# A Common Rationale for Global Sensitivity Analysis

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ABSTRACT: We show that variance-based, density-based, expected-value of information based sensitivity measures rest on the same rationale, namely, information updating. We prove general results concerning their properties. We then show that they can all be estimated by the same design. The design is suitable in the presence of correlated inputs and makes the estimation cost independent of the number of model inputs and depending solely on the sample size. Results of numerical experiments are proposed.

## 1 INTRODUCTION

Reliability analysts use complex models implemented in computer programs frequently to support reliability assessment problems. Due to their complexity, the models run the risk of becoming black boxes to decision-makers. This is why a *process starts of finding out what it was about the inputs that made the outputs come out as they did* (Little 1970, p. B469). Sensitivity analysis methods allow us to carry out this process. Under uncertainty, global methods are the appropriate sensitivity techniques to be used. However, computational burden might hinder a fully-fledged global sensitivity analysis. The designs proposed by (Plischke, Borgonovo, & Smith 2013) and (Strong & Oakley 2012) obtain expected-value-of-information-based (henceforth, EVPI-based), variance- and density-based sensitivity measures at an estimation cost equal to the Monte Carlo sample size.

In this work, we argue that a common rationale binds global sensitivity measures. It is shown that they can be seen as operators between the conditional and unconditional model output distributions. We analyze the properties that make theses shift measures distances or divergences between distributions. In particular, EVPI-based measures share the properties of distances between distributions.

We then prove a general consistency result for estimating global measures by a single loop design, which holds also in the presence of correlated model inputs.

We perform numerical test cases focusing on the case of correlated factors. New analytical results for variance-based, EVPI-based, density-based and distribution-based sensitivity measures are proposed.

The remainder of the paper is largely taken from (Borgonovo, Hazen, & Plischke 2013).

## 2 PROBABILISTIC SENSITIVITY ANALYSIS: REVIEW AND FRAMEWORK

The family of probabilistic sensitivity methods analysed in this work comprises variance-based (Wagner 1995), distribution-based (Baucells & Borgonovo 2013) and expected value of information (EVI)-based (Felli & Hazen 1998) sensitivity measures.

The computer code quantifies $A$ decision-support variables $Y_a$, $a = 1, 2, \ldots, A$:

$$g: \quad \mathbf{x} \mapsto \mathbf{y} = \mathbf{g}(\mathbf{x}), \qquad \mathcal{X} \to \mathbb{R}^A \tag{1}$$

$\mathcal{X} \subset \mathbb{R}^n$ is the model input space.

EVPI-based sensitivity measures are defined as follows:

$$\epsilon_i = \mathbb{E}\left[\max_{a=1,2,\ldots,A}\{\mathbb{E}[Y_a|X_i]\}\right] - \max_{a=1,2,\ldots,A}\{\mathbb{E}[Y_a]\} \tag{2}$$

$\mathbb{E}[\max_{a=1,2,\ldots,A}\{\mathbb{E}[Y_a|X_i]\}]$ is called *prior expected value of action posterior to perfect information* (Pratt, Raiffa, & Schlaifer 1995, p. 252) .

The model input associated with the highest value of $\epsilon_i$ is the one on which it is worth more to spend when gathering new information on the model inputs. (Pörn 1997) proposes EVPI as a probabilistic sensitivity measure in reliability analysis. See (Oakley 2009) and (Oakley, Brennan, Tappenden, & Chilcott 2010) for recent reviews.

Variance-based measures are defined independently in (Iman & Hora 1990), (Sobol´ 1993) and (Wagner 1995). Following (Wagner 1995), we write

$$\nu_i = \mathbb{V}[Y] - \mathbb{E}\left\{\mathbb{V}[Y|X_i]\right\} = \mathbb{V}\left\{\mathbb{E}[Y|X_i]\right\} \tag{3}$$

and

$$\tau_i = \mathbb{E}\left\{\mathbb{V}[Y|\mathbf{X}_{\sim i}]\right\} \tag{4}$$

where $Y$ is the (unique) output of interest, $\mathbf{X}_{\sim i}$ denotes that all factors are fixed but $X_i$. Their normalized versions,

$$\eta_i^2 = \frac{\nu_i}{\mathbb{V}[Y]} \tag{5}$$

and

$$\eta_i^T = \frac{\tau_i}{\mathbb{V}[Y]} \tag{6}$$

have been the subject of numerous studies and they have replaced the un-normalized version in the practice. $\eta_i^2$ is (Pearson 1905)'s correlation ratio. To overcome limitations in variance-based sensitivity indicators the $\delta$ importance indicator measures a distance between unconditional and conditional output densities and is defined as (Borgonovo 2007):

$$\begin{aligned}\delta_i &= \frac{1}{2}\mathbb{E}\left[\int_{\Omega_Y} |f_Y(y) - f_{Y|X_i}(y)|dy\right] \\ &= \frac{1}{2}\iint_{\Omega_{X_i}\times\Omega_Y} |f_Y(y)f_{X_i}(x_i) - f_{Y,X_i}(y,x_i)|dydx_i.\end{aligned} \tag{7}$$

By (7), $\delta_i = 0$ if and only if $Y$ is independent of $X_i$(Plischke & Borgonovo 2013). That is, $\delta_i = 0$ ensures that $Y$ is independent of $X_i$. The $\beta^{KS}$ importance measure is based on the Kolmogorov-Smirnov distance and is defined as:

$$\beta_i^{KS} = \mathbb{E}\left[\sup_y\{\left|F_Y(y) - F_{Y|X_i}(y)\right|\}\right]. \tag{8}$$

$\delta_i$ and $\beta_i^{KS}$ possess the monotonic invariance property, i.e., their value stays invariant under monotonic transformations of inputs and outputs.

## 3 A COMMON RATIONALE

The common rationale rests on considering the inner statistic as an operator between the unconditional and any conditional model output distribution:

$$\gamma_i(x_i) = \zeta(\mathbb{P}_Y, \mathbb{P}_{Y|X_i=x_i}) \tag{9}$$

$\gamma_i(x_i) : \mathcal{X}_i \to \mathbb{R}$ depends on the realized value of $X_i$. (Borgonovo, Hazen, & Plischke 2013) propose the following definitions:

**Definition 1** *We call*

$$\xi_i = \mathbb{E}[\gamma_i(X_i)] = \mathbb{E}[\zeta(\mathbb{P}_Y, \mathbb{P}_{Y|X_i})] \tag{10}$$

*the global sensitivity measure of $X_i$ based on operator $\zeta(\cdot,\cdot)$.*

**Definition 2** *We call $\gamma_i(x_i)$ the inner statistic of $\xi_i$.*

$\xi_i$ takes the decision-maker's degree of belief about $X_i = x_i$ into account. As in (Borgonovo, Hazen, & Plischke 2013), consider the following example:

**Example 1** *Setting $\zeta(\mathbb{P}_\mathbf{Y}, \mathbb{P}_{\mathbf{Y}|X_i=x_i})$ to either*

$$\max_{a=1,2,\ldots,A}\{\mathbb{E}[Y_a|X_i]\} - \max_{a=1,2,\ldots,A}\{\mathbb{E}_\mathbf{X}[Y_a]\} \tag{11}$$

*or*

$$\mathbb{E}[(Y-\mathbb{E}[Y])^2|X_i = x_i]] - \mathbb{V}[Y|X_i = x_i] \tag{12}$$

*or*

$$\frac{1}{2}\int_\mathcal{Y} |f_Y(y) - f_{Y|X_i=x_i}(y)|dy \tag{13}$$

*or*

$$\sup_y \left|F(y) - F_{Y|X_i=x_i}(y)\right| \tag{14}$$

*we obtain the inner statistics of $\epsilon_i$, $\nu_i$, $\delta_i$, and $\beta_i$ respectively.*

The following two Lemmas are proven in (Borgonovo, Hazen, & Plischke 2013).

**Lemma 1** *The conditions*
*a) $\gamma_i(x_i) \geq 0$ and*
*b) $\gamma_i(x_i) = 0$ for all values of $X_i$ if $Y$ is stochastically independent of $X_i$*
*are satisfied if $\zeta(\cdot,\cdot)$ is a divergence between probability distributions.*

**Lemma 2** *Under the hypotheses of Lemma 1, $\gamma_i(x_i)$ is independent of the order with which $\mathbb{P}_X$ and $\mathbb{P}_{Y|X_i=x_i}$ are considered if $\zeta(\cdot,\cdot)$ is a distance between probability distributions.*

Then, it is possible to see that $\epsilon_i$ is then also a distance between distributions. However, the inner statistic of variance-based sensitivity measures can be negative and therefore it is not a distance nor a divergence between probability distributions. Some authors have then modified the definition of the inner statistic of variance-based sensitivity measures to make it positive (Ruan, Lu, & Tian 2012). However, the modification removes the neat association between variance-decomposition and input-output mapping and conflicts with the original intuition of variance-based sensitivity measures.

Finally, it is possible to prove that a sensitivity measure is transformation invariant if and only if the inner statistic is.

## 4 ESTIMATION: A UNIFIED FRAMEWORK

We can use the common rationale discussed in Section 3 to come to a unified estimation design. The intuition is scatterplot smoothing (Figure 1).

Formally, we define:

**Definition 3** *Given a global sensitivity measure $\xi_i$ based on inner statistic $\gamma_i(x_i)$, a sample $[\mathbf{X}\,\mathbf{Y}]_{N\times(n+A)}$, a partition of $\mathcal{X}_i$ into $M$ classes and the corresponding scatterplot partitioning, we call the quantity*

$$\widehat{\xi}_i(M,N) = \sum_{m=1}^{M} \widehat{\gamma}_i(\mathcal{C}_i^m)\widehat{\mathbb{P}}_{X_i}(\mathcal{C}_i^m) \tag{15}$$

*where*

$$\widehat{\gamma}_i(\mathcal{C}_i^m) = \gamma_i(\widehat{\mathbb{P}}_{\mathbf{Y}}, \widehat{\mathbb{P}}_{\mathbf{Y}|\mathcal{C}_i^m}) \tag{16}$$

*class-conditional estimator of $\xi_i$.*

**Example 2** *Combining eqs.* (11), (12), (14), (16), *and* (15) *we obtain, respectively:*
*1) (Strong & Oakley 2012)'s estimator of EVPI-based sensitivity measures*

$$\widehat{\epsilon}_i = \sum_{m=1}^{M} \frac{n_m}{N} \cdot \max_{a=1,2,\ldots,A}(\widehat{\mu}_m^a) - \max_{a=1,2,\ldots,A}(\widehat{\mu}^a) \tag{17}$$

*where* $\widehat{\mu}_m^a = \dfrac{1}{n_m}\sum_{x\in\mathcal{C}_i^m} g_a(x)$ *and* $\widehat{\mu}^a = \dfrac{1}{N}\sum_{x\in\Omega_i} g_a(x)$*;*
*2) Pearson's estimator of $\eta_i^2$ (Pearson 1905, Plischke 2012) ($A=1$)*

$$\widehat{\eta}_i^2 = \left(\frac{1}{N-1}\sum_{i=1}^{n}(g(x_i)-\widehat{\mu})^2\right)^{-1} \sum_{m=1}^{M}\frac{n_m}{N}\cdot(\widehat{\mu}_m-\widehat{\mu})^2 \tag{18}$$

*and*
*3) (Baucells & Borgonovo 2013)'s estimator of $\beta_i^{KS}$ ($A=1$)*

$$\widehat{\beta}_i^{KS} = \sum_{m=1}^{M} \max_{x_i\in\mathcal{C}_i^m}\left|\widehat{F}_Y(g(x_i)) - \widehat{F}_{Y|\mathcal{C}_i^m}(g(x_i))\right| \cdot \frac{n_m}{N} \tag{19}$$

*Here $\widehat{F}_Y$ and $\widehat{F}_{Y|\mathcal{C}_i^m}$ are empirical cumulative distribution functions.*

where $\widehat{\gamma}_i(\mathcal{C}_i^m)$ replaces the point condition $X_i = x_i$ with the class condition $X_i \in \mathcal{C}_i^m$, where $\mathcal{C}_i^m$ is an element of the partition of the $X_i$-axis of the scatterplot.

(Borgonovo, Hazen, & Plischke 2013) introduce the notion of *partition refinement strategy* as follows:

**Definition 4** *Let $\mathcal{P}_{j(N)} = \{\mathcal{C}_i^{m_j}; m=1,\ldots,M_{j(N)}\}$ denote a sequence of partitions. A* partition refinement strategy *is any sequence of partitions such that, with increasing sample size $N$, for each $x_i$ from the support of $X_i$ there exists a $m_j$ among the $M(N)$ partitions such that $x_i \in \mathcal{C}_i^{m_j}$ and $\bigcap_N \mathcal{C}_i^{m_{j(N)}} = \{x_i\}$.*

They prove that a partition refinement strategy exists, $X_i$ being either discrete, continuous or mixed. Then, they come to the following theorem.

**Theorem 1** *Given the estimators in Definition 3, a family of partitions and a refinement strategy as in Definition 4, then*

$$\lim_{N\to\infty} \sum_{m=1}^{M_{j(N)}} \widehat{\xi}_i(M_{j(N)},N) = \mathbb{E}_i[\gamma_i(X_i)] = \xi_i. \tag{20}$$

## 5 RESULTS FOR CORRELATED FACTORS

The presence of correlations among factors is, traditionally, a challenge in probabilistic sensitivity analysis. We consider the following example (Borgonovo, Hazen, & Plischke 2013).

**Example 3** *Let $g_i(X_i) = \phi_i X_i$ with $\phi_i \in \mathbb{R}$, $i = 1,2,\ldots,n$, $\mathbf{X} \sim \mathcal{N}(\mu,\Sigma)$, normally distributed with expected values $\mu = (\mu_1,\mu_2,\ldots,\mu_n)$, ($\mu_i = \mathbb{E}[X_i]$) and non-degenerate covariance matrix $\Sigma = [\ \sigma_{i,\ell}\quad i,\ell = 1,2,\ldots,n\ ]$ ($\det\Sigma \neq 0$).Then,*

$$\eta_i^2 = \mathbb{V}^{-1}[Y]\sum_{\ell=1}^{n}\phi_\ell\phi_i\sigma_{i,\ell}.$$

*If the decision-problem is to select the maximum between $Y$ and $0$ then*

$$\epsilon_i = \int_{x_i^*}^{\infty} f_{X_i}(s)\left(s\phi_i + \sum_{\ell=1,\ell\neq i}^{n}\phi_\ell\left(\mu_\ell + (s-\mu_i)\frac{\sigma_{i,\ell}}{\sigma_{i,i}}\right)\right)ds - \mathbb{E}[Y]$$

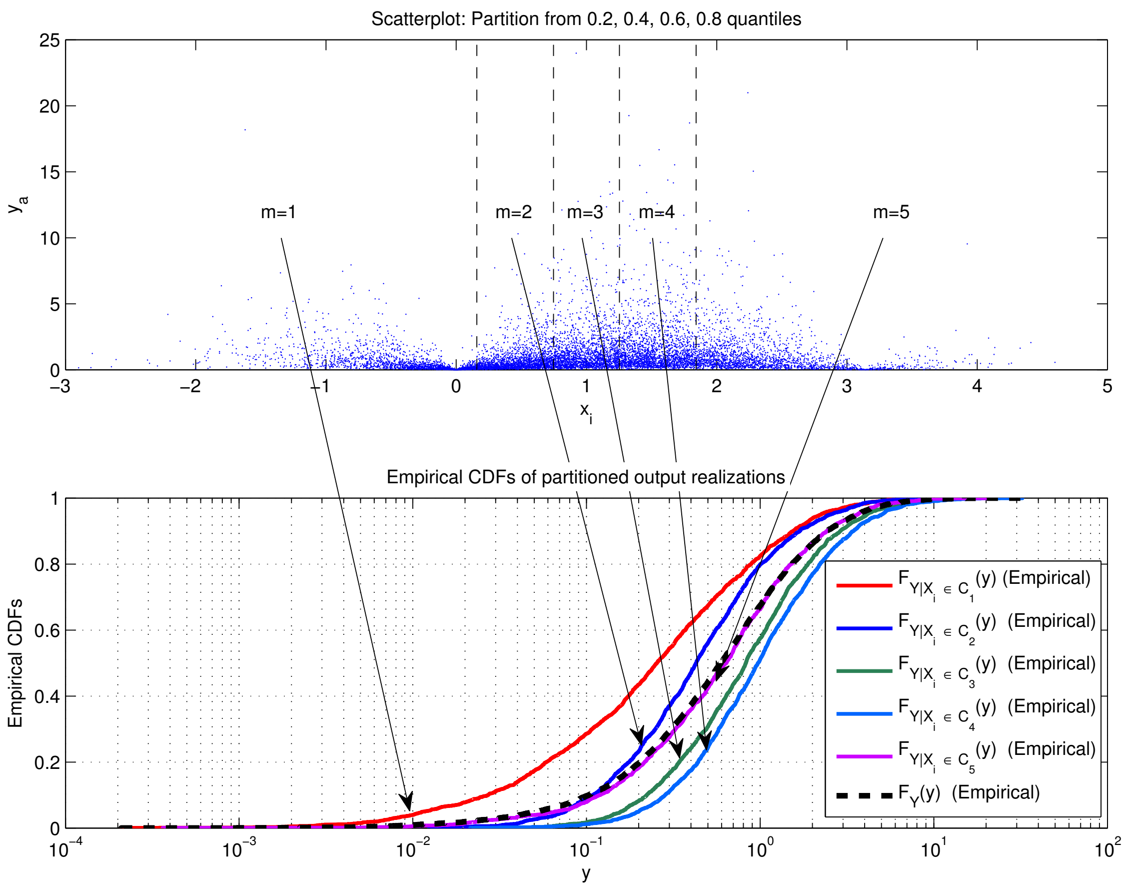


Figure 1: Intuition concerning scatterplot smoothing.

*where*

$$x_i^* = \left( \sum_{\ell=1,\ell\neq i}^{n} \mu_i \frac{\sigma_{i,\ell}\phi_\ell}{\sigma_{i,i}\phi_i} - \sum_{\ell=1,\ell\neq i}^{n} \mu_\ell \frac{\phi_\ell}{\phi_i} \right) \cdot \left( \sum_{\ell=1}^{n} \frac{\sigma_{i,\ell}\phi_\ell}{\sigma_{i,i}\phi_i} \right)^{-1}$$

*and $f_{X_i}(s)$ is the normal density.*

*Analytical expressions for $\delta_i$ and $\beta_i$ can be found in (Borgonovo, Hazen, & Plischke 2013). Analytical expressions for $\delta_i$ and $\beta_i$ can be found in (Borgonovo, Hazen, & Plischke 2013).*

We now consider the model

$$Y = \phi \cdot \mathbf{X} \qquad \mathbf{X} \sim \mathcal{N}(\mu, \Sigma)$$
$$\Sigma = \begin{pmatrix} 1 & .5 & \dots & .5 \\ .5 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & .5 \\ .5 & \dots & .5 & 1 \end{pmatrix} \tag{21}$$

with $n = 21$, $\phi_1 = \dots = \phi_7 = -4$, $\phi_8 = \dots = \phi_{14} = 2$, $\phi_{15} = \dots = \phi_{21} = 1$, $\mu \equiv 0$. The analytical values of the sensitivity measures are given in Table 1.

Figure 2 confirms that the estimators of all sensitivity measures approximate the respective analytical values (dashed lines) as $N$ increases [Theorem 1 ].

Table 1: Analytical values for the importance measures of example (21).

| Factor group | 1–7 | 8–14 | 15–21 |
|---|---|---|---|
| Exp. value of partial info. | 0.265 | 0.002 | 0.001 |
| Correlation ratio | 0.309 | 0.064 | 0.092 |
| Kolmogorov Smirnov | 0.205 | 0.083 | 0.101 |
| $L^1$ density distance | 0.212 | 0.084 | 0.102 |

# 6 BUILDING YOUR OWN IMPORTANCE MEASURES

Nonparametric tests on independent samples involve the Wilcoxon/Mann-Whitney, the Kolmogorov-Smirnov and the Wald-Wolfowitz tests. Item 3 of Example 2 shows the use of Kolmogorov-Smirnov as a distance measure. To show the flexibility of our proposed approach we propose an importance measure which is not based on the notion of distance but derived from the Wald-Wolfowitz test (Wald & Wolfowitz 1940). Clearly, as we deal with sub-sampling the default setup of this test has to be modified. Under the null hypothesis that the subset selection of $n_m$ out of $n$ samples is purely random (default setup: $n_m$ out of the pooled sample of size $n + n_m$) we can derive formulas for the expected number of runs in the sample. The Wald-Wolfowitz test proceeds as follows: The sample consisting of pairs $(\mathbf{x}, y)$ is sorted according to $y$. All $n_m$ realizations with $x_{\cdot,i} \in \mathcal{C}_{m,i}$

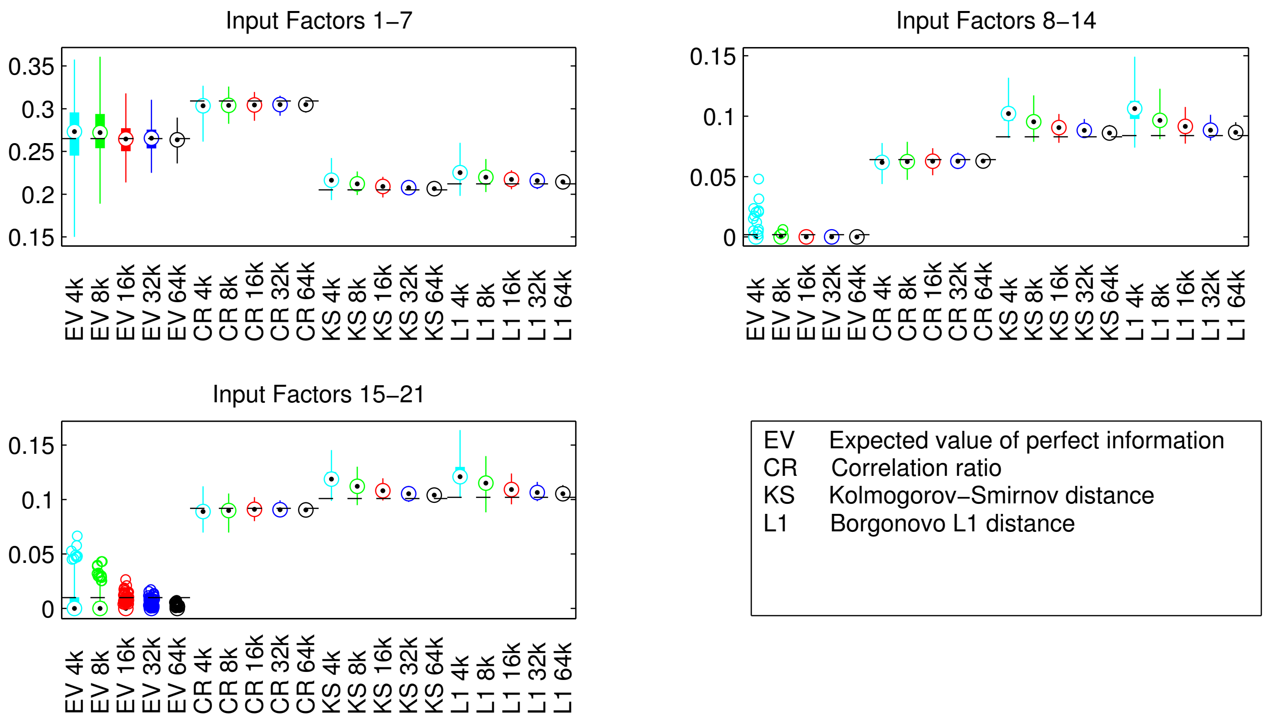


Figure 2: Convergence of different partition based sensitivity indicators.

are marked. Then the total number of runs $R_{m,i}$ of unmarked/marked realizations in the ordered sample is determined.

The test statistics for a given interval $\mathcal{C}_{m,i}$ is computed by

$$W_{m,i} = \frac{R_{m,i} - \mu}{\sqrt{\frac{(\mu-1)(\mu-2)}{n-1}}} \tag{22}$$

with $\mu = 2\frac{(n-n_m)n_m}{n} + 1$. It is asymptotically normal under the null hypothesis.

We can use $W_{m,i}$ as an inner statistic $\hat{\gamma}_i(\mathcal{C}_{m,i}) = W_{m,i}$ for an importance measure based upon the Wald-Wolfowitz runs test. A value deviating from 0 indicates an important contribution in the sense that the number of runs in the subsamples differ from their expected values. This usage is in compliance with Definition 3.

## 7 CONCLUSIONS

This work has demonstrated that variance-based, density-, distribution- and EVPI based global sensitivity measures rest on a common rationale. The rationale, this, comprises the most important classes of probabilistic sensitivity measures. The common rationale allows us to explore the properties of sensitivity measures when regarded as operators among probability distributions. The fact that they are joined by a common rationale also shows that they can all be estimated through a common design. Traditionally a double loop approach is assumed. However, it has been discussed here a single loop approach based on class conditioning if the random model input is continuous and on the support of the model input itself, if the model input is discrete. New analytical findings concerning the value of all expected value of information-based and distribution-based sensitivity measures in the presence of correlations are obtained. We perform numerical experiments in the presence of correlated inputs, that demonstrate the consistency of the estimators.

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