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A new uncertainty importance measure

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Abstract

Uncertainty in parameters is present in many risk assessment problems and leads to uncertainty in model predictions. In this work, we introduce a global sensitivity indicator which looks at the influence of input uncertainty on the entire output distribution without reference to a specific moment of the output (moment independence) and which can be defined also in the presence of correlations among the parameters. We discuss its mathematical properties and highlight the differences between the present indicator, variance-based uncertainty importance measures and a moment independent sensitivity indicator previously introduced in the literature. Numerical results are discussed with application to the probabilistic risk assessment model on which Iman [A matrix-based approach to uncertainty and sensitivity analysis for fault trees. Risk Anal 1987;7(1):22–33] first introduced uncertainty importance measures.

Keywords: Importance measures; Uncertainty analysis; Global sensitivity analysis; Uncertainty importance measures; Probabilistic risk assessment

1. Introduction

Dealing with uncertainty is one of the challenges of many quantitative risk assessment problems [1]. As Hammit and Shiyakhter [2] underline, it is often "*the lack or sparsity of data*" which prevents the analyst/decision-maker from assigning a certain value to the parameters. Uncertainty in the inputs is reflected in uncertainty in model results and predictions [3].

Saltelli [4] defines sensitivity analysis (SA) as the study of how "*uncertainty in the output of a model* (*numerical or otherwise*) *can be apportioned to different sources of uncertainty in the model input*." With this respect, Saltelli [4] remarks that SA techniques to be utilized in the context of uncertainty analysis should satisfy the following three requirements: "*global*, *quantitative and model free*." By global one means that the technique allows to take into consideration the entire input distribution. By model independent one means that no assumptions on the model functional relationship to its inputs is necessary in order for the SA method to produce accurate results.

Saltelli [4] shows that variance-based methods provide a set of tools that share the three above-mentioned requirements. The works of Saltelli et al. [5], Sobol' [6–8], Rabitz et al. [9], Rabitz and Alis [10] and Alis and Rabitz [11] have established the theoretical and numerical background for the utilization of variance-based techniques. The demonstrated merits of variance-based global SA methods are the consideration of the entire range of variation of the inputs and the ability to identify individual parameter contributions and parameter interactions in a model independent fashion. Since Sobol' decomposition method rests on the assumption of independent inputs, a limitation of a technical nature appears when one performs variance decomposition in the presence of input correlations. More precisely, Bedford [12] proves that "*the values taken on by the indices depend on the ordering of the variables*." The problem has been later tackled by Tarantola [13], Ratto et al. [14] and Saltelli and Tarantola [15], who thoroughly discuss the use of variance-based uncertainty importance measures in the presence of correlations among the parameters.

However, it has been recognized that the interpretation of global SA based on the sole variance as a way of indicating how "*the total uncertainty in model prediction is apportioned to uncertainty in the model input parameters*

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[16]" or "*the expected percentage reduction in the uncertainty …that is attributable to each of the input variables* [17]" is not entirely satisfactory. In fact, Saltelli [4] underlines that variance-based methods "*implicitly assume that this moment* (variance) *is sufficient to describe output variability.*" Indeed, a decision-maker/analyst state of knowledge on a parameter or on a model output is represented by the entire uncertainty distribution [18]. With this respect, Helton and Davis [19, Section 2, p. 25] underline that any moment of a random variable "*provides a summary*" of its distribution with the inevitable "*loss of resolution*" that occurs when the information contained in the distribution is mapped into a single number. Thus, if an analyst aims at assessing which parameter influences the decision-maker state of knowledge the most, a sensitivity indicator should refer to the entire output distribution and not to one of its moments. With this respect, inspection of the whole decision-maker uncertainty requires to add a fourth feature to Saltelli's three requirements, namely, moment independence.

In this work, we analyze how these issues can be addressed. To do so, we propose a global SA indicator (called δ) that considers the entire distribution both of the input and of the output (global) in a moment independent fashion (Fig. 1). We define δ so that its computation is well posed in the presence of correlations among the parameters. We derive analytically the main mathematical properties of δ, showing that the importance of a parameter equals zero when the output is independent of the parameter and that δ equals unity when the set of all inputs is considered. We propose an algorithm for its computation and analyze the numerical procedure.

We then compare δ to both variance-based indicators and to the moment independent sensitivity indicator introduced by Chun et al. [20]. With this respect, we show that the main difference between δ and the Chun–Han–Tak (CHT) importance measure is that CHT requires to hypothesize a "*sensitivity case* [20, p. 314]," while δ does not. Thus, CHT is investigating which of the parameters influence output uncertainty the most given the hypothesized change, while δ does not require to pre-suppose a sensitivity case.

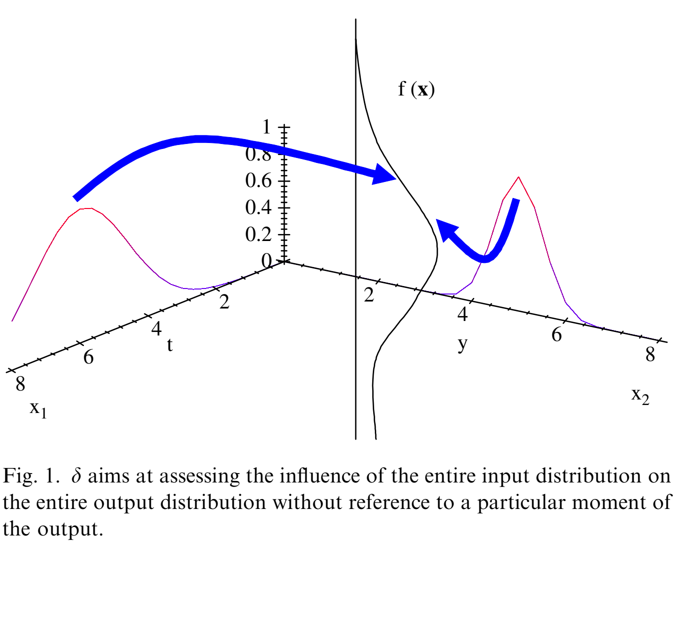

Fig. 1. δ aims at assessing the influence of the entire input distribution on the entire output distribution without reference to a particular moment of the output.

The application to the Ishigami test function [21,16] details the comparison of the ranking obtained with δ to the ranking obtained with the importance indicators of Iman–Hora [22], the global sensitivity indices [23] and CHT [20].

We then discuss the application of δ to the uncertainty and global SA of a probabilistic safety assessment model first introduced in [24] and next utilized as a test case in several works [20]. In this analysis, we also focus on the importance of parameter groups and interactions, which shall enable us to further highlight the difference between δ and variance-based approaches.

Results of both applications show that variance-based global SA indicators and δ agree in identifying the less relevant parameters with respect to (w.r.t.) the output uncertainty. However, differences in the ranking of the most relevant parameters emerge, due to the different scope of the indicators.

In Section 2, we present an overview of global SA as used in risk analysis, starting with variance-based techniques and ending with a moment independent SA indicator introduced in [20]. Section 3 proposes a new moment independent importance measure and discusses its mathematical properties. In Section 4, the application to the Ishigami test function is discussed with the purpose of illustrating the properties of the new indicator and comparing results with those of the other uncertainty importance measures presented in Section 2. In Section 5 the application to the uncertainty analysis of the probabilistic risk assessment model on which uncertainty importance measures were first introduced by Iman [24] is detailed. Section 6 deals with computational aspects and presents perspectives of future research. Section 7 offers conclusions.

2. Global sensitivity analysis

Global SA is the term utilized to denote the set of techniques aimed at determining which of the input parameters influence output the most when uncertainty in the parameters is propagated through the model [22,24–28,19]. In the family of global SA indicators one can include non-parametric techniques [29,30,19], variance-based techniques [31,24,6–11,32,5], and moment independent techniques [33,20]. Indicators created for global SA purposes are called global importance measures [16] or uncertainty importance measures [34,22,16,20] to differentiate them from local importance indicators [35–37], and screening methods [38,39].

With reference to Saltelli's requirements, several authors have underlined that non-parametric methods often lack model independence. For example, regression-based methods are appropriate when a linear input–output relationship exists (Frey and Patil [40] discuss limitations). Saltelli and Marivoet [29] and Hora and Helton [41] underline the fact that ranking provided for by the Spearman rank correlation coefficient would be significant if a monotone input/output relationship were to hold. To overcome this limitation, a test for non-monotone relationship is introduced in [41].

As an alternative way of measuring uncertainty importance, after the early works of Nakashima and Yamato [21] and Bier [34], particular attention is deserved by the Iman and Hora indicator [31,24,22], defined as follows:

$$\mathrm{IH}_i = V[Y] - E\{V[Y|X_i]\} = V\{E[Y|X_i]\}, \tag{1}$$

where $V[Y]$ is the variance of the model output Y, and $E\{V[Y|X_i]\}$ is the conditional expected value of $V[Y]$ given X_i and the expectation is taken over the possible values of X_i, weighted by the appropriate density. It can be proven that the Iman–Hora uncertainty importance measure (IH_i from now on) is the expected reduction in output variance that can be achieved if uncertainty in X_i is eliminated [4,5].

As Saltelli et al. [5] underline, robustness problems connected with IH_i have been solved through the global importance measures introduced in the works of Sobol' [6] and further developed by Homma and Saltelli [16], Sobol' [7,8], Rabitz and Alis [10] and Alis and Rabitz [11]. In these works it is shown that, letting $\underline{X} \in [0,1]^n$ be a set of random independent variables uniformly distributed in the unitary hypercube, and

$$Y = g(\underline{X}) \tag{2}$$

a square-integrable function, then $g(\underline{X})$ can be uniquely decomposed as follows:

$$g(\underline{X}) - g_0 = \sum_{i=1}^{n} g_i(X_i) + \sum_{i<j} g_{i,j}(X_i, X_j) + \cdots + g_{1,2,\ldots,n}(X_1, X_2, \ldots, X_n) \tag{3}$$

and the variance of Y can be decomposed in the following sum:

$$V[Y] = \sum_{i=1}^{n} V_i + \sum_{i<j} V_{i,j} + \sum_{i<j<m} V_{i,j,m} \ldots + V_{1,2,\ldots,n}, \tag{4}$$

where

$$\begin{cases} V_i = \int \cdots \int [g_i(\underline{X})]^2 \, \mathrm{d}X_i, \\ V_{i,j} = \int \cdots \int [g_{i,j}(X_i, X_j)]^2 \, \mathrm{d}X_i \, \mathrm{d}X_j, \\ \ldots \\ V_{i,j,\ldots,m} = \int \cdots \int [g_{i,j,\ldots,m}(X_i, X_j, \ldots, X_m)]^2 \prod_{k=i,j,\ldots,m} \mathrm{d}X_k. \end{cases} \tag{5}$$

Each of the integrands $g_{i,j,\ldots,m}(X_i, X_j, \ldots, X_m)$ in Eq. (5) is found by iterative expectations on Y [6,12]. Eqs. (3) and (4) imply that, in the absence of input correlations, variance decomposition directly mirrors the model structure, evidencing the presence of interactions and the contribution to the model output due to individual and parameter groups.

It turns out that the first order terms, V_i, are the "*expected amount of variance reduction that would be achieved for Y, if we were able to specify X_i exactly* [12,5]" and, therefore, coincide with the IH_i indicator (Eq. (1)).

Sobol' [6] introduced the "*sensitivity estimates*" of order r:

$$S_{i_1,i_2,\ldots,i_r} \equiv \frac{V_{i_1,i_2,\ldots,i_r}}{V[Y]}. \tag{6}$$

$S_{i_1,i_2,\ldots,i_r}$ are the ratios of the interaction terms of order r, $V_{i_1,i_2,\ldots,i_r}$ in Eq. (4), and $V[Y]$. Homma and Saltelli [23] introduced the concept of global sensitivity indices. Particular interest is deserved by the interpretation of the first order ($S1_i$) and total order sensitivity indices (ST_i)—or "*total effects*" in [4]. The first order indices

$$S1_i \equiv \frac{V_i}{V[Y]} \tag{7}$$

represent the expected percentage reduction in $V[Y]$ which is obtained when uncertainty in X_i is eliminated [4]. Note that if one selects $S1_i$ as uncertainty importance measure of X_i, one would obtain the same ranking as with IH_i.

The total effects

$$\mathrm{ST}_i \equiv \sum_{r=1}^{n} \sum_{l_1,\ldots,l_r} S_{l_1,\ldots,l_r} \; (l_1 = i) \tag{8}$$

represent the expected percentage of variance that remains if all parameters were known but X_i [4]. Selecting ST_i as uncertainty importance measure one would be measuring the importance of a parameter as the percentage of the output variance associated with the parameter [16,23,32,5].

Several studies have been performed on the computation of the global sensitivity indices: estimation procedures are the Extended FAST [32], the method of Sobol' [7], and others (see [16,23,11]).

We note that Sobol' theorem holds under the assumption that inputs are independent. Oakley and O'Hagan [42] evidence that in the case of uncorrelated inputs "*the representation* (i.e. Sobol' decomposition) *reflects the structure of the model itself*," while it does not reflect the model structure when correlations emerge. In the case of dependent inputs, Bedford [12] shows that the function decomposition is no more unique, and "*the values taken on by the indices depend on the ordering of the variables*." This problem has then been addressed by Saltelli and Tarantola [15], which have identified two lottery settings for SA in the presence and absence of correlations. The first setting consists in identifying the factor that, if determined, would lead to the greatest reduction in the variance of Y. The idea is that, by fixing $X_i = x_i^*$, one would obtain a new output distribution, namely $f_{Y|X_i}(y)$, that would produce a new output variance (Fig. 2):

$$V[Y|X_i = x_i^*]. \tag{9}$$

However, (see [15]), since X_i is a random variable, $V[Y|X_i = x_i^*]$ is in its turn a random variable. Then

$$E_{X_i}\{V[Y|X_i]\} \tag{10}$$

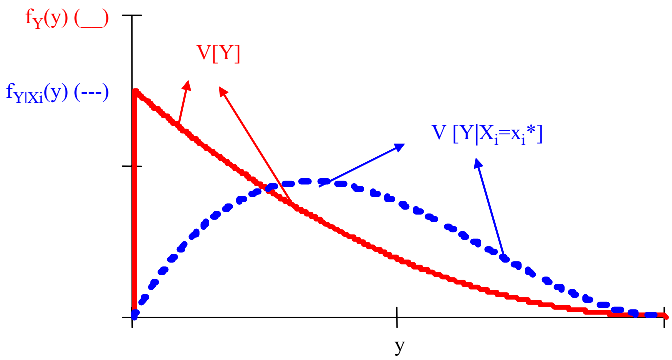

Fig. 2. Unconditional ($V[Y]$) and conditional variance ($V[Y|X_i = x_i^*]$) of Y when X_i is fixed at x_i^*.

is the expected remaining variance if one came to know X_i exactly. Utilizing Eq. (1), one notes that the factor associated with the lowest $E_{X_i}\{V[Y|X_i]\}$ are the more effective in reducing output variance [5].

The second lottery setting of Saltelli and Tarantola [15] parallels the first, and consists in betting on the sets of factors that lead to

$$V[Y] < V_{\text{tar}}, \tag{11}$$

where V_{tar} is a target variance. In this case, the terms $V[Y|X_i, X_j, \ldots, X_m]$ matter, and by extension of Eq. (1), the sensitivity measures become

$$V_{i,j,\ldots,m} = V[E(Y|X_i, X_j, \ldots, X_m)]. \tag{12}$$

We note that, based on classical utility theory, variance is not sufficient to the determination of the decision-maker state of knowledge in general. According to the theory, variance is sufficient to describe uncertainty in the following two cases: (a) the decision-maker possesses a quadratic utility function; (b) the random variable is normally distributed [43, Chapter 3, pp. 61–62]. Hence, identifying which of the parameters reduces variance the most is not equivalent to identify which parameters influence the decision-maker state of knowledge of the output the most, since $V[Y]$ is just one of the moments of the output distribution.

Following this line of thought, Chun et al. [20] introduced a global sensitivity indicator which is moment independent and looks at the entire distribution of the model output. The definition of the CHT indicator is as follows:

$$\text{CHT}_i = \left[\int (y_\alpha^i - y_\alpha^0)^2 \, \mathrm{d}\alpha\right]^{1/2} \Big/ E[Y^0], \tag{13}$$

where y_α^i is the αth quantile of Y for the sensitivity case, and y_α^0 is the αth quantile of Y for the base case. CHT_i is expressed in terms of the cumulative distribution function of Y (F_Y), and, intuitively speaking, represents the (square of the) area related to a shift in F_Y from the base case to the sensitivity case. By sensitivity case it is meant a recomputation of the model when: "(1) *the uncertainty in a parameter is completely eliminated*; (2) *the uncertainty range is changed*; *and* (3) *the type of distribution is changed*" [20]. All three cases reflect a change in the state of knowledge of the analyst regarding the input parameters.

It is useful to remark two main differences in the definitions of CHT_i on the one side and ST_i/IH_i on the other side:

- CHT_i requires the performance of a sensitivity case, while ST_i and IH_i do not;
- ST_i and IH_i refer to a particular moment of the distribution of Y, namely, $V[Y]$, while CHT_i does not.

In other words, the question answered by CHT_i concerns the parameter that provokes the greatest change in the distribution of Y when, for example, the uncertainty in all the parameters is reduced by, say, a factor of 10 [20]. ST_i and IH_i measure the relevance of the parameter contribution to $V[Y]$ given the current state of knowledge, i.e. without requiring to specify a sensitivity case that reflects an hypothetical decision-maker state of knowledge change.

In the next section, we introduce a global sensitivity indicator, which is independent of the moments of the model output and independent of the sensitivity case.

3. A moment independent importance measure

In this section, we present an uncertainty importance measure with the following characteristics: it does not refer to a particular moment of Y—and with this respect is similar to CHT_i but different from ST_i—and does not require a "sensitivity case"—with this respect it is similar to ST_i but different from CHT_i. We also try and define the new indicator in such a way that its definition is properly posed in the presence of correlations among the parameters.

We start with the relevant notation. Let

1. $$\underline{X} = (X_1, X_2, \ldots, X_n) \in R^n \tag{14}$$
   be the set of uncertain input parameters;
2. $$Y = g(\underline{X}), g(\underline{X}) : E \subseteq \mathbb{R}^n \longrightarrow \mathbb{R} \tag{15}$$
   be the functional relationship between output Y and input $\underline{X}$;
3. $\underline{x} = (x_1, x_2, \ldots, x_n)$ a realization of $\underline{X}$;
4. $F_{\underline{X}}(\underline{x})$ the (subjective) cumulative distribution of $\underline{X}$, i.e. the joint cumulative distribution of the X_i. $F_{\underline{X}}(\underline{x})$ expresses the analyst state of knowledge on $\underline{X}$;
5. $f_{\underline{X}}(\underline{x})$ the corresponding joint density of $\underline{X}$;

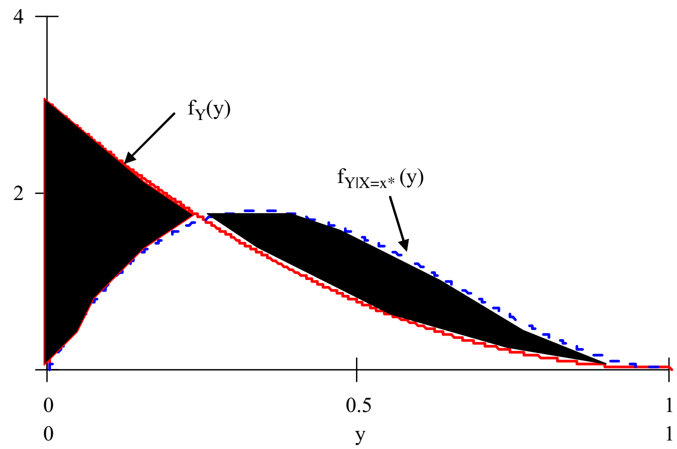

Fig. 3. $f_Y(y)$ (continuous) and $f_{Y|X_j=x_j^*}(y)$ (dashed). The shift between the two densities is measured by the shaded regions.

6. $f_{X_i}(x_i)$ the marginal density of x_i. As it is well known it is related to the joint density by

$$f_{X_i}(x_i) = \int \dots \int f_{\underline{X}}(\underline{x}) \prod_{s \neq i} \mathrm{d}x_s; \tag{16}$$

7. $F_Y(y)$ the cumulative distribution function of the model output Y;
8. $f_Y(y)$ the corresponding density;
9. $f_{Y|X_i}(y)$ the conditional density of Y given that one of the parameters, X_i, assumes a fixed value.

The rationale behind the definition of the following moment independent importance indicator is as follows. The unconditional density/cumulative distribution of Y obtained with all parameters free to vary in their uncertainty range are $f_Y(y)/F_Y(y)$ (the continuous line in Fig. 3 shows an example of density $f_Y(y)$). Suppose now that we are able to fix one of the inputs at, say, x_i^*. We would obtain the conditional density/distribution of Y given that X_i is fixed at x_i^*, namely $f_{Y|X_i}(y)/F_{Y|X_i}(y)$ (dashed line in Fig. 3).

The shift between $f_Y(y)$ and $f_{Y|X_i}(y)$ can be measured by the total area evidenced in Fig. 3. Such an area is given by

$$s(X_i) = \int |f_Y(y) - f_{Y|X_i}(y)|\, \mathrm{d}y. \tag{17}$$

Eq. (17) shows that $s(X_i)$ is dependent on X_i, and as such, it is a function of random variable. The expected shift is given by

$$E_{X_i}[s(X_i)] = \int f_{X_i}(x_i) \left[\int |f_Y(y) - f_{Y|X_i}(y)|\, \mathrm{d}y \right] \mathrm{d}x_i. \tag{18}$$

We then propose the following definition.

Definition 1. We name the quantity

$$\delta_i = \frac{1}{2} E_{X_i}[s(X_i)] \tag{19}$$

moment independent sensitivity indicator of parameter X_i w.r.t. output Y.[1] δ_i represents the normalized expected shift in the distribution of Y provoked by X_i.

We now discuss some of the properties of δ_i (Table 1). Property no. 1 in Table 1 bounds the possible values that the δ_i of an individual parameter can assume: it can be proven that δ_i lies between 0 and 1 (the proof is in Section A.1 in the Appendix). In particular, one finds that δ_i is zero when Y is independent of X_i (Property 2 in Table 1). In fact, if Y is independent of X_i, one would not get any change in $f_Y(y)$ for any value x_i assumed by X_i. Thus, $f_{Y|X_i}(y) = f_Y(y)$ and the integrand in Eq. (18) is null for all x_i.

Property no. 3 suggests that δ of all parameters equals unity. To prove the property, however, we need to extend the definition of δ from an individual parameter to a group of parameters. This is done as follows.

Definition 2. Let $\underline{R} = (X_{i_1}, X_{i_2}, \dots, X_{i_r})$ be any group of parameters. Then

$$\delta_{i_1,i_2,\dots,i_r} = \tfrac{1}{2} E_{\underline{R}}[s(\underline{R})] = \int f_{X_{i_1},X_{i_2},\dots,X_{i_r}}(x_{i_1}, x_{i_2}, \dots, x_{i_r}) \times \left[\int |f_Y(y) - f_{Y|X_{i_1},X_{i_2},\dots,X_{i_r}}(y)|\, \mathrm{d}y \right] \mathrm{d}x_{i_1}\, \mathrm{d}x_{i_2} \dots \mathrm{d}x_{i_r}, \tag{21}$$

where

$$f_{X_{i_1},X_{i_2},\dots,X_{i_r}}(x_{i_1}, x_{i_2}, \dots, x_{i_r}) = \int \dots \int f_{\underline{X}}(\underline{x}) \prod_{k \neq i_1, i_2, \dots, i_r} \mathrm{d}x_k. \tag{22}$$

The above definition then enables to prove Property 3 in Table 1 which states that

$$\delta_{1,2,\dots,n} = 1, \tag{23}$$

i.e. the joint importance of all parameters equals unity (for the proof, see Section A.2 in the Appendix).

One can summarize these three properties as follows. The δ of an individual parameter or of a group can assume values between 0 and 1. It will equal 0 when Y is independent of the parameter or group of parameters at hand. It will equal 1 when the group including all inputs is considered.

A couple of remarks. As far as correlations are concerned, we observe that Definitions 1 and 2 hold independently of whether the parameters are correlated. In fact, Eqs. (19) and (21) require the specification of the joint density, $f_{\underline{X}}(\underline{x})$, without reference to the eventual independence of the parameters.

[1] A more technical definition of δ_i is as follows:

$$\delta_i = \frac{1}{2} E_{X_i} \left[\int |\mathrm{d}\mu_Y - \mathrm{d}\mu_{Y|X_i}| \right], \tag{20}$$

where μ_Y and $\mu_{Y|X_i}$ are, respectively, the unconditional and conditional measures of Y.

Table 1
Properties of the uncertainty importance measure introduced in this work

No.	Property	Meaning	Proof
1	$0 \leqslant \delta_i \leqslant 1$	Bounds the possible values δ_i can assume	Section A.1
2	$\delta_i = 0$	If Y is independent of X_i then $\delta = 0$	Main body
3	$\delta_{1,2,\ldots,n} = 1$	The importance of all parameters equals unity	Section A.2
4	$\delta_{ij} = \delta_i$	If Y is dependent on X_i but independent of X_j then $\delta_{ij} = \delta_i$	Footnote
5	$\delta_i \leqslant \delta_{ij} \leqslant \delta_i + \delta_{j\mid i}$	Bounds the possible values δ_{ij} can assume	Section A.3

Let us now study the interpretation of Definitions 1 and 2 in terms of SA settings. One can see that Definition 1 resembles Setting 1 of [15] with a main similarity and a main difference. The similarity is that both settings involve conditioning w.r.t. $X_i = x_i^*$. The difference lies in the fact that Setting 1 of [15] looks for the parameters that achieve the greatest reduction in the variance of Y, while the setting implied by Definition 1 is the identification of the parameters that influence the entire distribution the most. Similarly, Definition 2 parallels Setting 2 of [15] in so far groups are concerned. However, we note that Setting 2 of [15] again refers to variance reduction, while Definition 2 concerns influence w.r.t. the entire distribution.

We now discuss the computation of δ for a simple example, with the purpose of illustrating its definition.

Example 1. Suppose that the unconditional density of $Y = g(\underline{X})$ is

$$f_Y(y) = Beta(y; 1, 3). \tag{24}$$

Suppose further that one of the parameters, X_i is a discrete random variable than can assume four values, namely, x_i^1, x_i^2, x_i^3, x_i^4 with $P(X_i = x_i^m) = \frac{1}{4}\,(m = 1, \ldots, 4)$. Suppose that either analytically or numerically, you are able to obtain the four conditional distributions of Y given that $X_i = x^m$ and that they are as follows:

$$f_{Y|X_i=x_i^m}(y) = \begin{cases} f_{Y|X_i=x_i^1}(y) = Beta(y; 2, 3), \\ f_{Y|X_i=x_i^2}(y) = Beta(y; 5, 3), \\ f_{Y|X_i=x_i^3}(y) = Beta(y; 7, 3), \\ f_{Y|X_i=x_i^4}(y) = Beta(y; 9, 3). \end{cases} \tag{25}$$

Fig. 4 shows the unconditional and conditional distributions named above.

Let us compute δ_i. For each of the conditional distributions we have (Eq. (17))

$$s(x_i^m) = \int |f_Y(y) - f_{Y|X_i=x_i^m}(y)|\,\mathrm{d}y, \quad m = 1, \ldots, 4. \tag{26}$$

For $X_i = x_i^1$, we have

$$s(x_i^1) = \int_0^1 |\beta(y, 1, 3) - \beta(y, 2, 3)|\,\mathrm{d}y = 0.6. \tag{27}$$

$s(x_i^2)$, $s(x_i^3)$, $s(x_i^4)$ are computed in a similar fashion (Fig. 4). The resulting value of δ_i is found as $\delta_i = \frac{1}{2}\left[\frac{1}{4}s(x_i^1) + \frac{1}{4}s(x_i^2) + \frac{1}{4}s(x_i^3) + \frac{1}{4}s(x_i^4)\right] = 0.75$.

Definitions 1, 2 and the example can be utilized to indicate a possible algorithm for the numerical computation of δ_i. Preliminary step is an uncertainty propagation leading to the determination of the unconditional density of Y; second step is the sampling of a value of x_i from $f_{X_i}(x_i)$; third step is the sampling of the conditional distribution of Y given X_i, i.e. $f_{Y|X_i}(y)$; fourth step is the computation of $s(X_i)$; fifth step the estimation of δ_i from the computed $s(x_i)$'s.

In the remainder of this section, we detail some observation on properties of the importance of parameter groups ($\delta_{\underline{R}}$, Definition 2). To do so, we begin with groups of two parameters, $\underline{R} = (X_i, X_j)$.

According to Definition 2, the delta of X_i and X_j is given by

$$\delta_{ij} = \frac{1}{2} E_{X_i X_j}[s(X_i, X_j)], \tag{28}$$

where

$$s(X_i, X_j) = \int |f_Y(y) - f_{Y|X_i X_j}(y)|\,\mathrm{d}y \tag{29}$$

is the shift obtained fixing X_i at x_i and X_j at x_j. Based on the above discussion, it is immediate to observe that, if Y is independent of X_j, then (Property 4, Table 1)

$$\delta_{ij} = \delta_i. \tag{30}$$

Eq. (30) simply re-states the fact that no contribution to model uncertainty comes from X_j if Y does not depend upon it.[2]

However, if there is a contribution to uncertainty coming from X_j, one would expect δ_{ij} to increase. Indeed, let us think of $s(X_i, X_j)$ as obtained in two steps. The first step is given by fixing X_i at x_i and the second step is obtained by then fixing of X_j at x_j (Fig. 5). We limit ourselves to an intuitive explanation; a formal treatment is offered in Section A.3. Note that from a mathematical viewpoint δ shares the properties of a distance (see [44] for definition of distance). Hence, δ_i represents the expected distance between the density of Y and the conditional density of Y given X_i. Similarly, δ_{ij} is the distance between the density of Y and the conditional density of Y given X_i and X_j.

[2] In fact, if Y is independent of X_j, then $|f_Y(y) - f_{Y|X_i X_j}(y)| = |f_Y(y) - f_{Y|X_i}(y)|$ that leads to Eq. (30) by definition of δ.

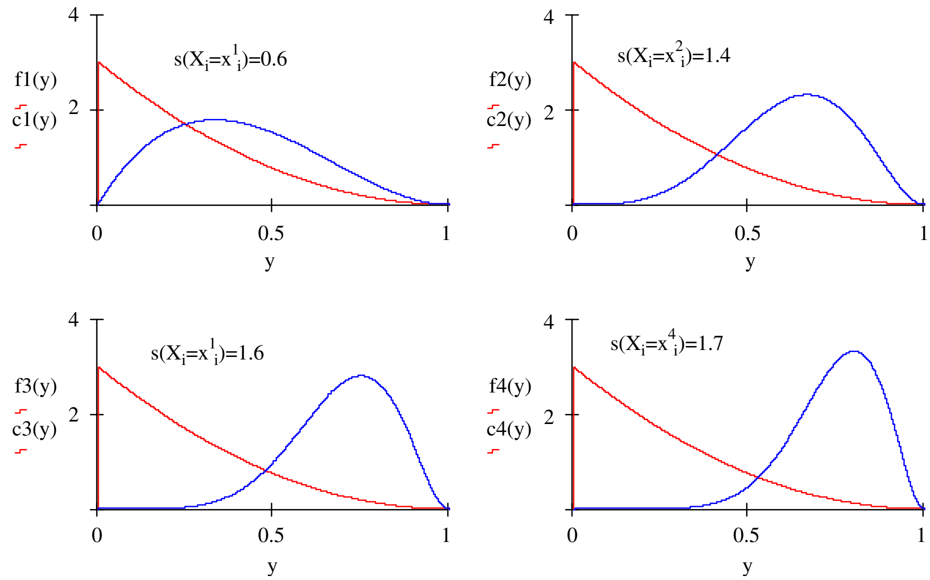

Fig. 4. $f_Y(y), f_{Y|X_i=x_i^*}(y)$ and $s(x_i)$ for the example.

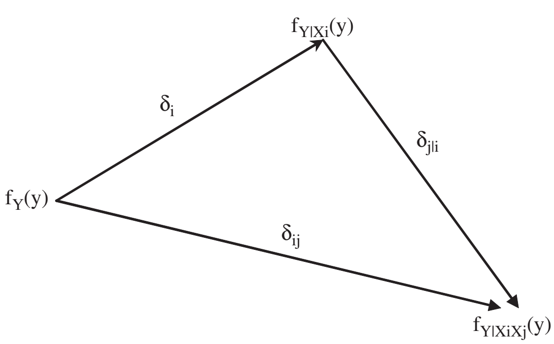

Fig. 5. Geometric interpretation of Property no. 5.

Now, geometrically, going from $f_Y(y)$ to $f_{Y|X_iX_j}(y)$ through $f_{Y|X_i}(y)$ is the same as moving from point A to point C but first going through point B. The length of path AB–BC is greater then the length of AC, unless the three points lie on the same line.

With this in mind, one can write

$$f_Y(y) - f_{Y|X_iX_j}(y) = [f_Y(y) - f_{Y|X_i}(y)] + [f_{Y|X_i}(y) - f_{Y|X_iX_j}(y)] \tag{31}$$

and interpret $[f_Y(y) - f_{Y|X_i}(y)]$ (first difference in the right-hand side of Eq. (31)) as the difference between the unconditional density of Y and the conditional density found fixing X_i and $f_{Y|X_i}(y) - f_{Y|X_iX_j}(y)$ as the residual difference between $f_{Y|X_i}(y)$ and $f_{Y|X_iX_j}(y)$ obtained fixing X_j after X_i has been fixed. Now, defining the conditional δ for the second step as

$$\delta_{j|i} = \frac{1}{2}E_{X_iX_j}\left[\int |f_{Y|X_i}(y) - f_{Y|X_iX_j}(y)|\,\mathrm{d}y\right]. \tag{32}$$

Noting $\delta_{j|i} \geqslant 0$ and that $\delta_{j|i} = 0$, if Y is independent of X_j, it is possible to see that (Appendix, Section A.3):

$$\delta_i \leqslant \delta_{ij} \leqslant \delta_i + \delta_{j|i}, \tag{33}$$

which states that the joint importance of X_i and X_j is greater than the individual importance of X_i, but limited by the importance of the residual term $\delta_{j|i}$.

Suppose now that the observed shift in uncertainty due to X_j is always independent of the value assumed by X_i. In that case, one would expect $\delta_{j|i} = \delta_j$. If it happens that

$$\delta_{ij} = \delta_j + \delta_i, \tag{34}$$

i.e. the three points lie on the same line, we say that the effects of the uncertainty in X_i and X_j on $f_Y(y)$ are separable.

The next section describes the application of δ to the global SA of the Ishigami test function, highlights the computational aspects in greater detail and illustrates a first comparison of δ with the previously introduced importance measures listed in Section 2.

4. A test function analysis

This section describes the numerical computation of δ and the comparison with variance-based techniques and the CHT indicator by studying the application of δ to the Ishigami test function [20]. The mathematical expression of the function is

$$Y = g(\underline{X}) = \sin X_1 + a\sin^2 X_2 + bX_3^4 \sin X_1 \tag{35}$$

and the X_i are assumed independent and uniformly distributed between $-\pi$ and π. The input distributions, the sample size ($N = 1000$) and the values of the constants a and b (5 and 0.1, respectively) are the same as in [20] to allow for a direct comparison.

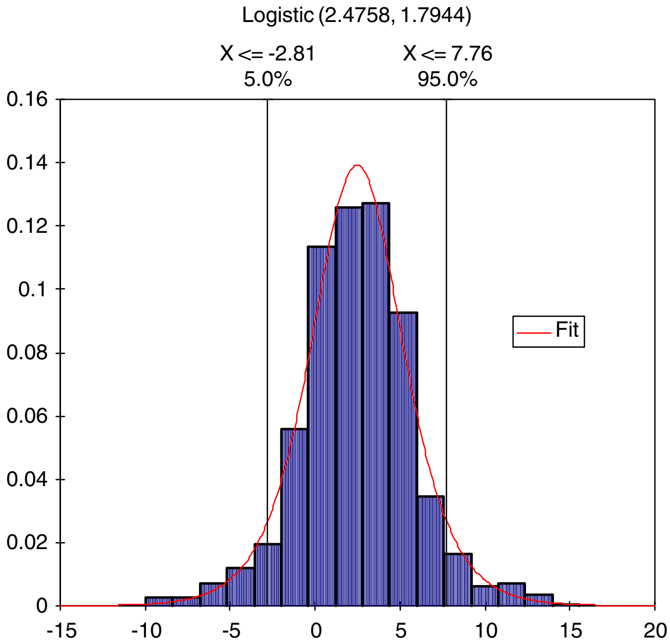

Fig. 6. The uncertainty propagation in the example results in a logistic distribution for $f_Y(y)$.

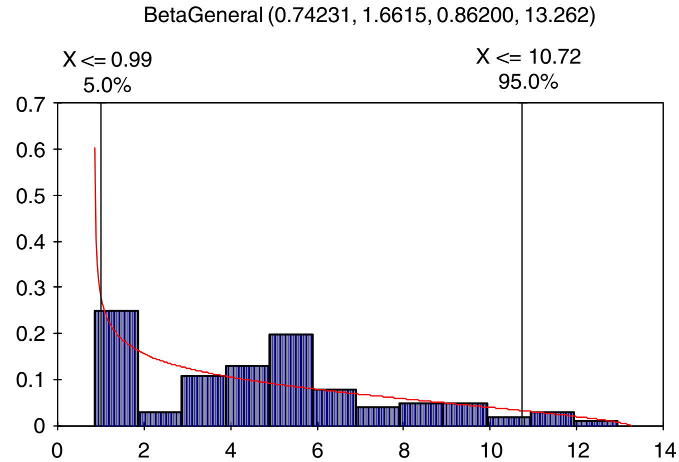

Fig. 7. Conditional density given $X_1 = 1.0219$, $f_{Y|X_1=1.029}(y)$.

Table 2
Parameter global importance measured with delta

Parameter	δ_i	$S1_i$	ST_i	CHT_i
X_1	0.33	0.39	0.62	0.66
X_2	0.39	0.29	0.34	0.98
X_3	0.28	0.02	0.28	0.67

Let us first discuss the uncertainty analysis of Y. Uncertainty propagation (Fig. 6) produces $f_Y(y)$ best fitted by a logistic density, with a Kolmogorov–Smirnov statistics equal to 0.02.

We now describe the computation of $\delta(X_1)$. One first generates a value for X_1, namely x_1^1 sampling from $f_{X_1}(x_1)$. In our first generation, we get $x_1^1 = 1.029$. Given this value, the conditional density of Y is obtained by propagating uncertainty in the model keeping $X_1 = x_1^1$. The resulting density, $f_{Y|X_1=x_1^1}(y)$, is shown in Fig. 7.

$f_{Y|X_1=1.029}(y)$ is now fitted by a beta distribution (the parameters are illustrated in Fig. 7) with a Kolmogorov–Smirnov statistics of 0.07. $s(x_1^1)$ is, then, computed from a simple numerical integration of the absolute value of the difference between the unconditional (Fig. 6) and the conditional density (Fig. 7). In this case, it turns out that $s(x_1^1) = 0.638$. The next step is to repeat the procedure to produce x_1^2 (equal to 2.84 in our second run), determine the new conditional density of Y and compute $s(x_1^2)$, which, in this case, turns out to be equal to 0.58. Repeating this steps for a 1000 times, δ_i is then estimated to be $\delta_i = 0.33$.

Proceeding in a similar fashion for X_2 and X_3, the moment independent indicators for X_2 and X_3 are computed. The results are reported in Table 2.

Table 2 shows that X_2 is the most influential parameter, followed by X_1 and X_3. As far as interactions are concerned, one can observe also that $\delta_1 + \delta_2 + \delta_3 \cong 1$, in this case. Recalling Property 3 in Table 1, then it holds that $\delta_{123} = \delta_1 + \delta_2 + \delta_3$, i.e., using the terminology introduced in Section 3, Eq. (34), the effects of uncertainty in the parameters on the uncertainty in Y are separable—for this model and for the given input distributions.

We now discuss the comparison of the above results to the ones obtained for the CHT_i indicator and for variance-based techniques, $S1_i$ and ST_i (Table 2).

The fourth column of Table 2 shows the total sensitivity indices of the three parameters estimated with the Sobol' method, utilizing the software SIMLAB [45]. The third column shows the result for the $S1_i$ indicator (Eq. (1)) and the fifth column for the CHT indicator (Eq. (13)), as reported in [20].[3] We note that ST_i and $S1_i$ produce the same ranking, while δ_i and CHT_i produce different ranking w.r.t. the other indicators (see also Fig. 8).

The different ranking between $\mathrm{ST}_i/S1_i$ and δ_i/CHT_i is explained by the fact that ST_i and $S1_i$ are variance-based, while δ_i and CHT_i are moment independent. This result confirms that a parameter which influences variance the most is not necessarily the parameter that influences the output distribution the most. The difference between the ranking produced by δ_i and CHT_i can be explained as follows. CHT_i results in Table 2 are the importance of the parameters when uncertainty in each of them, one at a time, is completely eliminated (Table 3). Hence, CHT_i ranks inputs given that an hypothesized change in the state of knowledge of the decision-maker happens. On the other hand, δ_i represents the importance of the entire distribution of X_i w.r.t. the entire distributionof Y, given the current state of knowledge and without considering an artificially hypothesized change.

[3]Note that $\mathrm{IH}_i = S1_i \cdot V[Y]$; hence the ranking obtained with $S1_i$ is the same as the ranking obtained with IH_i. Such ranking is reported in [20].

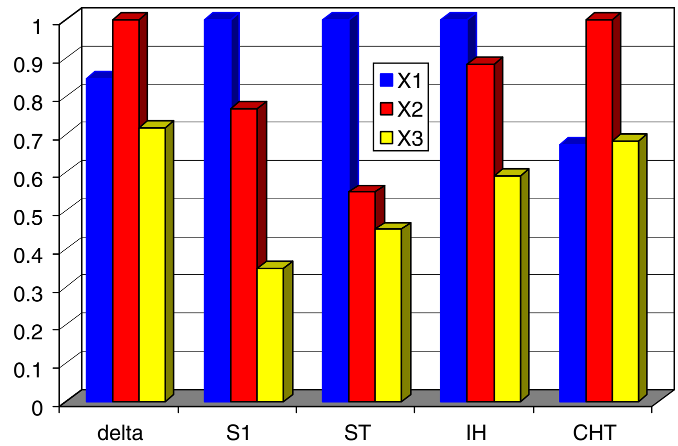

Fig. 8. Parameter ranking comparison.

Table 3
Distributions for the parameters of the PRA model of Iman [24]

Parameter	Distribution	Mean	Error factor
X_1	Lognormal	2	2
X_2	Lognormal	3	2
X_3	Lognormal	1×10^{-3}	2
X_4	Lognormal	2×10^{-3}	2
X_5	Lognormal	4×10^{-3}	2
X_6	Lognormal	5×10^{-3}	2
X_7	Lognormal	3×10^{-3}	2

Finally, given the above discussion, comparing the ranks obtained with the four indicators in Table 2 enables one to conclude that X_2 is the most important parameter when the entire output distribution is considered (it ranks first with both δ and CHT), while X_1 is the most important parameter in explaining the variance of the model output.

5. Application to a probabilistic risk assessment model

The purpose of this section is to illustrate the application of δ to the probabilistic risk assessment (PRA) model utilized in [24] where uncertainty importance measures were first introduced. The model has also been utilized in [20] (see for a comparison of the CHT indicator with the Iman–Hora importance measure). Besides computing the δ for the model parameters, we also estimate the first and total order global sensitivity indices, to highlight the differences between Sobol' interactions and δ-interactions ($\delta_{j|i}$).

The probability of the top event is written as [24]

$$\begin{aligned} Y_{\text{Top}} = {} & X_1X_3X_5 + X_1X_3X_6 + X_1X_4X_5 + X_1X_4X_6 \\ & + X_2X_3X_4 + X_2X_3X_5 + X_2X_4X_5 \\ & + X_2X_5X_6 + X_2X_4X_7 + X_2X_6X_7. \end{aligned} \tag{36}$$

The numerical values of the input distributions utilized in this analysis are the same as the ones used in [20] and are presented in Table 3.

The result of uncertainty propagation with a sample of size $N = 1000$ are displayed in Fig. 9. Fig. 9 shows that $f_{Y_{\text{Top}}}(y)$ is lognormal, with mean equal to $2E-6$ and error factor equal to 2.4.

The calculation of the δ importance measure for the parameters has been performed in accordance with the computation algorithm proposed in Section 3. We have found the results of Table 4.

Table 4 shows that X_6 is the most relevant parameter, followed by X_5, X_2, X_4, X_7, X_1 and X_3. Thus, we can say that X_6 is the most influential parameter on the top event while X_3 is the least influential.

We then compare the above results to the ones obtained by making use of the Sobol' total effects, the CHT_i and $S1_i$ indicators. Table 5 shows the results. The rankings obtained with CHT_i have been computed in [20] and are as such reported in Table 5, while $S1_i$ and ST_i have been computed with the Software SIMLAB [45].

To analyze the agreement among the ranking obtained with the four importance measures, we computed the Savage Score Correlation Coefficients (SSCC) (first introduced in [25]; for an illustration see also [46]) on the ranking in Table 5. The result is reported in Table 6.

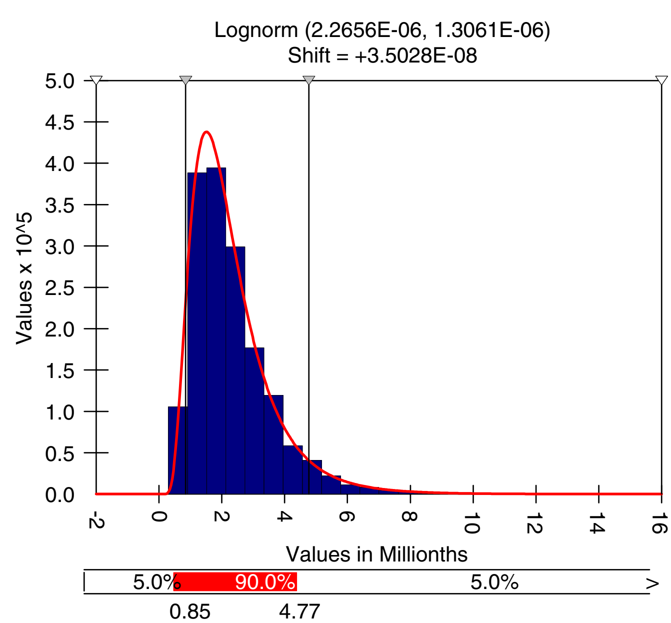

Fig. 9. $f_{Y_{\text{Top}}}(y)$ as a result of uncertainty analysis.

Table 4
Delta for the parameters of the PRA model of Iman [24]

Parameter	X_1	X_2	X_3	X_4	X_5	X_6	X_7
δ_i	0.11	0.17	0.09	0.13	0.18	0.20	0.11

Table 5
Parameter ranking with the four uncertainty importance measures

Parameter	δ_i	$S1_i$	ST_i	CHT_i
X_1	6	6	5	6
X_2	3	1	1	1
X_3	7	7	7	7
X_4	4	4	4	4
X_5	2	2	3	2
X_6	1	3	2	3
X_7	5	5	6	5

Table 6
SSCC matrix for the four importance measures used in Section 5

	δ_i	$S1_i$	ST_i	CHT_i
δ_i	1	0.49	0.59	0.49
ST_i	0.59	0.93	1	0.93
CHT_i	0.49	1	0.93	1
$S1_i$	0.49	1	0.93	1

One notes that the ranking of CHT_i coincides with that of $S1_i$, while it differs from both the δ_i and the ST_i ranking. Table 6 also shows that δ_i results are in a higher agreement with ST_i results then with CHT_i and $S1_i$.

We now turn our attention to a more detailed comparison of the global sensitivity indices and δ. We start with the ranking obtained with ST_i and δ_i. One notes that both indicators agree in the identification of the least relevant parameters: X_3 ranks 7th according to both indicators, X_1 6th, X_7 5th and X_4 4th. Some difference in the agreement is found on the ranking of the most relevant parameters: X_6 ranks first according to δ_i, while it ranks second according to ST_i;X_5 ranks 2nd according to δ_i, while it ranks 3rd according to ST_i;X_2 ranks 3rd according to δ_i, while it ranks 1st according to ST_i. Since the ranking difference ought to be attributed to the different meaning of the importance indicators, the following summary of the result becomes natural: (i)X_3, X_1, X_7 and X_4 are non-relevant on the model uncertainty, both when the entire distribution (δ_i) or its variance (ST_i) are considered; (ii) the most relevant parameter w.r.t. the entire output distribution is X_6, while the most relevant w.r.t. the output variance is X_2.

We then discuss how δ and global sensitivity indices interpret interactions. From Table 4 one notes that $\sum_{i=1}^{7}\delta_i = 0.99$. Recalling that $\delta_{1,2,\ldots,7} = 1$, we have that $\delta_{1,2,\ldots,7} \simeq \sum_{i=1}^{7}\delta_i$, i.e. interactions play a minor role according to δ. Using the terminology introduced in Section 3, we could say that the effect of uncertainty in the X_i on uncertainty in the top event are separable. Let us now examine the relevance of interactions that is revealed by Sobol' variance decomposition. Fig. 10 shows the comparison between the total effects of each of the parameters and the first order indices.

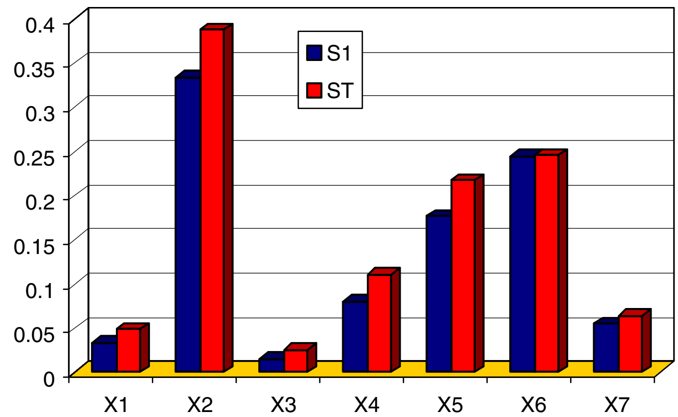

Fig. 10. The comparison of first order ($S1$) and total order (ST) sensitivity indices shows the low relevance of interactions for the model at hand when the error factor equals 2.

From Fig. 10 one notes that the percentage of interaction terms in each of the parameter importance is not as relevant. In fact, $\sum_{i=1}^{7} S1_i = 94\%$, indicating that almost all of the model variance is explained by individual effects. Hence, results of Sobol' indices show that the model responds additively to the input uncertainty. Thus, in this case both separability and additivity play a role. We then performed additional calculations to verify whether the above conclusion on interactions was robust w.r.t. the choice of the input distributions. We increased all error factors in Table 3 from 2 to 6. Results now show that given the new distributions $\sum_{i=1}^{7} S1_i = 57\%$, signaling that a significant portion of the model variance is now explained by interaction terms. On the other hand, $\sum_{i=1}^{7}\delta_i = 86\%$, implying that the output uncertainty is mainly attributable to individual parameter contributions, although it is not completely separable, as in the previous case.

6. Computational aspects: an overview of current methods and opportunity for future research

Although the primary purpose of this work is to introduce the definition, properties and meaning of δ, let us touch upon computational aspects of δ. The computational cost of a technique is defined in terms of number of model runs necessary to estimate the sensitivity measure.

The estimation of δ for the above-mentioned models did not pose any particular numerical issues. However, the cost for estimating δ_i using the algorithm proposed in Section 3 is equal to $nN_{\mathrm{o}}N_{\mathrm{i}}$where n is the number of parameters, N_{o} is the number of runs necessary for the outer integration and N_{i} the number of integrals necessary for the internal integration. Thus for computationally intensive models or models requiring sample sizes of $N > 1000$,[4] the estimation of δ_i can raise the "*curse of dimensionality* [10]" problem

[4]This sample size is also used in [10] as a threshold for numerical complexity.

which affects most of global SA techniques (as an example, see the investigations of Frey and Patil [40] and Patil and Frey [47]). The trade-off between computational complexity and amount of uncertainty information delivered by an SA technique is being and has been extensively dealt with in the literature. For example Rabitz and Alis [10] report that the cost of computing all the sensitivity indices in Sobol' decomposition is equal to $N \times \sum_{i=0}^{n} n!/(n-i)!i!$, which grows exponentially with the number of parameters. After the works of Homma and Saltelli [23], at least three approaches have been envisioned to ease the estimation of the global sensitivity indices: (i) Saltelli et al. [32] proposed the Extended FAST, which enables one to compute the first order and the total order indices at a cost equal to N, with a gain of $\sum_{i=0}^{n} n!/(n-i)!i!$ model runs; (ii) Rabitz and Alis [10] and Alis and Rabitz [11] propose a two step approach based on finite difference decomposition; (iii) Oakley and O'Hagan [42] demonstrate that further savings can be obtained if one adopts a Bayesian approach.

Besides the estimation of variance-based indicators, several authors have dealt with the problem of increasing the efficacy of sampling methods in uncertainty propagation for computationally intensive models. Some examples are: (i) Sobol' quasi-random sequence generator [48] applied by Homma and Saltelli [16] in the computation of the Iman–Hora importance measure of Eq. (1); (ii) Latin Hypercube sampling, first introduced in McKay et al. [49], and thoroughly discussed in [30,19].

Another way of circumventing the curse of dimensionality is to make use of screening methods. Screening methods are SA tools that enable to identify non-relevant parameters and therefore to eliminate from the analysis variables that do not deserve further attention. We refer the reader to the methods of Morris [38] and the ones described in [39].

As far as the estimation of δ is concerned, one can think of utilizing combinations of techniques to reduce either n or N_i/N_o or both. A first way is utilizing the algorithm used in this work together with a sampling method (Latin Hypercube Sampling or Sobol' quasi-random lpτ); this should allow to maintain N_i and N_o at their lowest size. A second way is applying a two-step method a la Alis and Rabitz [11]; this would reduce n. A third way is adopting a Bayesian approach a la Oakley and O'Hagan [42]; this would be effective in reducing $N_i N_o$. A fourth way is utilizing screening methods first to screen out non-relevant inputs and then applying a full-fledged estimation of delta, eventually with an appropriate sampling method: in this case both n and N_i and N_o would be reduced. The refinement of computational strategies for δ shall be the subject of future research by the author.

7. Conclusions

When uncertainty in model parameters is present, the problem of assessing which of the inputs influences output uncertainty the most is properly addressed by global SA.

The most recent literature development has assisted to the refinement and establishment of the theoretical and computational framework of variance-based techniques. We have seen that variance decomposition reflects model structure when the inputs are uncorrelated and provides guidance in data collection when an analyst wants to achieve a pre-determined variance reduction (even when parameters are correlated). However, in terms of uncertainty analysis, a limitation of a variance-based global SA is the fact that variance is just one of the moments of the output distribution and, as such, cannot be elected as representative of the whole decision-maker state of knowledge. In addition, when parameters are correlated, the direct relationship between variance and model structure does not hold.

In this work, we have addressed these issues by introducing a moment independent uncertainty indicator (δ) that looks at the entire input/output distribution and whose definition is well posed also in the presence of correlations among the parameters. We have discussed the mathematical properties of δ. We have seen that it is always between 0 and 1, it equals 0 if the output is not dependent upon an input, it is readily defined for parameter groups and it equals unity if the group of all inputs is considered. We have seen that its definition is well posed in the presence of correlations among the parameters, since one needs to specify a joint distribution of the inputs without requiring independence. We have also shown that the indicator does not pre-suppose a sensitivity case, i.e. a change in the decision-maker uncertainty, but reflects the current analyst/decision-maker state of knowledge.

We have illustrated the numerical aspects of the computation of δ. We have compared its results to those of first and total order sensitivity indices, the Chun–Han–Tak and the Iman–Hora indicators by studying the application of these techniques to the Ishigami test function.

We have then discussed the application of the above techniques to the PRA model analyzed in [20] and introduced in [24].

Results of both applications show that variance-based indicators and δ agree in identifying the less relevant parameters w.r.t. the output uncertainty. Discrepancies in ranking between the relevant parameters reveal that factors influencing variance the most are not necessarily the ones that influence the entire output distribution the most.

In summary, the analysis has shown that if one utilizes the moment independent importance measure introduced in this work one gains insights on which of the parameters influence uncertainty the most. Utilizing the new measure jointly with variance-based indicators would also enable the analyst to obtain insights on the parameters that achieve the greatest variance reduction and, when parameters are independent, on the model structure and interactions.

The work also paves the way to further research. The first line of research concerns the selection of the appropriate computational algorithm in the estimation of δ for numerically intensive models (see the discussion on alternative approaches illustrated in Section 6). A second line of research is represented by exploring the conditions on model structure and input distributions under which separability holds (i.e. $\delta_{1,2,\ldots,n} = \delta_1 + \delta_2 + \cdots + \delta_n$) and whether, under the same conditions, additivity holds (i.e. $(V = \sum_{i=1}^{n} V_i)$).

Acknowledgments

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Appendix A

A.1. Proof of Property 1

Proof. We prove first that $\delta_i \leqslant 1$. By the triangle inequality,

$$|f_Y(y) - f_{Y|X_i}(y)| \leqslant |f_Y(y)| + |f_{Y|X_i}(y)|. \tag{37}$$

Hence,

$$\int |f_Y(y) - f_{Y|X_i}(y)|\,\mathrm{d}y \leqslant \int |f_Y(y)|\,\mathrm{d}y + \int |f_{Y|X_i}(y)|\,\mathrm{d}y. \tag{38}$$

Since, $\int |f_Y(y)|\,\mathrm{d}y = 1$ and $\int |f_{Y|X_i}(y)|\,\mathrm{d}y = 1$, we have

$$\int |f_Y(y) - f_{Y|X_i}(y)|\,\mathrm{d}y \leqslant 2. \tag{39}$$

Hence,

$$E_{X_i}[s(X_i)] = E_{X_i}\left[\int |f_Y(y) - f_{Y|X_i}(y)|\,\mathrm{d}y\right] \leqslant E_{X_i}[2] = 2. \tag{40}$$

Applying Definition 2 (Eq. (19)) there follows that $\delta_i \leqslant 1$.

The fact that $\delta_i \geqslant 0$ follows from the monotonicity property of integrals, since $|f_Y(y) - f_{Y|X_i}(y)| \geqslant 0$. □

A.2. Proof of Property 3

Proof. We prove that $\delta_{1,2,\ldots,n} = 1$. By definition, when $\underline{X}$ is fixed at $\underline{X}^*$, $y^* = g(\underline{X}^*)$ and $P(Y = y^*) = 1$. That is $f_{Y|\underline{X}=\underline{X}^*}(y)$ is a *delta-Dirac* measure on y^*. Consider then a finite but small interval around y^* and write (Fig. 11):

$$\tilde{f}_{Y|\underline{X}=\underline{X}^*}(y; y_1, y_2) = \begin{cases} \dfrac{1}{y_2 - y_1} & \text{if } y_1 < y < y_2, \\ 0 & \text{otherwise.} \end{cases} \tag{41}$$

Note that $f_{Y|\underline{X}=\underline{X}^*}(y) = \lim_{y_1 \to y_2} \tilde{f}_{Y|\underline{X}=\underline{X}^*}(y; y_1, y_2)$. Now, consider still a small interval around y^* and compute the total shift when y belongs to such small interval around y^*:

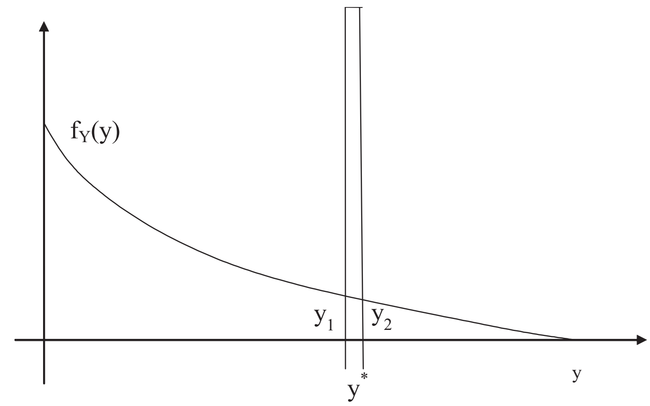

Fig. 11. Unconditional density and conditional density when all the parameters are in a small interval around $\underline{X}^*$.

$$s(\underline{X}) = \lim_{y_1 \to y_2} \int |f_Y(y) - \tilde{f}_{Y|\underline{X}}(y; y_1, y_2)|\,\mathrm{d}y. \tag{42}$$

Applying Eq. (41) one gets

$$s(\underline{X}) = \lim_{y_1 \to y_2} \int_{-\infty}^{y_1} |f_Y(y)|\,\mathrm{d}y + \int_{y_1}^{y_2} \left|f_Y(y) - \frac{1}{y_1 - y_2}\right| \mathrm{d}y + \int_{y_2}^{\infty} |f_Y(y)|\,\mathrm{d}y, \tag{43}$$

which is equivalent to

$$s(\underline{X}) = \lim_{y_1 \to y_2} \int_{-\infty}^{y_1} |f_Y(y)|\,\mathrm{d}y + \int_{y_2}^{\infty} |f_Y(y)|\,\mathrm{d}y + \int_{y_1}^{y_2} \left|f_Y(y) - \frac{1}{y_1 - y_2}\right| \mathrm{d}y. \tag{44}$$

Noting that

$$\lim_{y_1 \to y_2} \int_{-\infty}^{y_1} |f_Y(y)|\,\mathrm{d}y + \int_{y_2}^{\infty} |f_Y(y)|\,\mathrm{d}y = \int_{-\infty}^{\infty} f_Y(y)\,\mathrm{d}y = 1 \tag{45}$$

and that $f_Y(y)\,\mathrm{d}y \to 0$ as $y_1 \to y_2$, we have

$$\lim_{y_1 \to y_2} \int_{y_1}^{y_2} \left|f_Y(y) - \frac{1}{y_1 - y_2}\right| \mathrm{d}y = \lim_{y_1 \to y_2} \int_{y_1}^{y_2} \left|\frac{1}{y_2 - y_1}\right| \mathrm{d}y = 1. \tag{46}$$

Substituting back into Eq. (44) one finds

$$s(\underline{X}) = 1 + 1 = 2. \tag{47}$$

There follows that

$$\delta_{1,2,\ldots,n} = \frac{1}{2}E_{\underline{X}}[s(\underline{X})] = \frac{1}{2}E_{\underline{X}}[2] = 1. \qquad \square \tag{48}$$

A.3. Proof of Property 5

Proof. Note that

$$|f_Y(y) - f_{Y|X_iX_j}(y)| \leqslant |f_Y(y) - f_{Y|X_i}(y)| + |f_{Y|X_i}(y) - f_{Y|X_iX_j}(y)|. \tag{49}$$

Taking the integral of both sides

$$\int |f_Y(y) - f_{Y|X_iX_j}(y)|\,\mathrm{d}y \leqslant \int |f_Y(y) - f_{Y|X_i}(y)|\,\mathrm{d}y + \int |f_{Y|X_i}(y) - f_{Y|X_iX_j}(y)|\,\mathrm{d}y. \tag{50}$$

Now, one can take the expectation, to get

$$E_{X_iX_j}\left[\int |f_Y(y) - f_{Y|X_iX_j}(y)|\,\mathrm{d}y\right] \leqslant E_{X_iX_j}\left[\int |f_Y(y) - f_{Y|X_i}(y)|\,\mathrm{d}y\right] + E_{X_iX_j}\left[\int |f_{Y|X_i}(y) - f_{Y|X_iX_j}(y)|\,\mathrm{d}y\right]. \tag{51}$$

Since $f_{Y|X_i}(y)$ depends on X_i and not on X_j, it is true that

$$E_{X_iX_j}\left[\int |f_Y(y) - f_{Y|X_i}(y)|\,\mathrm{d}y\right] = E_{X_i}\left[\int |f_Y(y) - f_{Y|X_i}(y)|\,\mathrm{d}y\right] = 2\delta(X_i). \tag{52}$$

On the other side,

$$E_{X_iX_j}\left[\int |f_{Y|X_i}(y) - f_{Y|X_jX_i}(y)|\,\mathrm{d}y\right] \tag{53}$$

is a positive term, representing the expected shift between the distribution of Y given X_i and the distribution of Y conditional on X_i. We denote this term as

$$E_{X_iX_j}\left[\int |f_{Y|X_i}(y) - f_{Y|X_jX_j}(y)|\,\mathrm{d}y\right] = 2\delta_{j|i}. \tag{54}$$

Again note that $E_{X_iX_j}[\int |f_{Y|X_i}(y) - f_{Y|X_iX_j}(y)|\,\mathrm{d}y] \geqslant 0$ and that $E_{X_iX_j}[\int |f_{Y|X_i}(y) - f_{Y|X_iX_j}(y)|\,\mathrm{d}y] = 0$ if Y is independent of X_j. Combining this facts gives

$$\delta_{ij} \leqslant \delta_i + \delta_{j|i}. \tag{55}$$

Note that combining Eqs. (55) and (30) one can rewrite Eq. (55) equivalently as

$$\delta_i \leqslant \delta_{ij} \leqslant \delta_i + \delta_{j|i} \tag{56}$$

since $\delta_{j|i} \geqslant 0$, which is the thesis. $\square$

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