requires to characterize the response surface, which can be done either through meta-models, that is, less computationally expensive models that emulate the response surface (e.g., Kriging models, [9,10]), or via sampling the actual response surface. The quality of the results of the first approach will depend on the meta-model's capacity to capture the original model's behaviour. As a consequence, analysts usually put big efforts in defining an accurate meta-model, which can be time-consuming and requires a certain level of expertise. Regarding the second approach, sampling strategies very often rely on the widely-known Monte Carlo simulations to obtain a representative sample of the model response. Although some tailored sampling strategies have been developed to alleviate the computational burden associated with

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the Monte Carlo simulations, still many approaches present limited applicability in real life. When dealing with the extreme response, either meta-model or sampling strategy should be directed to a specific area of the response surface that is usually of very low occurrence probability, which makes the process especially challenging. See [11] for a more detailed discussion on the computational complexity of SA.

A common approach to performing a non-exhaustive SA of extreme-based problems is based on scenarios. Usually, the worst-case or best-case scenario is considered [12]. Once the scenario is identified, the sensitivity analysis is conducted for the corresponding values of the input factors. This approach implies a good knowledge of the model response. Some authors (e.g., [13]) analyse the extreme values of the input factors, which can or cannot yield the extreme response. [14] propose a Kriging model to identify a large set of extreme model responses, and [15] solves an optimization problem to determine the worst case. [16] identifies the input factors that produce the extreme response of axial forces in jacket platforms through stochastic simulations by Latin Hypercube sampling technique. Then, the sample response is fitted to a probabilistic distribution and the sensitivity analysis conducted by a regression method. This approach requires the probabilistic distribution of the factors. Moreover, in the case of non-smooth response surfaces, the stochastic simulation along with the fit of the extreme response to a given probabilistic distribution can mislead the results.

This paper concerns the SA of extreme-based engineering problems, that is, those problems whose outcome of interest is their extreme response. These type of problems are of relevance for reliability-based design. SA over the extreme response of a model is conducted with a two-fold objective; (a) the identification and ranking of the most relevant input factors that contribute the most to the variability of the extreme response (global perspective), and (b) the identification of the range of the input variability space that affects the most to the extreme response (local perspective). To address the two questions, this paper presents an efficient and robust sensitivity method to analyse high-dimensional models addressing problems of extreme values in Engineering.

The main novelties of this method include:

- it allows to visualize and measure the main effects of the input factors on the extreme response;
- it is conceptually simple, easy to apply and requires low computational efforts within the context of problems dealing with extreme values, even in the case of high-dimensional problems. For this reason, it does not require preliminary work for the dimensional reduction of the problem;
- the impact of altering a single input factor over the system failure can be determined without conducting further evaluations;
- the method is independent of the input factor's distribution and assumptions on model properties; and
- it can be applied to engineering problems involving continuous and discrete factors that can be independent or dependent among them.

The remaining document is organized as follows; Section 2 gives an overview of the existing sensitivity approaches, and discuss their suitability in the context of extreme-based problems. Section 3 presents the new method for sensitivity analysis of extreme-based problems, and in Section 4, a related importance measure is introduced. The application of the method is shown in Section 5, showing the good performance of the method in case of high-dimensional engineering problems. Final remarks are given in Section 6 and in Section 7, some conclusions and future research lines are drawn.

2. Review of sensitivity analysis methods

Sensitivity methods are usually classified into local and global methods. Most of the cases, they do not compete with each other, as they

provide solutions with different resolution. To do so, they consider two different perspectives of the sensitivity concept, which underlie how these methods address the sensitivity analysis.

Let us assume a d -dimensional mathematical model $f(\cdot)$, where a set of input factors $\mathbf{X} = X_1, X_2, \dots, X_d \in \mathcal{R}^d$ yields a response surface Y ;

$$Y = f(\mathbf{X}). \quad (1)$$

Each input factor is continuous and defined within a given interval, $X_i \in [X_i^l, X_i^u]$.

2.1. Local methods

Under the perspective of the local methods, the concept of sensitivity refers to the amount of change given on a response surface when a small change is introduced in an input factor. This concept is mathematically formalized by the partial derivative of the model response with respect to the factor at stake, X_i , i.e., $\frac{\partial f(\mathbf{X})}{\partial X_i}$, or by finite differences when working on the discrete domain, that is, $\frac{\Delta f(\mathbf{x})}{\Delta x_i}$. Note that the lowercase is used to denote the discrete factors.

Local sensitivity methods are based on this idea. They are usually referred as Once At a Time¹ (OAT) methods because they approach the SA by perturbing once factor at each time, while the rest of the factors are fixed in a given nominal value. Because the surface response is studied around the nominal point \mathbf{X}^0 , the local sensitivity is \mathbf{X}^0 -point specific, which can be expressed as follows

$$S_i^{local}(X_i^{0+}; X_{\sim i}^0) = \left. \frac{\partial f(\mathbf{X})}{\partial X_i} \right|_{\mathbf{X}^0} \simeq \left. \frac{\Delta f(\mathbf{x})}{\Delta x_i} \right|_{\mathbf{X}^0} \quad X_i \in [X_i^l, X_i^u], \forall X_i \quad (2)$$

where $X_{\sim i}$ denotes all the factors except X_i . Given that the value of the partial derivative with respect to X_i changes for different nominal values, a well-established grid of nominal points should be studied to obtain a good picture of the sensitivity of the response surface. If the sensitivity scores are then combined and jointly analysed, e.g., by calculating the mean of the absolute [17] or squared [18] sensitivity scores, the approach would be considered as a global method.

For the sake of illustration of the local approach and its limitations, let us assume the model

$$f(X_1, X_2, X_3) = \cos(X_1)(X_2 - X_3^2)^2, \quad (3)$$

defined for the input variability space $X_1 \in [-\frac{3\pi}{4}, \frac{5\pi}{4}]$, $X_2 \in [-20, 20]$ and $X_3 \in [-1, 1.5]$.

Fig. 1 shows the local sensitivity of the model to the input factor X_2 considering $50 \times 50 = 2500$ possible combinations of nominal values of x_1 and x_3 within the input variability space. When the selected nominal value corresponds to the middle point within the definition range of X_1 and X_3 (i.e., mean values, $x_1 = -\pi/4$ and $x_3 = 0.25$), it is observed that the sensitivity of the response surface to X_2 increases with increasing absolute values of x_2 , with a maximum sensitivity value of ± 28.26 reached at $x_2 = \pm 20$. Nevertheless, this sensitivity assessment is meaningless, because when another combination of nominal values is selected, the sensitivity measure can change. For instance, when the nominal combination $x_1 = 0$, $x_3 = 1.5$ is selected, which corresponds to the minimal value of the response surface, a maximum sensitivity value of -46.75 is obtained for $x_2 = -20$.

Thus, to determine the largest sensitivity of a model to the input factors, the analysis should be conducted by combining all the factors involved. Fig. 2 depicts, with thin lines the local sensitivity of the response surface to the input factors for the different nominal combination of values; and highlighted with a thicker line, the envelope of the sensitivity curves for the three factors analysed.

¹ Note that the OAT term refers to the sampling strategy used.

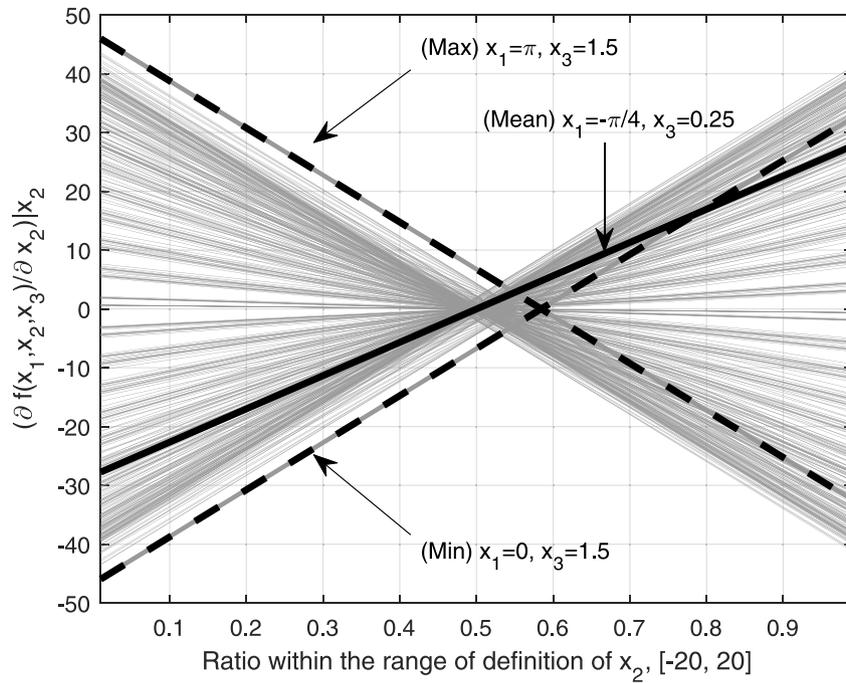


Fig. 1. Local sensitivity of $f(x_1, x_2, x_3) = \cos(x_1)(x_2 - x_3^2)$ to x_2 for 2500 combinations of nominal values of x_1 and x_3 .

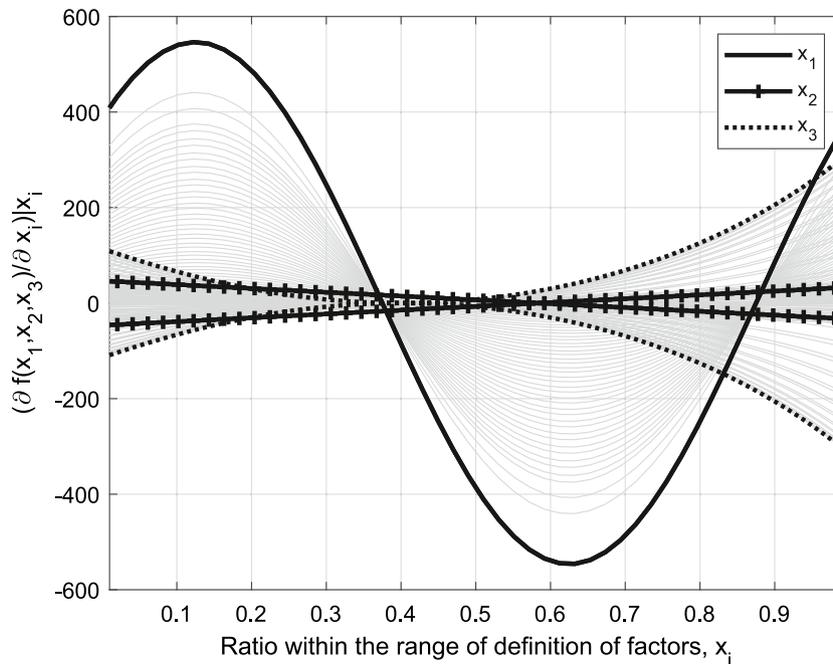


Fig. 2. Envelopes of the local sensitivity of $f(x_1, x_2, x_3) = \cos(x_1)(x_2 - x_3^2)$ to the three input factors.

In the case of dimensionless factors, the largest absolute value of the derivatives can be used to rank the importance of the factors in terms of sensitivity, that is, as an importance measure. Based on Fig. 2, and assuming dimensionless factors, x_1 is the most important factor, followed by x_3 and x_2 . Such conclusion required $50^3 = 125,000$ evaluations, which shows the clear limitation of the local sensitivity methods when dealing with large dimensional problems. Nonetheless, for low dimensional problems, local methods are useful tools to visualize and better understand the model behaviour. If the factors have units, it is not mathematically consistent to compare the derivatives of the three factors and ranking their importance accordingly. To avoid this problem, standardization of the variables should be conducted.

For relevant contributions in the context of derivative-based sensitivity methods, the reader is referred to [19] who proposes a sort of stratified OAT, and [20] who introduces an analytical approach of the equations defining the model. Adjoint-based methods are also included within this group (see, e.g., [21]). [18] discusses the derivative-based sensitivity measures, showing their link with the global Sobol's indices, which will be discussed in the following section.

2.2. Global methods

Global methods, which are more suitable for large-dimensional problems, study the influence on the model response of each input

factor and the combination of them, based on statistical analyses. Thus, under the perspective of the global methods, the concept of sensitivity is a measure of the response surface variability introduced by an input factor, or a combination of them, when they vary within their definition range. The variability, understood as amount of change, can be measured using the mean of a sample of partial derivatives, the comparison of conditional and unconditional distributions, etc.

In most of the global methods, all factors are perturbed at the same time (All at A Time, AAT), and the surface response is studied based on correlation analysis, analysis of variance, etc. For a meaningful sensitivity analysis, the probabilistic distribution of the input factors should be known. If appropriate probabilistic distributions are assigned to the input factors (being consistent with the support of the probabilistic distribution), it is not necessary to define their upper and lower bounds.

The main advantage of the global methods is that they yield importance measures to rank the factors in terms of sensitivity. Probably, the most popular importance measure is the Sobol's indices [22], which are based on the functional decomposition of the variance measuring the contribution of each factor to the total variance of the model response. The first-order indices, also called main-effect indices, are obtained as follows,

$$I_i^{Sobol} = \frac{Var_{X_i} (E_{X_{-i}} [y|x_i])}{Var(y)}. \quad (4)$$

As mentioned before, importance measures should be independent of factors' units, as is the case of the Sobol indices. See [23–25] for a detailed discussion on the importance of the dimensional-related issues.

For the illustrative case of Eq. (3), and assuming uniform distributions for the three factors, $I_1^{Sobol} = 0.57$, $I_2^{Sobol} = 2 \times 10^{-4}$ and $I_3^{Sobol} = 0$; thus the most important factor is X_1 and the least is X_3 , which is not in agreement with the ranking obtained with the local approach. The reason is that the first result considered the largest sensitivity, understood as the largest slope of the response surface, to rank the factor's importance, whereas Sobol's indices use the average response (conditioned to each factor) to rank them.

To understand the implications of considering the average response, Fig. 3 shows the box plots of the surface response for each factor (this sensitivity method is used by [26]) along with the expected value of the response for each X_i (red thick line). In the case of X_3 , although some variability exists in the response when moving through the definition range of X_3 , the symmetry of the surface response with respect to the horizontal axis makes the Sobol's index zero. Thus, for very symmetrical response surfaces, considering the aggregated data (e.g., average value) results in dismissing relevant information. In this regard, [27] notes that to avoid non-informative conclusions, the analysis should be complemented with other sensitivity indicators. For instance, to decide if a factor is not relevant and can be removed, Sobol indices of orders higher than one can be used to assess the influence of the interactions among factors. This analysis could unveil the hidden role of some influential variables. For the illustrative example, the second-order indices are $S_{12} = 0.43$, $S_{13} = 0.002$ and $S_{23} = 0$, which, along with the first-order indices, sum up 1 [22]. When the number of factors is too large, it is more convenient to use the total-effect indices that measure the fraction of variance of the surface response that remains unexplained when varying just one input factor over its definition range. Based on this complementary information, factor X_3 is unimportant from a global perspective, although it was the second most important factor from a local perspective. This highlights the consequences of considering aggregated values.

This section has presented the existing sensitivity methods from a broad perspective, paying attention to those aspects that are of interest in the context of extreme-based problems. The interested reader is referred to [11,28–30] for comprehensive reviews of these methods.

3. Sensitivity analysis of extreme-based problems

Many engineering problems are interested in the extreme response of a given model, that is, either the maximum or the minimum response, rather than the average behaviour of the model. The previous section has shown that Sobol's indices, which are based on aggregated data, might not be the most appropriate to characterize the extreme response. Sobol's indices relate to the expected value (red curve in Fig. 3), which can hide information about how the extreme curve behaves (e.g., the U-shape of the maximum response values when moving through X_2 in the middle plot of Fig. 3). Furthermore, extreme-based problems pose a special challenge concerning the sampling methods, as they have to guarantee that the extreme region is properly captured. On the other hand, local approaches do not seem to be suitable methods, as the number of input factors of real problems is usually significant. In this context, this section presents a new sensitivity method specifically designed for extreme-based problems.

3.1. A-IAT (all minus one at a time) upon the extreme response surface

The effect that an input factor has on a response surface can be studied by perturbing just the target factor while the rest of the factors remain fixed (OAT approach). Nonetheless, the same effect can be determined if the target factor is fixed and the rest is perturbed. This is the idea behind the proposed method.

In order to analyse the sensitivity of the extreme response surface, either the maximal or the minimal, this method proposes to fix one factor at each time and to study how this affects the extreme response surface. Therefore, for each fixed factor, it is required to obtain the value of the extreme response. This method can be defined as an A-IAT (all minus one at a time) approach.

For the sake of illustration, let us analyse the function given by [31] and further discussed in [32]. Given that only two input factors are involved, it allows the visualization of the results. This D-function is defined as follows;

$$Y = 0.2 \exp(X_1 - 3) + 2.2|X_2| + 1.3X_2^6 - 2X_2^2 - 0.5X_2^4 - 0.5X_1^4 + 2.5X_1^2 + 0.7X_1^3 + \frac{3}{(8X_1 - 2)^2 + (5X_2 - 3)^2 + 1} + \sin(5X_1) \cos(3X_1^2), \quad (5)$$

with both input factors defined in the $[-1, 1]$ interval. Fig. 4(a) shows the 3D response surface of the D-function.

Fig. 4(b) depicts the extreme response (maximal and minimal) of the D-function when fixing each factor at a time. Note that the obtained curves are the envelope of the D-function for the input factors, that is, they capture the extreme response surface when all the factors vary minus the one analysed.

Once the extreme surface is determined for each factor, the finite differences of the corresponding extreme surface can be evaluated to determine the sensitivity (i.e., slope) of this curve. Fig. 5 shows the obtained sensitivity of the extreme response surface for different values of X_1 and X_2 . They are also compared with the envelopes of the local sensitivity analysis of the D-function for $50 \times 50 = 2500$ combinations of different nominal values of x_1 and x_2 . It is interesting to see how the sensitivity of the extreme surfaces does not correspond with the maximum sensitivity of the function. This is evident in the case of the sensitivity with respect to X_2 for the second half of its definition range, that is, $[0, 1]$. The reader is referred to Fig. 4(a) and (b) to appreciate the difference between the largest local sensitivity (slope) of the response surface with respect to X_2 , which occurs along the silhouette edges of the central cone, and the sensitivity of the maximal response surface, which corresponds mostly to the function at $X_1 = 1$. In the case the extreme response is of interest, the variability of the response surface that does not provide an extreme response can be disregarded.

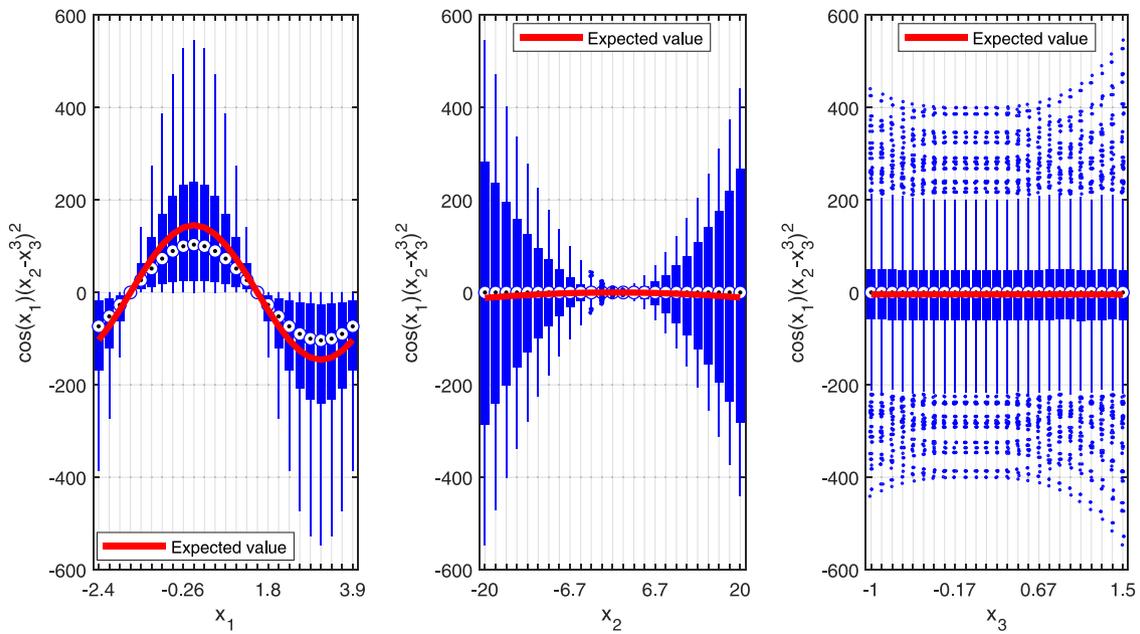


Fig. 3. Box plots of the surface response of $f(X_1, X_2, X_3) = \cos(X_1)(X_2 - X_3^2)^2$ with respect to each analysed factor.

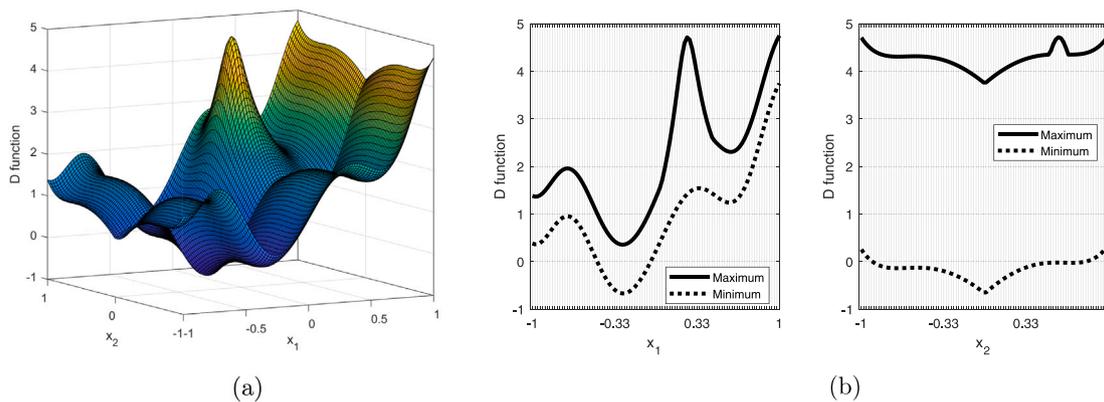


Fig. 4. (a) 3D representation of the response surface of D-function, Eq. (5). (b) Extreme response of D-function for different input factors.

Fig. 4 has shown that when varying all inputs of a problem space of d dimensions at a time minus input X_i (A-1AT), the extreme response of the reduced dimensional space can be identified. In this manner, the relevant information of the reduced dimensional space associated with $X_i = x_i^0$ is condensed into a maximum or minimum value. In other words, the $d - 1$ dimensional space is now represented by just one value. The variation of this value with the studied input, X_i , informs about the sensitivity of the entire dimensional space to variable X_i . Varying an input at a time (OAT) would transform the 1-dimensional space associated with X_i into one value, requiring many evaluations to characterize the extreme response. The following section formalizes mathematically the A-1AT approach for extreme-based problems.

3.2. Mathematical formulation

Let \bar{Y}_i denote the extreme (either maximal or minimal) response surface of $Y = f(\mathbf{X})$ for a given point x_i^0 , thus the sensitivity of the extreme response surface at this point can be expressed as follows;

$$S_i^{Ext}(x_i^0, X_{\sim i}) \approx \left. \frac{\Delta \bar{Y}_i(x_i^0, X_{\sim i})}{\Delta x_i} \right|_{x_i^0} \quad x_i^0 \in [X_i^l, X_i^u], \forall X_i \quad (6)$$

Note that Eq. (6) is expressed in terms of finite differences, rather than exact derivatives. Since a maximum or minimum operator is involved,

the derivative may not exist. Thus, each input factor that is analysed should be discretized in n_i points, $\{x_i^0\}$, where the extreme response surface has to be defined. The extreme response surface, $\bar{Y}_i(x_i^0, X_{\sim i})$, can be obtained either by gradient-based methods or (meta)heuristics (e.g., genetic algorithms), depending on the complexity of the model. The optimum search is independent of the level of discretization of the non-fixed factors (note that they have been denoted by capital $X_{\sim i}$ in Eq. (6)), which avoids the problem of dismissing some extreme values due to a non-adequate discretization. If a technique based on Monte Carlo simulation is used to sample the response surface and pick the extreme value (which is possible for simple models), it would result in enormous computational costs, and the potential neglect of some extreme values given by the discretization of the non-fixed factors.

Regarding the definition range of the input factors, $[X_i^l, X_i^u]$, this can be chosen according to different criteria. For example, if the physical domain of the variable is considered, a wave height could be defined in the range of $[0, 20]$ m (other values would make no physical sense). If the domain of interest of the engineer is considered, the diameter of a pipe could be defined, for instance, in the range of $[0.50, 1.50]$ m, because other values might not be possible due to other design constraints. Also, the range can be linked to a statistical parameter, such as a number of times the deviation with respect to the mean, and

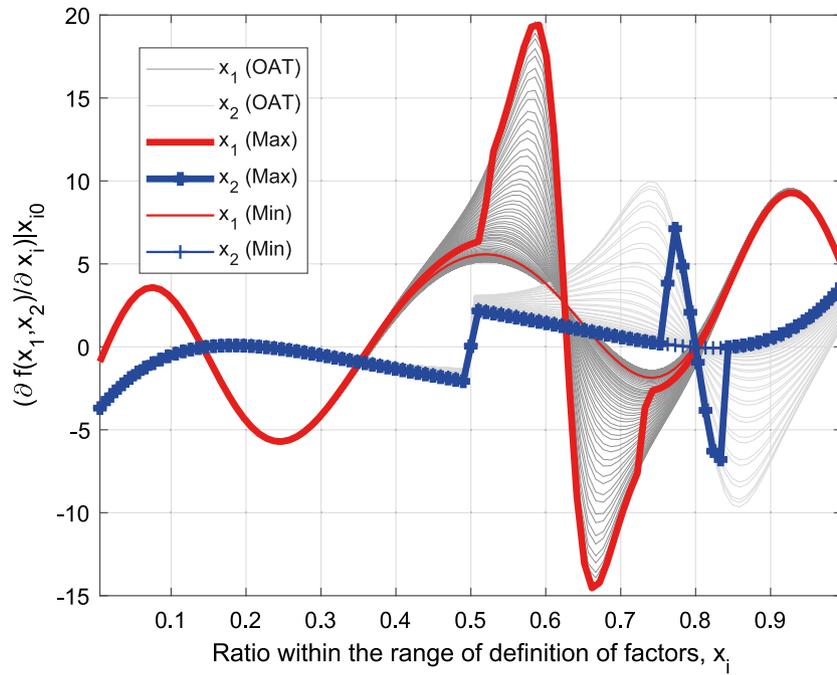


Fig. 5. Envelopes of the local sensitivity (partial derivatives) of D-function for 2500 combinations of nominal values of x_1 and x_2 , and sensitivity of the extreme surface response (maximal and minimal) obtained with the A-1AT approach.

a given percentile (e.g., P95). In any case, the probability distributions of the factors are not required.

The method requires a total number of optimizations that is of the order of $\mathcal{O}(n \times d)$, where n is the average number of discrete points in which the factors are discretized and d is the number of input factors.

Therefore, the A-1AT sensitivity analysis for extreme response surface can be summarized as the estimation of how the extreme response surface varies with respect to each analysed factor. The following section provides the algorithm to evaluate the sensitivity according to this approach.

3.3. Algorithm for sensitivity analysis

Algorithm 1 describes the proposed sensitivity method. The first step is to discretize the factor X_i in n_i points within the $[X_i^l, X_i^u]$ interval (line 1). Then, for each discrete value of X_i , the extreme value (maximum or minimum) of the model is obtained for all the factors $X_{\sim i}$ defined in their corresponding interval, $[X_{\sim i}^l, X_{\sim i}^u]$, and X_i fixed, i.e., defined in an interval whose lower and upper bounds take the same value, $[x_i(j), x_i(j)]$ (line 3). The optimal value is saved. Once the optimal value is determined for all the discrete points of X_i , the sensitivity is calculated according to Eq. (6) (line 6).

Algorithm 1 A-1AT sensitivity of X_i for extreme problems

- 1: $x_i \leftarrow \text{DiscretizeFactor}(X_i^l, X_i^u, n_i)$
 - 2: **for** $j = 1 \rightarrow n_i$ **do**
 - 3: $\bar{Z} \leftarrow \text{Optimize}(Y, X_i \in [x_i(j), x_i(j)], X_{\sim i} \in [X_{\sim i}^l, X_{\sim i}^u])$
 - 4: $\bar{Y}_{i,j} \leftarrow \text{Add}(\bar{Z})$
 - 5: **end for**
 - 6: $S_i^{Ext} \leftarrow \text{FiniteDifferences}(\bar{Y}_{i,j}, x_i)$
 - 7: **return** S_i^{Ext}
-

4. Importance measure

The previous section has presented a method to visualize the sensitivity of the extreme response of a model to each factor involved. As occurred in the case of the local sensitivity, the results can be also used

to rank the importance of the factors in the case all of them are dimensionless. Nonetheless, given that most of the engineering problems involve dimensional factors, an importance measure is required to rank the sensitivity of the extreme response of the model to the different factors.

Based on the concept behind Sobol's indices, the following importance measure is proposed;

$$I_i^{Ext} = \frac{Var_{X_i}(\bar{Y}|x_i)}{\sum_i Var_{X_i}(\bar{Y}|x_i)} \quad (7)$$

The index, which is defined between $[0, 1]$, allows ranking input factors according to its contribution to the total variability introduced by the individual factors to the extreme response surface. The indices of all the input factors sum up 1. In contrast to the variability of the expected response considered by Sobol, the variability of the extreme response associated with each factor, $Var_{X_i}(\bar{Y}|x_i)$, is here considered. The proposed index is dimensionless, and thus, stable to factor's scale changes. Nevertheless, it can present instabilities due to the factor's discretization process. In order to avoid this issue, a weighted variance is proposed where the weight is given by the distance between the discrete points. In this way, the variance of each factor is calculated as follows

$$Var_{X_i}(\bar{Y}|x_i) = \sum_{j=1}^N \frac{w_j}{\sum_{j=1}^N w_j} (\bar{Y}_j - \bar{\mu})^2 \quad (8)$$

with

$$\bar{\mu} = \sum_{j=1}^N \frac{w_j}{\sum_{j=1}^N w_j} \bar{Y}_j \quad (9)$$

where N is the number of discrete points in which factor X_i is discretized and \bar{Y}_j is the value that the maximal response surface takes at the j th discrete point. The weights are calculated according to

$$w_j = \frac{1}{2}(x_{i,j+1} - x_{i,j-1}) \quad \forall j \in [2, N - 1] \quad (10)$$

and $w_1 = \frac{1}{2}(x_{i,2} - x_{i,1})$ and $w_N = \frac{1}{2}(x_{i,N} - x_{i,N-1})$ for the first and last points of the discrete factor. Note that if the discretization of a

Table 1
Importance measures for the illustrative example in Eq. (3) and the D-function.

| Case | Factors | Range | Index (minimal) | Index (maximal) | Sobol (expected value) |
|--------------|---------|-------------------------------------|-----------------|-----------------|------------------------|
| Illustrative | X_1 | $[-\frac{3\pi}{4}, \frac{3\pi}{4}]$ | 0.659 | 0.658 | 0.57 |
| | X_2 | $[-20.0, 20.0]$ | 0.322 | 0.323 | 2×10^{-4} |
| | X_3 | $[-1.0, 1.5]$ | 0.019 | 0.019 | 0.00 |
| D-function | X_1 | $[-1.0, 1.0]$ | 0.962 | 0.973 | 0.91 |
| | X_2 | $[-1.0, 1.0]$ | 0.038 | 0.027 | 0.06 |

Table 2
Input factors, definition range, discretization of the factors and importance measures for the case of flooding risk.

| Factor | Range | Discretization | I_i^{Ext} (Eq. (7)) |
|-------------------------|-------------------------|----------------------------|-----------------------|
| Q (m ³ /s) | [500, 3000] | 20 points (log spaced) | 0.594 |
| Z_v (m) | [49, 51] | 20 points (equally spaced) | 0.244 |
| H_d (m) | [2, 4] | 20 points (equally spaced) | 0.106 |
| Z_m (m) | [54, 56] | 20 points (equally spaced) | 0.028 |
| C_b | [55, 56] | 20 points (equally spaced) | 0.027 |
| B (m) | [295, 305] | 20 points (equally spaced) | 6×10^{-4} |
| L (m) | [4990, 5010] | 20 points (equally spaced) | 2×10^{-6} |
| K_s (-) | [15, 10 ¹⁰] | 200 points (log spaced) | 1×10^{-7} |

factor is equally distributed, the weighted variance becomes the regular variance.

Table 1 provides the value of the proposed importance measure for the maximal and minimal response surface, and it compares to the Sobol’s indices for the illustrative example in Eq. (3) and the D-function. For the illustrative example, note that the symmetry in the maximal and minimal response surface of X_3 is captured by the proposed index, which results in a Sobol index equal to zero.

A relevant aspect to consider when using an importance measure is its robustness regarding the sampling method and/or the number of evaluations. In the context of the proposed method, the robustness is studied against the degree of discretization of x_i . The next section presents two large-dimensional examples, and the robustness of the importance measure is then further discussed.

5. Application to large dimensional cases

5.1. Flooding risk model

5.1.1. Problem description

The case of flooding risk due to dyke overtopping is analysed. To do so, a simplification of the Saint-Venant equation is proposed, Eq. (11), which provides the overflow, F , in metres.

$$F = Z_v + H - H_d - C_b, \tag{11}$$

with

$$H = \left(\frac{Q}{K_s B} \sqrt{\frac{L}{Z_m - Z_v}} \right)^{3/5}. \tag{12}$$

H , c_b and H_d denote the water level, bank level and dyke high, respectively, Q is the flow rate, B , L and K_s the width, length and bed friction coefficient of the watercourse, respectively, and the bottom watercourse levels upstream and downstream are given by the Z_m and Z_v . Positive values of F means that overtopping occurs. The quantity of interest here is the maximal value of F , therefore, the sensitivity analysis should study the extreme response, and not the average response. The domains of definition of the input factors are indicated in Table 2, which are based on the values provided by [29]. Given that K_s is upper unbounded, an upper bound of $K_s^u = 1 \times 10^{10}$ is taken because of computational reasons. It is assumed that they are independent factors.

5.1.2. Sensitivity analysis

The discretization of the input factors is indicated in the third column of Table 2. Note that discrete points for the factors with the largest ranges are distributed using a log-scale. Also, in the case of K_s , which is upper unbounded, 200 points have been selected. Given that the optimization of the function is conducted at each point, the number of required optimal evaluations is given by the summation of the number of discrete points, 340 in this case. A generalized pattern search method has been used to identify the optimal curves, \bar{F}_i , with the absolute optimal point given as an initial search point. More precisely, the Matlab algorithm “patternsearch” and poll method “GPSPositive-Basis2N” have been used. The average number of model runs per optimization using “patternsearch” has been 448. The 340×448 model runs, which were conducted in Matlab2018b, took 7.6 sec. with a CPU @1.90 GHz, and 8.00 GB of RAM.

Fig. 6 shows the maximal overflow for each fixed factor, \bar{F}_i . The horizontal dot lines highlight the zero level, i.e., when the overtopping event occurs. For the input variability space considered, C_b , B , Z_m and L are not critical because independently of the value they take, the associated curve of \bar{F}_i is above the zero value; thus, overtopping will occur for any value of those factors within their domains of definition. On the contrary, the rest of the factors might play a critical role in the risk of overtopping. Guaranteeing either $Z_v < 50.2$ m, $H_d > 3.4$ m, $Q < 2100$ m³/s or $K_s > 100$, overtopping will be avoided. Overtopping can be also avoided if a combination of input factors are modified even when they are not critical (e.g., C_b and B), however identifying the effective combinations will require further analysis.

Q and Z_v have the largest influence according to the importance measure indicated in the last column of Table 2. B and L have a negligible effect as supported by the small range (in comparative terms) that \bar{F}_i takes for these factors (see Fig. 6), indicating that \bar{F}_i is not very sensitive to the variability of these factors. Q causes a large variability of the output; this contribution is roughly constant over its domain of definition. If the first half of the range is considered, i.e., [500, 1500], the importance measure obtained for Q would be roughly half (0.3). The large range of K_s is penalizing its importance because the response is very insensitive to large values of the K_s . Its contribution to the variability of the output is mainly concentrated in the first half of its domain of definition (see Fig. 6). If only the range of [15, 1000] were considered, K_s would be ranked as the second more important parameter after Q . In relation to the risk of overtopping (i.e., the point where \bar{F}_i cuts the zero-level dashed line), K_s presents the larger slope, thus, special attention should be paid to this input factor when taking values smaller than 100.

Fig. 7 shows the robustness of the importance measures of the 8 input factors when different levels of discretization are selected. Equally-, log- and randomly spaced discretizations of the factors Q and K_s are considered, while the discretization of the rest of the factors is equally distributed. It can be seen that when log-spaced discretization is chosen, a small number of total discrete points guarantee stable values. In the case of the linear and random discretizations, more discrete points are needed, and thus, more model evaluations are needed. In any case, the order of importance of the factors remains constant after 1500 total points. This shows the level of robustness of the method. Therefore, the optimal discretization degree will depend on the regularity of the model and the criterion used to discretize the input factors (e.g., linear scale or log scale). Section 6 discusses some recommendations to maximize the robustness of the results.

5.1.3. Discussion

This model has been used by other authors to discuss different sensitivity methods. For instance, [29], after removing L , B and Z_m as a result of an initial factor screening to reduce the dimensional complexity, use Monte Carlo sampling involving 10^5 evaluations to obtain the first-order Sobol’s indices of the remaining factors. The resulting importance ranking is as follows, $Q(0.35) > H_d(0.28) >$

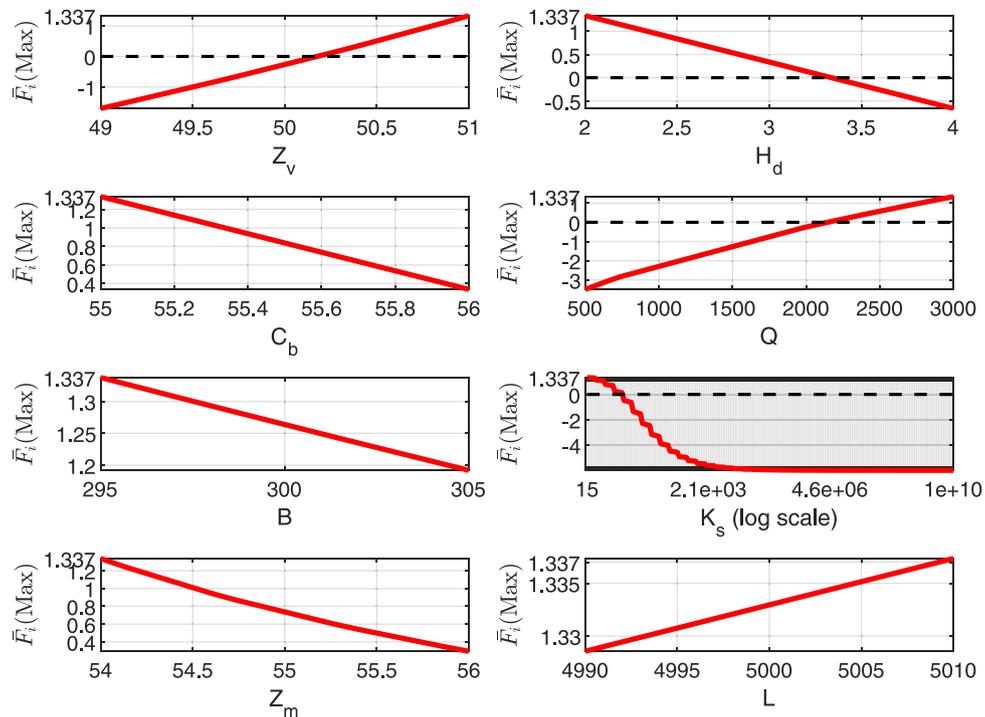


Fig. 6. Maximal response surface for each fixed factor (\bar{F}_i expressed in metres).

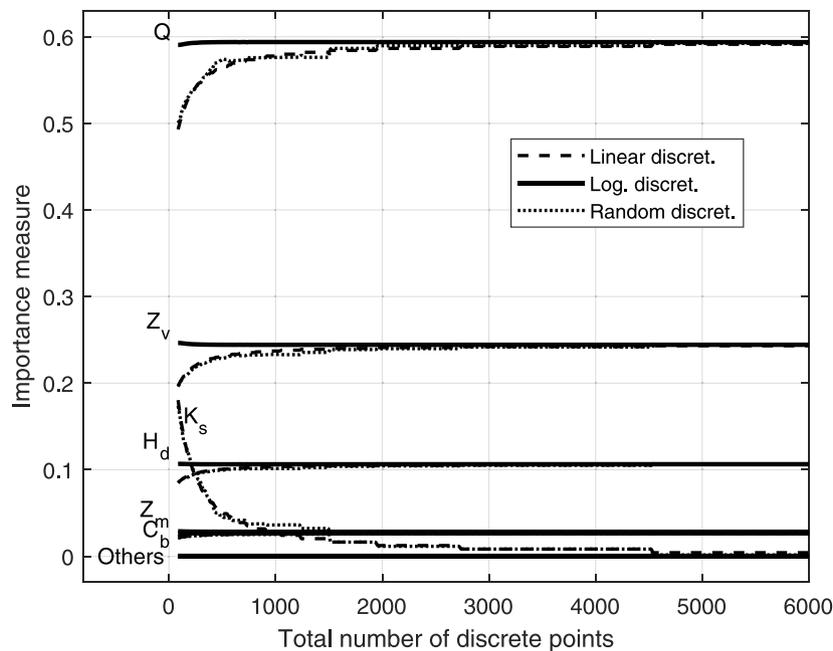


Fig. 7. Importance measure for different types and degrees of discretization. Linear (i.e., equally spaced), log-spaced and random discretization have been considered for Q and K_s .

$Z_v(0.19) > K_s(0.13) > C_b(0.03)$. As mentioned before, this ranking considers the influence of the input factors based on the average response of the model, thus the differences with the ranking given in Table 2 are justified. Practitioners should reflect on the type of problem they have in hand in advance, that is if they are interested in the mean response or the extreme response.

A simplified version of this model is analysed in [33]; only the influence of Q , K_s , Z_v and Z_m on H is studied. They assess the influence of the input factor distributions on the overtopping probability. To do so, they assume that the extreme values of the input factors cause

failure, which can be considered as an analysis of the maximum values, rather than the average response. They use Monte Carlo sampling involving 10^5 evaluations. According to the analyses conducted, K_s is the most relevant factor followed by Q .

5.2. Structural frame

5.2.1. Problem description

The second large case deals with the 8-storey building shown in Fig. 8, involving a total of 40 input factors, namely, the Young modulus

Table 3
Definition range and discretization of the input factors for the structural frame.

| Factor | Data proposed by [8] | | | Range [$P_{0.001}$, $P_{0.999}$] | Discretization |
|------------------------------------|----------------------|----------------------|-------------------|---|----------------------------|
| | Distribution | Mean | Std. Dev. | | |
| $E_{i,v}$ (Pa) ($i = 1 \dots 8$) | Lognormal | 3.0×10^{10} | 2.0×10^9 | $[2.44 \times 10^{10}, 3.7 \times 10^{10}]$ | 10 points (log spaced) |
| $b_{i,v}$ (m) ($i = 1 \dots 8$) | Lognormal | 0.4 | 0.015 | [0.36, 0.45] | 10 points (equally spaced) |
| $E_{i,h}$ (Pa) ($i = 1 \dots 8$) | Lognormal | 3.0×10^{10} | 2.0×10^9 | $[2.44 \times 10^{10}, 3.7 \times 10^{10}]$ | 10 points (log spaced) |
| $b_{i,h}$ (m) ($i = 1 \dots 8$) | Lognormal | 0.2 | 0.01 | [0.17, 0.23] | 10 points (equally spaced) |
| P_1 (N) | GEV Type I | 1.0×10^4 | 3.0×10^3 | [-4800, 15900] | 50 points (equally spaced) |
| P_2 (N) | GEV Type I | 1.5×10^4 | 3.5×10^3 | [-2300, 21800] | 50 points (equally spaced) |
| P_i (N) ($i = 3 \dots 8$) | GEV Type I | 2.0×10^4 | 4.0×10^3 | [-2180, 21800] | 50 points (equally spaced) |

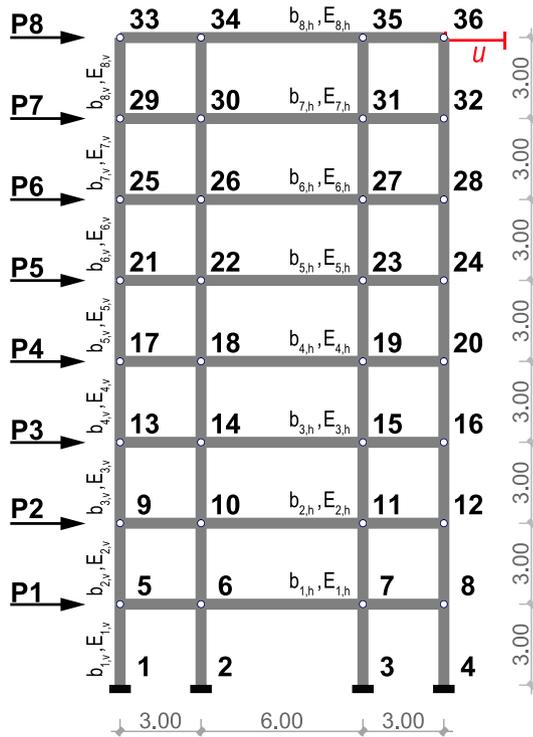


Fig. 8. Geometry, mechanical properties and loads of the structural frame.

and the dimension of the horizontal and vertical members (assuming a squared cross-section) and the horizontal forces applied to the left side of the building. The quantity of interest is the maximal horizontal displacement of Node 36, either to the right or to the left. Therefore, the sensitivity analysis focuses on the extreme response, that is, $\max(u)$, u being the absolute value of the displacement. This large example is discussed by [8] and is selected as it allows the comparison with their results. The domains of definition and the discretization of the input factors are indicated in Table 3. The domain of definition corresponds with the percentiles 0.001 and 0.999 of the probability distributions proposed by [8]. The horizontal forces have been more finely discretized than the rest of factors because, after an initial analysis with a uniform number of discrete points for all the factors, non-monotonic response of the model in relation to the horizontal forces (i.e., first decreasing and then increasing) was observed (see Fig. 9). All factors are assumed to be independent.

5.2.2. Sensitivity analysis

A pattern-search method has been used to identify the optimal curves, \bar{u}_i , executed twice, with two different initial search points, namely, the horizontal forces pushing the structure with the minimum structural stiffness, and the horizontal forces pulling the structure with the minimum stiffness. The Matlab algorithm used is “patternsearch” and the poll method, “GSSPositiveBasis2N”. The generating set search

(GSS) has been chosen because of its better performance when the optimum is close to the boundaries, as this is the case. The results are obtained with a total number of 720 optimizations. The average number of model runs per optimization using “patternsearch” has been 3900. The 720×3900 model runs took 5808 seconds in a laptop with a CPU @1.90 GHz, and 8.00 GB of RAM. Note that the number of evaluations is significantly low for SA dealing with extreme values. The number of model evaluations required by Monte Carlo simulations to address the problem with the same level of accuracy would have been unaffordable.

Fig. 9 shows the maximal response surface for each fixed factor, \bar{u}_i . Factors with the largest vertical range of \bar{u}_i , i.e., the horizontal forces, P_i , and the dimensions of the horizontal members, $b_{i,h}$, are the most relevant from the SA perspective. In the case that, for instance, the horizontal displacement of Node 36 is required not to exceed a given threshold, e.g., 0.25 m, this can be attained by guaranteeing that any of the factors intersecting the horizontal dashed line represented in Fig. 9 is defined within the range below the dashed line; E.g., $-13000 < P_8 < 10000$ (N) or $b_{3,h} \in [0.213, 0.23]$ (m). Varying the value of any other factor within their range of definition will not be enough to guarantee a horizontal displacement below this threshold. For instance, if $E_{1,v} = 3 \times 10^{10}$ Pa, then, the maximum displacement of Node 36 will be 0.281 m.

This analysis is consistent with the importance measure of the input factors obtained (Fig. 10). The horizontal forces P_8 and P_7 are the most relevant factors, followed by $b_{3,h}$ and $b_{4,h}$. The results are sound from the structural point of view, as the dimensions of the horizontal members can take (alarming) small values, making the structure especially vulnerable, with the horizontal members of the intermediate floors being the most critical. Also, the descendent importance order of P_i is consistent with the physical phenomenon. The stiffness of the lowest vertical members is significantly more important than the stiffness of the other vertical members as they are key elements to control the rotation of the structure.

Fig. 11 shows the robustness of the ranking of the importance measures of the 40 input factors involved. The order of the ranking is stable even using a very small number of discrete points and the importance measure is noticeably constant from 600 discrete points, i.e., an average of 15 discrete points per variable. Using different types of discretizations for $E_{i,v}$ and $E_{i,h}$ does not change the results given the linear maximal response surface for these factors (see Fig. 9).

5.2.3. Discussion

The importance measure of the input factors given by [8] are shown in Fig. 10 (right y-axis). The discrepancy between the results is because [8] uses Sobol’s indices, and thus, they implicitly consider the average response rather than the extreme. According to their classification, the stiffness of the vertical members of the highest level of the frame, given by the expression $\frac{E_{8,v} b_{8,v}^4}{12}$, has more influence on the horizontal displacement \bar{u}_i than the lowest levels, which is not easily justifiable from a structural point of view. Besides, they dismiss the importance of the cross-section of the horizontal members. This example highlights the importance of considering the most appropriate SA to conduct beforehand, as the result can vary significantly.

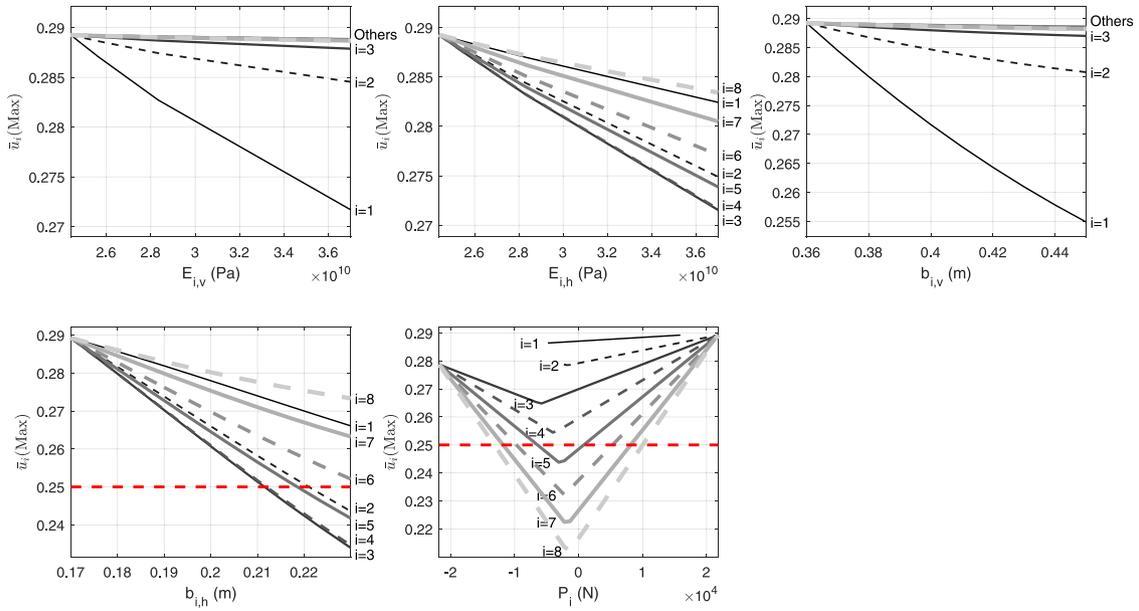


Fig. 9. Maximal response surface for each fixed factor for the structural frame (\bar{u}_i expressed in metres). The horizontal dashed line represents the maximum displacement of u permitted.

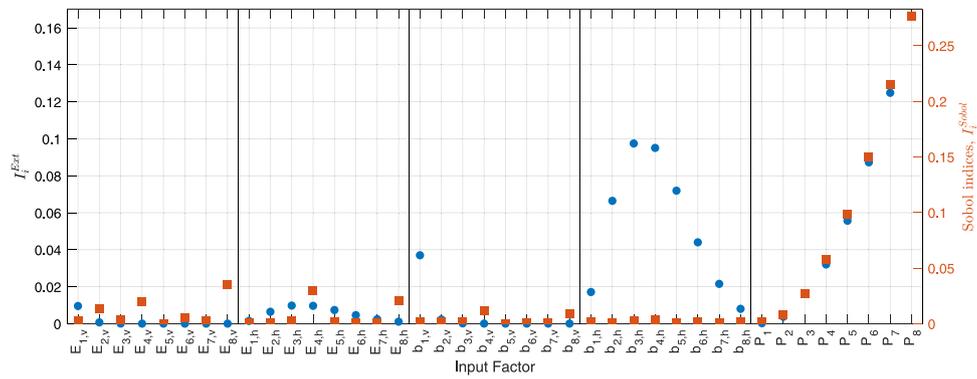


Fig. 10. Importance measure of the input factors; on the left y -axis and associated blue round marker, I_i^{Est} given by Eq. (7), and on the right y -axis and associated red squared marker, Sobol indices, I_i^{Sobol} , given by [8].

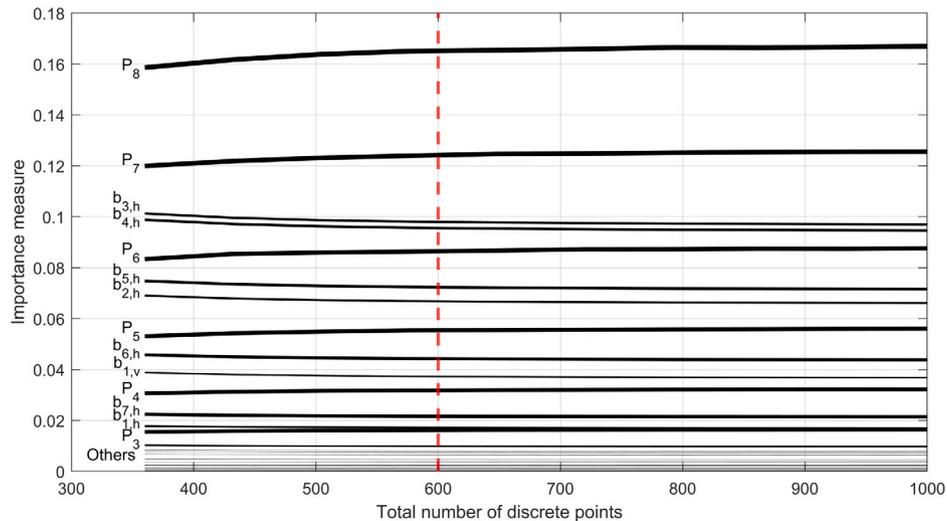


Fig. 11. Importance measure for different degrees of discretization.

6. Further considerations

The robustness of the results has been seen to depend on the discretization strategy. Coarse discretizations of the target factors might hide local optima. Missing some local optima does not impact the final result as much as missing the global optimum. Note that the global optimum is common for all the factors (see Figs. 3, 4, 6 and 9) and relevant to assess factors' importance given that the global optimum is the upper (lower in the case of minimum-related problems) bound of the response surface. To avoid dismissing the global optimum, an initial global optimization including all the factors can be conducted to identify the coordinates of the input factors where the global optimum occurs. Then, the discretization of the input factors should include these coordinates. Besides, searching for the optimum value of the response surface in advance can help to identify the best optimization method and to choose an adequate discretization strategy. Engineers can easily make use of their knowledge of the physical problem in hand to help the search of the optimum values.

The domain of definition of the factors is an important input in the proposed sensitivity method. Very often, not enough attention is paid to the selection of the range of values that the input factors can take, despite its relevance in many SA [6]. Once again, the engineer's expertise is required to choose reasonable values. For instance, in the case of the structural frame, assuming larger values of $b_{i,h}$ would result in a reduction of the importance measure of these factors, given that they would not be so critical in the extreme system response. In the case of extreme-related problems, it is common to find a relationship between the extreme surface response and the extremes of the domain of definition of the input variables. The presented method gives information on which side of the range is of relevance. In the case of the structural frame, the lower bounds of $E_{i,v}$, $E_{i,h}$, $b_{i,v}$ and $b_{i,h}$ result in the minimum structural stiffness. Regarding P_j , the two slopes of the associated curves show that both, the upper and the lower bounds are relevant.

In many cases, the input variability space can be defined by a set of variables that are dependent among them or even can include non-continuous variables. These aspects can be easily introduced in the optimization problem when defining the variables and by adding the corresponding constraints.

7. Conclusions

Sensitivity analyses are used for several reasons, such as identifying the input factors with larger influence on a model output allowing the prioritization of the factors, gaining insights into the model performance and output behaviour (e.g., its consistency), and calibration of the input factors. The selection of the most adequate sensitivity analysis method is not straightforward, as it will depend on the goal of the SA, but also the dimension of the problem on stake, the available information of the input factors, and the difficulty to evaluate the model. In general, the larger the dimension of the engineering problem is, the more complex the required sensitivity approach, implying a deeper analyst's mathematical and computational background. As a consequence, in real practice, many SA are conducted by a 3-step process of (1) dimension reduction, (2) Monte Carlo simulation sampling, and (3) importance ranking by Sobol's indices, given the conceptual simplicity of this approach. Nonetheless, this paper has shown how, for the case of extreme-based engineering problems, this type of approach is not providing meaningful information to the engineer.

This paper has presented a conceptually simple method to conduct SA of extreme-based engineering problems, permitting the visualization and measure of the influence of each input factor on the extreme model response. The method requires to iteratively maximize or minimize the model by fixing one factor at each time. Then, the variation of the optimal surface is evaluated. To maximize (or minimize) the model,

an optimization problem has to be solved for a defined range of the input factors with no other constraints.

The method provides the two ways of approaching a SA; first, sensitivity understood as a measure of how a small change in the input factor affects the output (local approach); this is given by Eq. (6), and depicted in Figs. 6 and 9. Secondly, sensitivity understood as a measure of the total contribution of the input factor to the output (global approach). In this case, this is assessed by importance measure given by Eq. (7).

The proposed method allows practitioners to determine the input factors that trigger the failure of the system, with no need for determining the probability distribution of those input factors. The difficulty of assessing the distributions and the uncertainty of the input factors usually puzzle practitioners [33]. Nonetheless, special attention should be paid to the adequate definition range of the factors involved, along with the possible relationships among them to avoid a non-realistic combination of input factors.

Moreover, given that the required optimization lacks of constraints, commonly used optimization algorithms can deliver the extreme response surface within very reasonable computational times in most of the cases. The advantage of using optimization techniques is the reduction of model evaluations when compared to the approaches based on Monte Carlo simulations. For instance, in the case of gradient-based methods, the search of the optimal value and thus, the model evaluations, are oriented by the gradient of the response surface. In any case, the number of evaluations is usually significantly smaller than a search based on scanning the input space. For very complex problems requiring simulations, simheuristics can provide good results in a very short time [34,35]. In this paper, analysing a 40-dimensional problem has required less than two hours on a regular laptop, which makes the approach very convenient to practitioners.

The method only provides the main effect of the input factors. The joint effect of the input factors has not been addressed in this paper. Further research in this direction will be conducted. Another extension of the method will include the stratification of the domains of definition of the input factors in conjunction with the probability distributions of these factors. In this way, the probability that a given factor reaches the lower or upper bound will be accounted, adding relevant information to the reliability problem.

CRedit authorship contribution statement

M. Nogal: Conceptualization, Methodology, Validation, Writing - review & editing. **A. Nogal:** Methodology, Software, Visualization, Writing - original draft.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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