Target and conditional sensitivity analysis with emphasis on dependence measures

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NEW STATISTICAL DEVELOPMENTS FOR TARGET AND CONDITIONAL SENSITIVITY ANALYSIS

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Abstract. In the context of sensitivity analysis of complex phenomena in presence of uncertainty, we motivate and precise the idea of orienting the analysis towards a critical domain of the studied phenomenon. For this, target and conditional sensitivity analyses are defined. We make a brief history of related approaches in the literature, and propose a more general and systematic approach. Nonparametric measures of dependence being well-suited to this approach, we also make a review of available methods and of their use for sensitivity analysis, and clarify some of their properties. Then, we focus our attention on sensitivity indices based on correlation ratio, namely Sobol' indices, and on two dependence measures: the kernel quadratic dependence measure also called Hilbert–Schmidt independence criterion and the Csiszár divergence dependence measure. We propose adapted versions of these tools for target and conditional analysis, by considering transformation of the output using hard or smooth weight functions. Finally, we show on synthetic numerical experiments both the interest of target and conditional sensitivity analysis, and the efficiency of the dependence measures. We also illustrate the relevance of the proposed smooth versions for conditional estimators.

Key words. Sensitivity analysis, computer experiments, target and conditional sensitivity analysis, dependence measure, correlation ratio

AMS subject classifications. 62G05, 62G99

1. Introduction. Nowadays, many phenomena are modeled by mathematical equations which are implemented and solved using complex computer programs. These numerical simulators are used to model and predict the underlying physical phenomena and their results can guide decisions, which can involve important financial, societal and safety stakes. However, they often take as inputs a high number of numerical, physical or even conception parameters. Because of a lack of phenomenon knowledge and characterization or a need to investigate various configurations, many of these input parameters are uncertain (or considered as such) and it is important to assess how these uncertainties can affect the model output. In a probabilistic framework, the uncertain parameters, also called factors, are modeled by random variables characterized by probabilistic distributions. Sensitivity analysis methods are performed to evaluate how input uncertainties contribute, qualitatively or quantitatively, to the variation of the output. The variety of approaches and applications of sensitivity analysis brings forth a diversity of objects and terms. Before presenting the goals of this document and the extent of our work, we introduce a few notations.

In the classical framework, we assume the modeling of a phenomenon Y depending on a set of *factors* $(X_i)_{1\leq i\leq d}$ following a deterministic relation $Y \overset{\text{def}}{=} f(X_1, \dots, X_d)$, f being the numerical simulator in our industrial applications and Y the output(s) of interest. Uncertainties are taken into account by modeling the factors as random variables, defined over the same implicit probability space $(\Omega, \mathfrak{F}, \mathrm{P})$ with Ω denoting the sample space, $\mathfrak{F}$ the set of events and P the associated probability measure. It will also be convenient to consider a generic random variable X, usually standing for a group of one or several factors. For such a variable, we note its range $\mathcal{X} \overset{\text{def}}{=} \mathrm{ran}(X)$ and its law $\mathrm{P}_X \overset{\text{def}}{=} \mathrm{P} \circ X^{-1}$ is the induced probability measure over $\mathcal{X}$. We also particularize the range of the output $\mathcal{Y} \overset{\text{def}}{=} \mathrm{ran}(Y)$.

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1.1. Global, target and conditional sensitivity analysis. *Global sensitivity analysis* aims at measuring how the variations of one or several factors contribute to the variation of the studied phenomenon, over the whole domain of possible values. Many authors agree with Saltelli et al. (2008) to distinguish several use of sensitivity analysis. First, the *ranking* of factors by importance is the starting point of any application. Identifying the factors which are most influential in a phenomenon might help understanding it or guide resource investment for controlling it. Then, *screening* the factors for insignificant ones is considered, for instance for the purpose of model simplification. This sometimes calls on statistical tests, which might be practical but cannot be satisfying for all applications. In our experience, screening is often in practice interpretation of ranking, either through the expertise of the practitioner or with some cross-validation process. Finally, *factor mapping* is often described as a finer identification of functional relationship between the specific domains of values of the factors and of the phenomenon. This last use of sensitivity analysis consists in determining *which values* of these factors are responsible of the occurrence of the phenomenon in a given domain.

In our work, we also focus on specific domains of values of the phenomenon but we want to determine *which factors* contribute most in the occurrence of the phenomenon in a given domain. For this, we first define the *target sensitivity analysis* which aims at measuring the influence of the factors over a restricted domain of the studied phenomenon, and in particular over the *occurrence* of the phenomenon in this restricted domain. Such domain of interest would usually be extreme and relatively rare, constituting a risk or an opportunity; we call it *critical domain*, noted $\mathcal{C} \subset \mathcal{Y}$ and associated to a *critical probability* $\mathrm{P}(Y \in \mathcal{C}) = \mathrm{P}_Y(\mathcal{C})$. Alternatively, we also define the *conditional sensitivity analysis* which evaluates the influence of the factors *within* the critical domain only, ignoring what happens outside. Let us underline that those two notions can widely differ; this point will be illustrated by the numerical applications proposed in this paper.

1.2. Goals and Structure of the Paper. In this paper, we aims at proposing news methods and tools for target and conditional sensitivity analysis. It seems to us that there are numerous, direct applications, especially for, but not restricted to, industrial safety. Still, while global sensitivity analysis has been an active research field for several decades, it seems that target sensitivity analysis is less understood, and until recently has not been studied systematically as such. This is why we sometimes introduce our own terminology, which we discuss along with the description of similar concepts that we identify in the literature. Finally, let us point out that we are mostly interested in phenomena influenced by many factors and of which only limited understanding is available. Typical situations include complex systems observed through heavy computer simulations or costly physical measures. These applicative constraints should be taken into account when selecting and proposing dedicated tools.

In section 2, we propose a review on the existing approaches and tools for target sensitivity analysis before introducing our contributions in this framework. Then, the actual sensitivity analysis tools on which our work relies are more precisely described in section 3. In section 4, we get back to our initial problematic of target and conditional sensitivity analysis: we propose a simple dedicated framework and describe some resulting tools. Finally, we give numerical evaluations of our methods along section 5, on various synthetic data.

2. Review on Existing Approaches. We propose here a coarse classification of methods relating to target sensitivity analysis, according to both chronological and methodological criteria.

2.1. Regional Sensitivity Analysis. The very notion of target sensitivity analysis dates back at least to Spear and Hornberger (1980), motivated by environmental science applications. The proposed methodology compares the distribution of the factors within the critical domain against their distribution outside. The authors choose to use the *Kolmogorov distance*, almost systematically reused ever since:

$$\sup_{x \in \mathcal{X}} \left| F_{X \mid Y \in \mathcal{C}}(x) - F_{X \mid Y \in \mathcal{Y} \setminus \mathcal{C}}(x) \right| ,$$

where $F_{X|A}$ is the *cumulative distribution function* of a real random variable X (i.e. $\mathcal{X} \subseteq \mathbb{R}$) conditioned by an event $A \in \mathfrak{F}$ of nonzero probability (see section 4.1.2 for details).

They call it *regional sensitivity analysis*, or sometimes generalized sensitivity analysis. The former name could fit our purpose, if it was not for two inconveniences. First, it evokes more of a sensitivity analysis within the critical domain (what we call conditional sensitivity analysis) rather than its occurrence; second, for the past three decades in the literature it referred exclusively to the above methodology. It appears to be the generalization of no other method, explaining why the alternative name is not used anymore. Finally, one may encounter the term *Monte Carlo Filtering*, which might be vague and restrictive.

Comparing distributions conditionally to the critical domain seems a good choice for target sensitivity analysis. It involves only two conditionings, which facilitates its estimation, for instance with Monte Carlo method. One difficulty, mentioned by the authors and common to all target sensitivity methods, arises when the critical probability is low. Another deficiency pointed out by the authors is the difficulty to study factors in interaction. From this viewpoint, observe that a metric comparing cumulative distribution functions can be extended to multidimensional settings, which would allow to regroup several factors. However, the particular metric used here, namely the supremum norm over the differences, is sensitive to outliers. Both aspects make it particularly unsuitable for categorical factors.

Strangely enough, regional sensitivity is mostly used in the literature as a mean of global sensitivity analysis, the partition of the domain of values of the phenomenon into several regions losing its original sense and becoming more or less arbitrary.

2.2. Reliability Sensitivity Analysis. Another field dealing with target sensitivity analysis is motivated by applications in structural reliability, where the term *reliability sensitivity analysis* is commonly used. In this context, critical domains are failure domains, and the developed methods are influenced by two typical features: failure probabilities are small in comparison to the number of available observations, and the probability distributions of the factors are assumed to be known.

The first methods developed seek, in a suitable transformation of the factors space, to determine a “most probable failure point”, and to estimate the critical probability from linear or quadratic approximations of the boundary of the critical domain around that point. This yields the *first-* and *second-order reliability methods*, reviewed by Rackwitz (2001). It is possible to give to each factor an importance measure based on the position of the most probable failure point. The geometrical assumption about the failure domain seems however restrictive, implying in particular that the factors have a monotonous effect on the phenomenon.

The sensitivity measures which later prevail in the field are based on derivatives of the critical probability, with respect to the parameters defining the probability laws of the factors or of their transformation. This framework seems once again restrictive for our purpose. Nonetheless, the approaches developed in parallel for dealing with low critical probabilities deserves to be incidentally noted, because they could be adapted to other sensitivity measures. Let us mention the methods based on *importance sampling* (see for instance the adaptation of Wu, 1994), as well as the approach of *sequential Monte Carlo* as proposed by Au and Beck (2001), who call it *subset simulation*. As further developed by Song et al. (2009) and Cérou et al. (2012), the latter is based on Markov chain Monte Carlo with the Metropolis–Hasting algorithm.

Still in the reliability context, the Ph.D. dissertation of Lemaître (2014) is the first systematic study of target sensitivity analysis. With this purpose in mind, the author compares more general methods of global sensitivity analysis, of which we give a brief overview below. We can already mention that he identifies the need to transform the variable modeling the phenomenon into a binary variable encoding the occurrence in the critical domain; that is $1_{\mathcal{C}}(Y)$, where $1_{\mathcal{C}} \colon y \mapsto 1$ if $y \in \mathcal{C}$, 0 otherwise. This is one of the approach on which we focus in this work (see subsection 4.1).

A first sensitivity analysis method considered is the estimation of (square) *correlation ratio* between the factors and the phenomenon (real, with finite variance),

$$\eta^2(X,Y) \overset{\text{def}}{=} \frac{\mathrm{V}(\mathrm{E}[Y \mid X])}{\mathrm{V}(Y)} \ . \tag{2.1}$$

Resulting quantities are often called Sobol' (1990, 1993) indices. These are nowadays standard for global sensitivity analysis, notably because they can be interpreted in terms of decomposition of the variance of the studied phenomenon. Lemaître shows how these indices applied to the binary transformation of the observed phenomenon, $\eta^2(X, 1_{\mathcal{C}}(Y))$, are relevant at least for cases that are simple and where the number of available observations is high enough.

A second method is based on the *total variation* which we develop later (see section 3.2.2), once again applied to the binary transformation. Unfortunately, the proposed estimation methods might be inadequate and the analysis is too brief; the author mentions a "positive bias" without further explanations.

Another set of methods is based on *binary classification trees*. The author lists many ways of defining classification trees, and even more ways of deducing sensitivity indices. This indicates a lack of generality and robustness, actually revealed by some numerical experiments. For the sake of brevity, we do not elaborate here and invite the interested reader to refer to the dissertation for more details.

Then, Lemaître takes over regional sensitivity described above with some modifications. He compares the probability laws conditionally to the critical domain against the (known) marginal probability laws. In addition to Kolmogorov distance, he tries other discrepancy measures between cumulative distribution functions classically used in statistical tests, namely Cramér–Von Mises and Anderson–Darling, and shows that this choice can influence the importance ranking of factors. More importantly, he suggests that sequential Monte Carlo approaches are well adapted to methods based on comparisons of factor distributions conditionally to the critical domain.

Finally, closer to the classical sensitivity measures for reliability mentioned above, the author proposes its own measures, quantifying how modifications of the factors probability laws impact on the critical probability. Although it has specific advantages, such as quantification of uncertainties due to estimation errors on the model's parameters, this framework seems somewhat artificial and restrictive.

Altogether, this Ph.D. dissertation is an interesting entry point to target sensitivity analysis. However, more numerical experiments seem necessary in order to conclude about the advantages and drawbacks of the different considered approaches, and those which should be retained for further improvements and comparisons are not clearly identified.

2.3. Sensitivity Analysis of a Specific Statistic. Another recent approach for target sensitivity analysis is due to Fort et al. (2013). Their formulation is more precise than ours: they are interested in the sensitivity of *an estimator of a statistical quantity* of the studied phenomenon. For this, they introduce the term of *goal-oriented sensibility analysis*.[1]

From the relations $\mathrm{V}\big(\mathrm{E}[Y \mid X]\big) = \mathrm{E}\Big(\big(\mathrm{E}[Y \mid X] - \mathrm{E}[Y]\big)^2\Big) = \mathrm{V}(Y) - \mathrm{E}\big(\mathrm{V}[Y \mid X]\big)$, the authors show how the correlation ratio, (2.1), is, in their sense, a measure adapted to the sensitivity of the *expectation* of the phenomenon: indeed, it measures a distance between expectations, quantified by a difference of variances. Now for a generic real random variable Y, expectation and variance can be defined through an optimization problem, $\mathrm{E}[Y] = \arg\min_{\theta\in\mathbb{R}} \mathrm{E}\Big((Y-\theta)^2\Big)$ and $\mathrm{V}[Y] = \min_{\theta\in\mathbb{R}} \mathrm{E}\Big((Y-\theta)^2\Big)$, where the functional $(y,\theta) \mapsto (y-\theta)^2$ plays the role of a *contrast function*.

The generalization of the correlation ratio to a statistic defined by another contrast function ψ becomes[2] $\min_{\theta\in\mathbb{R}} \mathrm{E}(\psi(Y,\theta)) - \mathrm{E}(\min_{\theta\in\mathbb{R}} \mathrm{E}[\psi(Y,\theta) \mid X])$. In practice, in order to study extreme values, they focus on the *quantiles* of the phenomenon, considering for a level $\alpha \in \,]0,1[$, the contrast function $(y,\theta) \mapsto (y-\theta)(1_{\{y\leq\theta\}} - \alpha)$. However, resulting indices turn out to be difficult to estimate, as shown by the recent developments of Browne et al. (2017) and Maume-Deschamps and Niang (2017).

Les us mention that Kucherenko and Song (2016) propose another adaptation of the correlation ratio to analysis of sensitivity of quantiles, more direct: expectations are simply replaced by quantiles[3] of level $\alpha \in \,]0,1[$, $\mathrm{E}\bigg(\Big(F^{-1}_{Y|X}(\alpha) - F^{-1}_{Y}(\alpha)\Big)^2\bigg)$, where F^{-1} is the generalized inverse of a cumulative distribution function. As its estimation is also difficult, the authors propose to approximate the quantiles conditionally to factors values by a rough form of kernel method.

At last, let us add that the quantile is a peculiar notion and in our opinion, its use for sensitivity analysis raises some troubles. Beyond difficulty of definition and estimation, these tools are adapted only to phenomena which are unidimensional and continuous. Moreover, the "sensitivity of a quantile" has a less straightforward interpretation than the sensitivity of the occurrence of a phenomenon, or of the variation of a phenomenon, in a critical domain.

2.4. Contributions. The majority of the methods previously described are originally developed for particular applications; we would like to make abstraction of the problem to get more general methods. To this end, rather than defining or enhancing specific methods, we seek modifications or generalizations of global sensitivity analysis tools, which would be adapted to target or conditional sensitivity analysis.

Such modifications boil down, for a given analysis tool considered, to weighting the observations according to the critical domain. The weights can operate following

[1] Beware that this term already exists in the literature referring to tools of different nature.

[2] Provided that the random variable $\min_{\theta\in\mathbb{R}} \mathrm{E}[\psi(Y,\theta) \mid X]$ is well defined.

[3] The random variable $F^{-1}_{Y|X}$ is now defined through conditional distribution.

two principles: either as a *transformation* of the phenomenon prior to the application of the tool, or as a *modification* of the parameters and objects which define the tool itself. This includes, but is not restricted to, the natural notion of conditioning. Several variations around these principles are presented along section 4; before that, the actual sensitivity analysis tools must be introduced.

3. Correlation Ratio and Dependence Measures for Sensitivity Analysis. We present here the measures of sensitivity analysis upon which we construct our tools. First, sensitivity indices based on correlation ratio, the popular *Sobol' indices*, are introduced. Now, it appears that sensitivity analysis based on *nonparametric dependence measures*, recently advocated by Da Veiga (2015), is particularly adapted to our framework. This will retain most our attention in the following, starting from subsection 3.2 where we review available methods for measuring statistical dependence and detail the use of some of them in the context of sensitivity analysis.

3.1. Correlation Ratio yielding Sobol' Indices. Given a group of factors $I \subset \{1,\ldots,d\}$, we write $X_I \overset{\text{def}}{=} (X_i)_{i\in I}$ for the corresponding random tuple, and ${}^{\complement}I \overset{\text{def}}{=} \{1,\ldots,d\} \setminus I$ for the complementary group of factors. Moreover, we abusively note the concatenation $\big(X_I, X_{\complement I}\big) \overset{\text{def}}{=} \big(X_i\big)_{1\leq i\leq d}$.

The use of correlation ratio for sensitivity analysis has been proposed by Iman and Hora (1990) and Ishigami and Homma (1990), and independently by Sobol' (1990, 1993). The latter was the most popularized, introducing modifications of correlation ratios of groups of factors to achieve a convenient decomposition of the total variance of the phenomenon, provided that the factors are independent; these are the Sobol' indices. While they are theoretically interesting for studying specific interactions of factors, in practice the most useful sensitivity indices are the *first-order indices* and the *total-order indices*. The former tends to evaluate the influence of a group of factor I on its own and is simply $\eta^2(X_I, Y)$, and the latter incorporate all possible interactions with other factors, defined as $1 - \eta^2\big(X_{\complement I}, Y\big)$.

Estimation of correlation ratio can be expensive because it involves the term $\mathrm{E}\big(\mathrm{E}[Y \,|\, X_I]^2\big)$. Most common efficient estimators develop the square conditional expectation as the product $\mathrm{E}\big[f(X_I, X_{\complement I}) \,\big|\, X_I\big]\, \mathrm{E}\big[f(X_I, X'_{\complement I}) \,\big|\, X_I\big]$ where $(X_I, X'_{\complement I})$ is distributed identically to $(X_I, X_{\complement I})$, which in turn is $\mathrm{E}\big[f(X_I, X_{\complement I}) f(X_I, X'_{\complement I}) \,\big|\, X_I\big]$, provided that $X_{\complement I}$ and $X'_{\complement I}$ are independent conditionally to X_I. In practice, this is ensured when the *input factors are independent*. The expectation of the last expression is nothing but $\mathrm{E}\big(f(X_I, X_{\complement I}) f(X_I, X'_{\complement I})\big)$, which is now easier to handle. Typical estimator consists in drawing $2n$ independent observations $\big(X_I^{(j)}, X_{\complement I}^{(j)}\big)_{1\leq j\leq 2n}$ distributed as $\big(X_I, X_{\complement I}\big)$, and evaluating the model at specifically chosen factors combinations, typically

$$\mathrm{E}\big(\mathrm{E}[Y \,|\, X_I]^2\big)_n \overset{\text{def}}{=} \frac{1}{n} \sum_{j=1}^{n} f\big(X_I^{(j)}, X_{\complement I}^{(j)}\big) f\big(X_I^{(j)}, X_{\complement I}^{(n+j)}\big) \ . \tag{3.1}$$

Let us mention that this approach, usually referred to as *pick-and-freeze*, has two drawbacks: first, this constrains the *experience design* (the set of points at which the model must be observed or computed), and second, the required number of model evaluations grows with the number of factors to be investigated.

3.2. Sensitivity Analysis with Dependence Measures. Sensitivity analysis based on correlation ratio as described above is fairly general and can be readily adapted for target and conditional analysis, as we propose later in sections 4.2.1 and 4.2.2. However, several weaknesses can be pointed out.

First, accurate estimation is known for requiring many observations. In addition, although statistical independence implies zero correlation ratio, some variables can be significantly related and yet their correlation ratio be zero as well; in such case, one must resort to total-order indices to identify a relationship. More generally, the statistical variance of the phenomenon might not be the most representative mode of variation. Finally, the above extension for multidimensional phenomenon might not be satisfying. In the classical probabilistic framework, we believe with Da Veiga (2015) that a more general and more versatile notion of sensitivity of a phenomenon to a group of factors can be captured by the notion of statistical dependence. Moreover, De Lozzo and Marrel (2016) recently investigated the use of dependence measures for sensitivity analysis of costly model and illustrated the efficiency of associated significance tests for screening purpose.

We propose somewhere else (Raguet and Marrel, 2018, §§ 3.1 and 3.2), a classification of dependence measures in general, and an extensive discussion on their use for sensitivity analysis in particular. We refer the interested reader to the above article for details; for now, let us focus on two important classes. Note that our choice is mainly guided by ease of implementation (notably the possibility of writing estimators as empirical expectations), aim for generality (factors and phenomenon of any nature and dimension), good invariance properties, and ease of adaptation for target and conditional sensitivity analysis. They both rely on the same principle: measuring the statistical dependence between two variables X and Y by comparing their joint distribution $\mathrm{P}_{X,Y}$ to their product $\mathrm{P}_X \otimes \mathrm{P}_Y$; the two being equal if, and only if, X and Y are independent.

3.2.1. Kernel Quadratic Dependence Measure also called Hilbert–Schmidt Independence Criterion. The first class of dependence measures which we consider arises in the literature from the comparison of the distributions according to their *probability density* or *characteristic functions*, with help of weighted L_2 norms. However, more recent interpretations in terms of *kernel embeddings* of probability distributions yield the *kernel quadratic dependence measure*, following the terminology of Achard et al. (2003) and Diks and Panchenko (2007), also called *Hilbert–Schmidt independence criterion* by Gretton et al. (2005).

In brief, if P is a probability distribution over a generic space $\mathcal{Z}$, and if $k\colon \mathcal{Z}^2 \to \mathbb{R}$ is a suitable *positive definite kernel*, then the mapping $z \mapsto \int k(z,z')\,\mathrm{dP}(z')$ is an element of the *reproducing kernel Hilbert space* induced by k (see the introduction of Berlinet and Thomas-Agnan, 2003, Chapter 4). The norm between such *kernel embeddings* of two different probability distributions is called their *kernel distance*.

A measure of the dependence between X and Y is thus defined by the kernel distance between $\mathrm{P}_{X,Y}$ and $\mathrm{P}_X \otimes \mathrm{P}_Y$. These are probability distributions over the space $\mathcal{X} \times \mathcal{Y}$; a useful particular case arises when the kernel k is separable as $((x,y),(x',y')) \mapsto k_{\mathcal{X}}(x,x')k_{\mathcal{Y}}(y,y')$, where $k_{\mathcal{X}}$ and $k_{\mathcal{Y}}$ are positive definite kernels over $\mathcal{X}$ and $\mathcal{Y}$, respectively. The square of the resulting kernel distance is the kernel quadratic dependence measure, and can be expressed as

$$\text{(3.2)}\quad \mathrm{QDM}_{k_{\mathcal{X}},k_{\mathcal{Y}}}(X,Y) \stackrel{\text{def}}{=} \mathrm{E}(k_{\mathcal{X}}(X,X')k_{\mathcal{Y}}(Y,Y')) + \mathrm{E}(k_{\mathcal{X}}(X,X'))\,\mathrm{E}(k_{\mathcal{Y}}(Y,Y')) - 2\,\mathrm{E}(k_{\mathcal{X}}(X,X')k_{\mathcal{Y}}(Y,Y''))\ ,$$

provided that (X',Y') is independent of, and distributed identically to, (X,Y), and Y'' is independent of X,Y,X',Y' and distributed identically to Y.

A straightforward estimator, given $\big(X^{(i)}, Y^{(i)}\big)_{1\le i\le n}$ independent observations distributed identically to (X, Y), is

$$\begin{aligned}\mathrm{QDM}_{k_\mathcal{X},k_\mathcal{Y}}(X,Y)_n \overset{\text{def}}{=} \frac{1}{n^2}\sum_{i,j=1}^{n} k_\mathcal{X}\big(X^{(i)},X^{(j)}\big)k_\mathcal{Y}\big(Y^{(i)},Y^{(j)}\big) \\ + \frac{1}{n^2}\left(\sum_{i,j=1}^{n} k_\mathcal{X}\big(X^{(i)},X^{(j)}\big)\right)\frac{1}{n^2}\left(\sum_{i,j=1}^{n} k_\mathcal{Y}\big(Y^{(i)},Y^{(j)}\big)\right) \\ - \frac{2}{n}\sum_{i=1}^{n}\left(\frac{1}{n}\sum_{j=1}^{n} k_\mathcal{X}\big(X^{(i)},X^{(j)}\big)\right)\left(\frac{1}{n}\sum_{j=1}^{n} k_\mathcal{Y}\big(Y^{(i)},Y^{(j)}\big)\right),\end{aligned}$$

which should be put under the following handier form for practical implementation,

$$\frac{1}{n^2}\sum_{i,j=1}^{n}\Big(k_\mathcal{X}\big(X^{(i)},X^{(j)}\big)-\frac{1}{n}\sum_{\ell=1}^{n}k_\mathcal{X}\big(X^{(i)},X^{(\ell)}\big)\Big)\Big(k_\mathcal{Y}\big(Y^{(i)},Y^{(j)}\big)-\frac{1}{n}\sum_{\ell=1}^{n}k_\mathcal{Y}\big(Y^{(\ell)},Y^{(j)}\big)\Big).$$

Note that some authors prefer normalizing with factors $n-1$ and $n-2$, or add some other debiasing modifications, which are of little interest here. The required number of computations grows as $O(n^2)$, which is acceptable in situations where the cost for obtaining each observation is large.

When $\mathcal{X}$ is a finite set, the *categorical kernel* $(x, x') \mapsto 1$ if $x = x'$, 0 otherwise, is most typically used. When $\mathcal{X}$ is a normed vector space, the *Gaussian kernel* $(x, x') \mapsto \exp\big(-\|x - x'\|^2/2\sigma^2\big)$ for some parameter $\sigma^2 \in \mathbb{R}$, dependent in practice on the data, is also typically used, but others variants are popular; Sejdinovic et al. (2013) show that the *distance covariance* of Székely et al. (2007) is a particular case.

These last authors propose to normalize their dependence measure in the spirit of the linear correlation coefficient, yielding the *distance correlation*, which is scale-invariant. When Da Veiga (2015) highlights the potential use of the quadratic dependence measure for sensitivity analysis, he also advocates for such normalization, leading to the sensitivity index

$$\overline{\mathrm{QDM}}_{k_\mathcal{X},k_\mathcal{Y}}(X,Y) \overset{\text{def}}{=} \frac{\mathrm{QDM}_{k_\mathcal{X},k_\mathcal{Y}}(X,Y)}{\sqrt{\mathrm{QDM}_{k_\mathcal{X},k_\mathcal{X}}(X,X)}\sqrt{\mathrm{QDM}_{k_\mathcal{Y},k_\mathcal{Y}}(Y,Y)}},$$

and similarly for its *plug-in* estimator $\overline{\mathrm{QDM}}_{k_\mathcal{X},k_\mathcal{Y}}(X,Y)_n$.

3.2.2. Csiszár Divergence Dependence Measure. The second class of dependence measures which we consider compares the distributions through *Csiszár (1972) divergences*. Considering again P, Q two probability distributions over a generic space $\mathcal{Z}$, a *Csiszár divergence* between P and Q can be defined as

$$\mathrm{div}_\phi(\mathrm{P},\mathrm{Q}) \overset{\text{def}}{=} \int \phi\left(\frac{\mathrm{dP}}{\mathrm{dQ}}\right)\mathrm{dQ},$$

where $\phi\colon \mathbb{R}_+ \to \mathbb{R}\cup\{+\infty\}$ is a convex function vanishing at unity, and $\frac{\mathrm{dP}}{\mathrm{dQ}}$ is the Radon–Nikodym derivative of P with respect to Q; note that this can be conveniently extended to cases where P is not dominated by Q. Notable examples include the *(reverse) Kullback–Leibler divergence* with $\phi\colon t \mapsto -\log(t)$ and the *total variation distance* with $\phi\colon t \mapsto |t-1|$.

Again, one can measure dependence between X and Y by measuring discrepancy between $\mathrm{P}_{X,Y}$ and $\mathrm{P}_X \otimes \mathrm{P}_Y$ with help of this tool, yielding *Csiszár divergence dependence measure*, $\mathrm{CDM}_\phi(X,Y) \stackrel{\text{def}}{=} \mathrm{div}_\phi(\mathrm{P}_X \otimes \mathrm{P}_Y, \mathrm{P}_{X,Y})$. The famous special case of the *mutual information*, stemming from the work of Shannon (1948), is obtained with the Kullback–Leibler divergence, $\mathrm{div}_{-\log}(\mathrm{P}_X \otimes \mathrm{P}_Y, \mathrm{P}_{X,Y})$. In the context of sensitivity analysis, Park and Ahn (1994) use a form of mutual information, and later Borgonovo (2007) uses the *total variation* dependence measure. In both cases, estimating the Csiszár divergence is problematic, and the authors must call on *ad hoc* parametric density fits.

In fact, estimations of Csiszár divergences have been studied in many contexts, often focused on specific versions defined by a given function ϕ or on specific knowledge about the involved distributions. In order to devise a general tool, we choose in the current work to rely on nonparametric estimations of the Radon–Nikodym derivatives. Densities at specific points can be estimated through *kernel* or *nearest-neighbors* methods, see for instance the monograph of Silverman (1986). Probabilities are estimated by empirical frequencies. Both can be combined if necessary.

We justify somewhere else (Raguet and Marrel, 2018, § 3.4.2) that a "support" version, $\mathrm{sCDM}_\phi(X,Y)$, where the integration is performed over the range of the joint variable (X,Y) rather than the whole product space $\mathcal{X} \times \mathcal{Y}$, is convenient. The corresponding estimator is

(3.3)
$$\mathrm{sCDM}_\phi(X,Y)_{k_\mathcal{X},k_\mathcal{Y},n} \stackrel{\text{def}}{=} \frac{1}{n}\sum_{i=1}^{n} \phi\left(\frac{\left(\frac{1}{n}\sum_{j=1}^{n} k_\mathcal{X}\left(X^{(i)},X^{(j)}\right)\right)\left(\frac{1}{n}\sum_{j=1}^{n} k_\mathcal{Y}\left(Y^{(i)},Y^{(j)}\right)\right)}{\frac{1}{n}\sum_{j=1}^{n} k_{\mathcal{X},\mathcal{Y}}\left(\left(X^{(i)},Y^{(i)}\right),\left(X^{(j)},Y^{(j)}\right)\right)}\right)$$

where $k_\mathcal{X}$, $k_\mathcal{Y}$ and $k_{\mathcal{X},\mathcal{Y}}$ are the kernels used for estimating densities or probabilities; typically (normalized) Gaussian and categorical, respectively. It has a computational cost of $O(n^2)$, just as for the kernel quadratic dependence measure.

Unfortunately, normalization is not as natural as for the kernel quadratic dependence measure which derives from a square norm. Consider moreover that, for instance, $\mathrm{sCDM}_\phi(X,X)$ might be infinite. We propose to normalize *the estimators* as

$$\overline{\mathrm{sCDM}}_\phi(X,Y)_{k_\mathcal{X},k_\mathcal{Y}n} \stackrel{\text{def}}{=} \frac{\mathrm{sCDM}_\phi(X,Y)_{k_\mathcal{X},k_\mathcal{Y},n}}{\mathrm{sCDM}_\phi(X,X)_{k_\mathcal{X},k_\mathcal{X},n}} \ .$$

Let us mention to the interested reader that this can be seen as a rough generalization of the normalization proposed by Joe (1989) for mutual information of categorical variables, because $\mathrm{sCDM}_{-\log}(X,X)$ is in that case the *Shannon entropy* of X.

4. Some Tools for Conditional and Target Sensitivity Analysis. All of the sensitivity measures detailed above can be easily adapted to target and conditional sensitivity analysis. We describe first general approaches which can be applied to any sensitivity measure. Further details are then given for each tool that we consider.

4.1. Transformations and Weights. Our general approaches are based on transformations of the variable quantifying the phenomenon and on conditioning; specific notions and notations are introduced here.

4.1.1. Targeting with Transformations. In order to study the *occurrences* of the phenomenon Y within the critical domain $\mathcal{C} \subset \mathcal{Y}$, the natural transformation which comes to mind is a binary random variable encoding directly the actual phenomenon of interest and suppressing uninformative fluctuations. This leads to consider the weight function $1_{\mathcal{C}} \colon \mathcal{Y} \to \{0, 1\} \colon y \mapsto 1$ if $y \in \mathcal{C}$, 0 otherwise.

Now, recall that a limited number of observations is usually assumed, so that estimation considerations cannot be ignored. The binary transformation above might result in a significant loss of the information conveyed by the relative values of Y. Indeed, when the critical probability $\mathrm{P}_Y(\mathcal{C})$ is low, most data is summed up to a bunch of zeroes.

Fortunately, a sensible relaxation of the binary assumption can be given as soon as one can evaluate some sort of distance $d_{\mathcal{C}} \colon \mathcal{Y} \to \mathbb{R}_+$ between each point in $\mathcal{Y}$ and the critical domain $\mathcal{C}$. One can compose it by a decreasing real function $\mathbb{R} \to [0,1]$, with the rationals that the closer is an observation to the critical domain, the more likely it is to convey similar information. This of course assumes some kind of regularity of the phenomenon's statistical properties. When $\mathcal{Y}$ lies in an Euclidean space, we typically consider the weight function $y \mapsto \exp(-d_{\mathcal{C}}(y)/s)$, where $d_{\mathcal{C}}(y) \overset{\text{def}}{=} \inf_{y' \in \mathcal{C}} \|y - y'\|$. Here, the exponential function encodes multiplicative contributions, and s is a smoothing parameter depending typically on a measure of dispersion of the values of Y.

In all the following, $w \colon \mathcal{Y} \to [0,1]$ is any kind of the above weight functions, either used deterministically, or as a transformation yielding a random variable through the composition $w(Y)$. Any sensitivity measure between a group of factors X and $w(Y)$ yields a target sensitivity measure.

4.1.2. Conditioning with Weighted Probabilities. Alternatively, in order to study the *behavior* of the phenomenon within the critical domain, a natural idea is *conditioning by the event* $\{Y \in \mathcal{C}\}$. Given an initial probability space $(\Omega, \mathfrak{F}, \mathrm{P})$, if $A \in \mathfrak{F}$ is an event of nonzero probability, then conditioning by A simply means *endowing the measurable space* $(\Omega, \mathfrak{F})$ *with the probability measure* $\mathrm{P}_{|A}$, defined as $\mathrm{P}_{|A}(B) \overset{\text{def}}{=} \mathrm{P}(B \cap A) / \mathrm{P}(A)$ for all $B \in \mathfrak{F}$. If X is a random variable over $(\Omega, \mathfrak{F}, \mathrm{P})$, then its law conditionally to A is the law of the mapping X over the conditioned probability space $\big(\Omega, \mathfrak{F}, \mathrm{P}_{|A}\big)$, that is $\mathrm{P}_{X|A} \overset{\text{def}}{=} \mathrm{P}_{|A} \circ X^{-1}$.

Just as we introduced smooth relaxation of the binary transformation above, it might be useful to consider extensions of conditioning allowing to take into account some of the information outside the critical domain. This can be easily done by observing that $\mathrm{P}_{|A}(B)$ can be expressed as $\int_B 1_A \,\mathrm{dP} \big/ \int_\Omega 1_A \,\mathrm{dP}$. If W is a positive nonzero random variable over $(\Omega, \mathfrak{F}, \mathrm{P})$ with finite expectation, we define the *probability* P *weighted by* W, noted P^W, with for all $B \in \mathfrak{F}$, $\mathrm{P}^W(B) \overset{\text{def}}{=} \int_B W \,\mathrm{dP} \big/ \int_\Omega W \,\mathrm{dP}$. In other words, P^W is the probability distribution absolutely continuous with respect to P whose density is proportional to W. In addition, if X is a generic random variable, we clarify that the notation P^W_X stands for the image measure $\big(\mathrm{P}^W\big)_X$; although strictly speaking, it cannot be confused with a weighted image measure $(\mathrm{P}_X)^W$ since W is defined over Ω and not over the range of X. Let us also exemplify the particular cases of weighted probabilities which are actual conditional probabilities, $\mathrm{P}_{|A} = \mathrm{P}^{1_A}$, and $\mathrm{P}_{X|A} = \mathrm{P}^{1_A}_X$.

In a probabilistic framework, any sensitivity measure is defined depending on a (usually implicit) probability space. When conditioning by weight W, we change the underlying probability measure, but the mappings defining the random variables are left unchanged; in such case, the notations are prefixed by $\big[\mathrm{P}^W\big]$. Let us underline here that, provided that the expectations exist, $\big[\mathrm{P}^W\big]\ \mathrm{E}(X) = \mathrm{E}(WX)/\mathrm{E}(W)$,.

For conditional sensitivity analysis, we typically use conditioning by weights $W \overset{\text{set}}{=} w(Y)$ as defined above.

4.2. Correlation Ratio. As presented in subsection 3.1, sensitivity indices based on correlation ratio (widely known as Sobol' indices) all consists in (possibly weighted sums of) correlation ratios of the phenomenon Y with well chosen groups of factors, noted generically X.

4.2.1. Target Correlation Ratio. Correlation ratios can be directly applied to the transformation $w(Y)$, yielding target sensitivity analysis indices based on $\eta^2(X, w(Y))$. Observe that even for multidimensional Y, the transformation $w(Y)$ takes values in [0,1], thus sparing us the trouble of interpreting multidimensional extensions of correlation ratio.

4.2.2. Proposition of Hybrid Conditional Correlation Ratio. Following section 4.1.2, the correlation ratio conditioned by the critical domain is the quantity $\left[\mathrm{P}^{w(Y)}\right]\ \eta\big(X, Y\big)$. It is important to note that even if the factors are independent under P, they usually are not under $\mathrm{P}^{w(Y)}$. The covariance estimator in (2.1) cannot be used anymore, hindering the estimation of the correlation ratio as explained in subsection 3.1.

Alternatively, it is possible to define a conditional correlation ratio by another transformation of Y. We have seen that $w(Y)$, keeping no memory of the actual values of Y, is more adapted to target sensitivity; for conditional sensitivity, it is preferable to weight multiplicatively the values, as $w(Y)Y$. However, the fact that w vanishes on regions away from the critical domain seems arbitrary: the value zero might not be meaningful for the phenomenon at hand. Since the correlation ratio is a measure of variance, it still seems relevant to set a constant value over these regions, but equal to the expectation of the resulting transformation; they would then not contribute to the variance of the phenomenon. We thus define the transformation

$$Y_w \overset{\text{def}}{=} w(Y)Y + (1 - w(Y))y_0 \quad \text{such that} \quad y_0 \overset{\text{def}}{=} \mathrm{E}(Y_w)\,; \quad \text{yielding} \quad y_0 = \frac{\mathrm{E}(w(Y)Y)}{\mathrm{E}(w(Y))}\,.$$

Observe that with $w \overset{\text{set}}{=} 1_{\mathcal{C}}$, $\mathrm{E}(w(Y)) = \mathrm{P}(Y \in \mathcal{C})$ and $y_0 = \mathrm{E}[Y \,|\, Y \in \mathcal{C}]$; more generally, we have $y_0 = \left[\mathrm{P}^{w(Y)}\right]\mathrm{E}(Y)$. In any case, it is easy to estimate with $\sum_{i=1}^{n} w(Y^{(i)})Y^{(i)} \big/ \sum_{i=1}^{n} w(Y^{(i)})$, and $\eta^2(X, Y_w)$ can be estimated in turn with any usual method, with the advantage over the conditional correlation ratio that even observations associated to null weight are somehow taken into account.

4.3. Kernel Quadratic Dependence Measure. We recall that this dependence measure is also known as Hilbert–Schmidt independence criterion, and is detailed in section 3.2.1.

4.3.1. Target Kernel Quadratic Dependence Measure. Just as with the correlation ratio, target sensitivity measure of a group of factors can be obtained through the weight transformations $w(Y)$, that is to say $\mathrm{QDM}_{k_{\mathcal{X}}, k_{w(\mathcal{Y})}}(X, w(Y))$. Our notation reminds that the kernels depend on the underlying spaces; in the particular case of the binary transformation $w \overset{\text{set}}{=} 1_{\mathcal{C}}$, it seems natural to use a categorical kernel for $k_{\{0,1\}}$. Let us mention that this last case was already suggested and briefly illustrated by Da Veiga (2015).

4.3.2. Conditional Kernel Quadratic Dependence Measure. The conditional version $\left[\mathrm{P}^{w(Y)}\right]\ \mathrm{QDM}_{k_{\mathcal{X}}, k_{\mathcal{Y}}}(X, Y)$ is defined through kernel distance and can be again expressed as expectations of kernels analogously to (3.2)

$$\begin{aligned}\mathrm{E}(k_{\mathcal{X}}(X,X')k_{\mathcal{Y}}(Y,Y')\bar{w}(Y)\bar{w}(Y'))\\ + \mathrm{E}(k_{\mathcal{X}}(X,X')\bar{w}(Y)\bar{w}(Y'))\,\mathrm{E}(k_{\mathcal{Y}}(Y,Y')\bar{w}(Y)\bar{w}(Y'))\\ - 2\,\mathrm{E}(k_{\mathcal{X}}(X,X')k_{\mathcal{Y}}(Y,Y'')\bar{w}(Y)\bar{w}(Y')\bar{w}(Y''))~,\end{aligned}$$

having taken care of normalizing the weights $\bar{w} \overset{\text{def}}{=} \mathrm{E}(w(Y))^{-1}w$. This can also be analogously estimated, by replacing empirical averages by weighted averages

$$\begin{aligned}\sum_{i,j=1}^{n}\Bigg(k_{\mathcal{X}}\big(X^{(i)},X^{(j)}\big) - \sum_{\ell=1}^{n}k_{\mathcal{X}}\big(X^{(i)},X^{(\ell)}\big)\hat{w}\big(Y^{(\ell)}\big)\Bigg)\\ \times\Bigg(k_{\mathcal{Y}}\big(Y^{(i)},Y^{(j)}\big) - \sum_{\ell=1}^{n}k_{\mathcal{Y}}\big(Y^{(\ell)},Y^{(j)}\big)\hat{w}\big(Y^{(\ell)}\big)\Bigg)\times\hat{w}\big(Y^{(i)}\big)\hat{w}\big(Y^{(j)}\big)~,\end{aligned}$$

with empirical normalized weights $\hat{w} \overset{\text{def}}{=} \big(\sum_{i=1}^{n} w\big(Y^{(i)}\big)\big)^{-1}w$.

4.4. Csiszár Divergence Dependence Measure. We refer to section 3.2.2 for the definitions of the "support" Csiszár divergence dependence measure.

4.4.1. Target Csiszár Divergence Dependence Measure. As previously, target sensitivity measure of a group of factors can be obtained through Csiszár divergence dependence measures of the transformations $w(Y)$, that is to say $\mathrm{sCDM}_\phi(X, w(Y))$. Let us emphasize that, in the case of the binary transformation $w \overset{\text{set}}{=} 1_{\mathcal{C}}$, Radon–Nikodym derivatives should be estimated with normalized categorical kernel.

4.4.2. Conditional Csiszár Divergence Dependence Measure. The conditional versions are respectively $\big[\mathrm{P}^{w(Y)}\big]~\mathrm{CDM}_\phi(X,Y) = \mathrm{div}_\phi\Big(\mathrm{P}^{w(Y)}_{X,Y}, \mathrm{P}^{w(Y)}_{X}\otimes\mathrm{P}^{w(Y)}_{Y}\Big)$ and $\big[\mathrm{P}^{w(Y)}\big]~\mathrm{sCDM}_\phi(X,Y) = \mathrm{sdiv}_\phi\Big(\mathrm{P}^{w(Y)}_{X}\otimes\mathrm{P}^{w(Y)}_{Y}, \mathrm{P}^{w(Y)}_{X,Y}\Big)$. In the estimator in (3.3), the weights are influencing the expectations in each density estimation and each integral, yielding with empirical normalized weights $\hat{w} \overset{\text{def}}{=} \big(\sum_{i=1}^{n} w\big(Y^{(i)}\big)\big)^{-1}w$,

$$\sum_{i=1}^{n}\phi\left(\frac{\Big(\sum_{j=1}^{n}k_{\mathcal{X}}\big(X^{(i)},X^{(j)}\big)\hat{w}\big(Y^{(j)}\big)\Big)\Big(\sum_{j=1}^{n}k_{\mathcal{Y}}\big(Y^{(i)},Y^{(j)}\big)\hat{w}\big(Y^{(j)}\big)\Big)}{\sum_{j=1}^{n}k_{\mathcal{X},\mathcal{Y}}\big(\big(X^{(i)},Y^{(i)}\big),\big(X^{(j)},Y^{(j)}\big)\hat{w}\big(Y^{(j)}\big)\big)}\right)\hat{w}\big(Y^{(i)}\big)~.$$

Versions with nearest-neighbors density estimation can also be easily adapted. For instance, the k-th nearest-neighbor distance of the point $(x,y)\in\mathcal{X}\times\mathcal{Y}$ is the smallest distance d_k such that the cumulative sum of the weights of the points within d_k distance to (x,y) reaches k. If copula transforms are used, recall that they are also modified by weighted probabilities.

5. Numerical Illustrations. We conduct here numerical illustrations and comparisons of the different adapted tools that we propose for target and conditional sensitivity analysis. These concise examples also demonstrate that target and conditional sensitivity analysis explore aspects of a model which are both different from global sensitivity analysis and valuable for practitioners.

Note that all the above tools are implemented in the language R, interfaced with C++ for some routines; we intend to integrate them to the *Sensitivity* package of R.

5.1. Presentation of Test Case Functions. To illustrate target and conditional sensitivity analysis, we first propose a model with a simple but strong nonlinearity, which we call *minimum-normal-uniform*. It is defined in dimension $d \overset{\text{set}}{=} 2$, with $f\colon x \mapsto \min(x_1, x_2)$, with independent factors conveniently noted $X_1 \overset{\text{set}}{=} N$ and $X_2 \overset{\text{set}}{=} U$, following respectively a standard normal distribution, and a uniform distribution over [0,1].

We then explore the more complicated Ishigami–Homma model which is well-known from the sensitivity analysis community. This model is defined in dimension $d \overset{\text{set}}{=} 3$ by

$$f\colon x \mapsto \sin(x_1) + a\sin^2(x_2) + b{x_3}^4\sin(x_1),$$

where $a, b \in \mathbb{R}_+$; all factors (X_1, X_2, X_3) are independent and uniformly distributed over $[-\pi,\pi]$. The influence of the factor X_2 is purely additive, its importance being modulated by the parameter a. The influence of the factor X_1 includes an additive part and an interaction with the factor X_3, the balance being tuned by parameter b. We set here the parameters $a \overset{\text{set}}{=} 5$ and $b \overset{\text{set}}{=} 0.1$, so that first-order Sobol' indices are $\eta^2(X_1, Y) = 0.40$, $\eta^2(X_2, Y) = 0.29$ and $\eta^2(X_3, Y) = 0$, while total-order ones are $1 - \eta^2(X_{^c\{1\}}, Y) = 0.71$, $1 - \eta^2(X_{^c\{2\}}, Y) = 0.29$, and $1 - \eta^2(X_{^c\{3\}}, Y) = 0.31$.

In both models, we suppose that the critical domain $\mathcal{C}$ is defined by Y exceeding a given critical value: $\mathcal{C} \overset{\text{set}}{=} \{y \in \mathcal{Y} \,|\, y \geq c\}$, chosen as the *ninth decile* of Y computed empirically, $c \overset{\text{set}}{=} F^{-1}_{Y,n}(0.9)$. Recall that target and conditional sensitivity measures are defined via weight functions $w\colon \mathcal{Y} \to [0,1]$ which depends on $\mathcal{C}$. In both models, we use the indicator function $1_{\mathcal{C}}$, and a smooth relaxation in accordance with the notion of distance over the reals,

$$w_{\mathcal{C}}\colon y \mapsto \exp\left(-\frac{\max(c-y,0)}{s\,\sigma_Y}\right)\;; \tag{5.1}$$

where σ_Y is an estimation of the standard deviation of Y, and $s \overset{\text{set}}{=} 1/5$ is a factor tuning the smoothness, chosen so that $w_{\mathcal{C}}$ almost vanishes one standard deviation away from $\mathcal{C}$.

5.2. Tested Target and Conditional Sensitivity Tools. Among the large choice of interesting sensitivity measures, we consider those in Table 5.1. Correlation ratios estimated with pick-and-freeze factors combinations are included because they are currently the most popular for global sensitivity analysis. Recall however from section 4.2.2 that they do not allow for proper conditional versions, because conditioning introduces dependence between factors. Consequently, we use what we call the "hybrid" version. We report here results only for the first-order indices, but we can mention that the total-order indices behave similarly for target and conditional sensitivity analysis of both analytical models.

Then, we include the quadratic dependence measure with Gaussian kernel, and the mutual information dependence measure with truncated nearest-neighbors copula density estimation Blumentritt and Schmid (2012). For the hard target versions, recall that $1_{\mathcal{C}}(Y)$ is a discrete random variable over $\{0, 1\}$. For the mutual information, its law is estimated by empirical frequencies and the law of the joint $(X_i, 1_{\mathcal{C}}(Y))$ is estimated by conditioning. For the quadratic dependence measure, we use a categorical kernel for $k_{\{0,1\}}$.

Table 5.1: Sensitivity measures used for target and conditional analysis experiments. The generic weight function w is either $1_{\mathcal{C}}$, or the smooth relaxation $w_{\mathcal{C}}$ defined in (5.1).

Notation	Definition	Expression for factor i
$\mathrm{S}_{\mathrm{PF}}^{(1,\mathrm{tgt},w)}$	First-order correlation ratio target sensitivity measure	$\eta^2(X_i, w(Y))_n$
$\mathrm{S}_{\mathrm{PF}}^{(1,\mathrm{hbd},w)}$	First-order correlation ratio hybrid sensitivity measure	$\eta^2(X_i, Y_w)_n$
$\mathrm{QDM}_{\mathrm{G}}^{(\mathrm{tgt},w)}$	Normalized target kernel quadratic dependence measure	$\overline{\mathrm{QDM}}_{k_{\mathcal{X}},k_{w(\mathcal{Y})}}(X_i, w(Y))_n$
$\mathrm{QDM}_{\mathrm{G}}^{(\mathrm{cnd},w)}$	Normalized conditional kernel quadratic dependence measure	$\left[\mathrm{P}^{w(Y)}\right] \overline{\mathrm{QDM}}_{k_{\mathcal{X}},k_{\mathcal{Y}}}(X_i, Y)_n$
$\mathrm{MI}_{\mathrm{c,nn}}^{(\mathrm{tgt},w)}$	Normalized target mutual information	$\overline{\mathrm{sCDM}}_{-\log}(X_i, w(Y))_{k_{\mathrm{nn}},n}$
$\mathrm{MI}_{\mathrm{c,nn}}^{(\mathrm{cnd},w)}$	Normalized conditional mutual information	$\left[\mathrm{P}^{w(Y)}\right] \overline{\mathrm{sCDM}}_{-\log}(X_i, Y)_{k_{\mathrm{nn}},n}$

5.3. Numerical Experiments and Results. For each model, we draw hundred different samples of size $n \overset{\text{set}}{=} 1\,000$ and schematize the resulting distribution of each conditional or target sensitivity measure, together with their global sensitivity counterpart, with Tuckey box plots on Figures 5.1 and 5.2.

On the minimum-normal-uniform model, the critical value is $c = 0.62$. The global analysis, on Figures 5.1(a) to 5.1(c), is unanimous: the factor N is much more important than the factor U. This is not surprising, since N presents more variability and takes values far below the minimum of U.

The target analysis indicates that the ordering of the factors is the same, although the relative importance difference is less drastic. This is again not surprising because N has a higher probability to be below the critical value than U, hence still determining again the outcome of interest here, but in the same time, the variability of N below the threshold has no influence anymore. The correlation ratio on Figure 5.1(d), is much less precise than the dependence measures (e) and (g). The target mutual information shows an important bias, but this does not impact the ordering of the factors. It can be noted that the smoothed versions present less variability while still ordering correctly the factors. However, it is unclear if this is thanks to better behavior of the smooth estimator, or simply because the estimated smoothed quantity is some kind of interpolation between target and global measures. In the latter case, this effect would turn out unfavorable if the ordering of the factors were different in both analysis. The smoothed target mutual information on Figure 5.1(i) is clearly problematic, as it yields the same importance measures as the global version (c). This can be explained by the fact that the density estimation is based on copula transforms, and that Y and $w_{\mathcal{C}}(Y)$ have very similar copula transforms with the level of smoothing that we used; in this case and for this particular estimator, smoothing is not judicious.

The conditional analysis tells a whole different story: now U is more important than N. Indeed, conditionally to both U and N being no less than c, U varies in $[c,1]$ while N varies in $[c,+\infty[$, in such a way that the former has more chance to determine

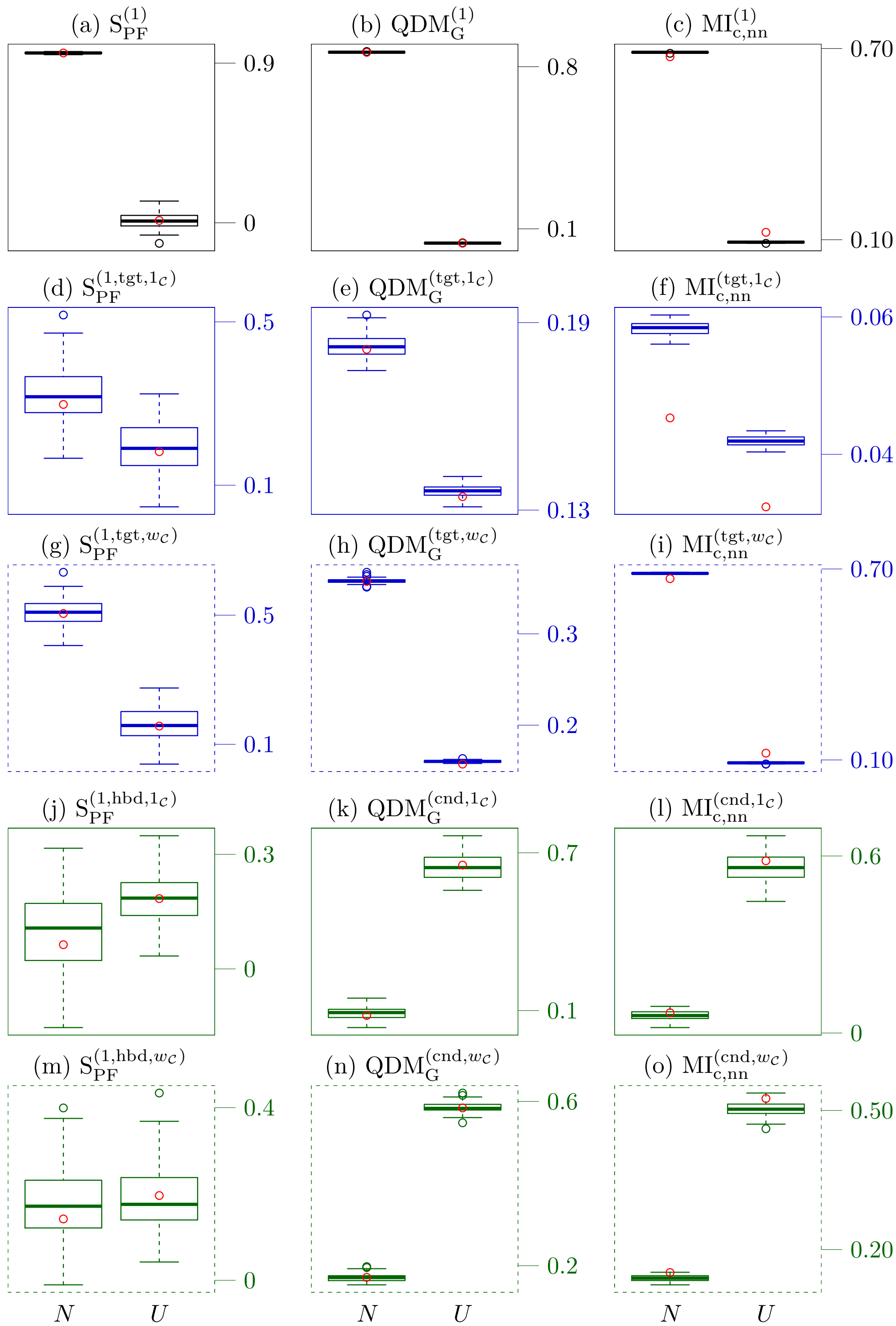

Figure 5.1: Global (black), target (blue) and conditional (green) sensitivity analysis of minimum-normal-uniform model on samples of size $n \overset{\text{set}}{=} 1\,000$. Red circles are asymptotic values estimated on samples of size $n \overset{\text{set}}{=} 10\,000$.

the value of their minimum. This is clearly captured by both dependence measures considered, on Figures 5.1(k) and (l), and moreover their smoothed conditional versions improve perceptibly their precision, as indicated by the relative height of the box plots in Figures 5.1(n) and (o), Hybrid correlation ratio adapted to pick-and-freeze estimator follows the same trend on Figures 5.1(j) and (m), but precision is not satisfying at all.

For the Ishigami–Homma model, the critical value is $c = 6.31$. Here, the relative importances of the factors are different in each analysis case. In the global analysis, the factor X_1 is the most important, and the factors X_2 and X_3 have lower importance, being ranked differently according to different sensibility measures (Figures 5.2(a), (b) and (f)).

In the target analysis, X_3 has now similar importance to X_1, while X_2 has much less. Indeed, the combined effect of X_1 and X_3 easily exceeds the critical value, while the isolated action of X_2 can merely approach the critical value (recall that the parameter $a \overset{\text{set}}{=} 5$ is significantly less than c). As previously, the dependence measures offer more precision than the correlation ratio with pick-and-freeze estimator. It can be noted that they do not agree exactly on the relative importance of X_1 and X_3 on Figures 5.2(e) and (f), and that the target kernel quadratic dependence measure does not differ much from its global version in (b). Once again, the smoothed versions for target analysis are not particularly relevant: even if they seem to slightly reduce the variability of the estimators of kernel quadratic dependence measures, they completely fail to improve the estimators of the mutual information computed through copula density.

In the conditional analysis, X_3 becomes the dominant factor: being raised to the fourth power, the corresponding term presents steep derivatives in the regime of high values. The mutual information on Figure 5.2(l) seems the most suitable method for putting this into evidence. Once again for conditional analysis, the smoothing techniques do improve the quality of both dependence measures considered, even enabling kernel quadratic dependence measure to capture the dominance of X_3.

6. Conclusion. In the context of sensitivity analysis of complex phenomena in presence of uncertainty, this work motivates and precises the idea of orienting the analysis towards a critical domain of the studied phenomenon. This gives rise to the notions of target and conditional sensitivity analysis. We show that many concepts in the literature relate to them, although usually in more specific frameworks depending on considered applications. Building up on modern statistical tools, we define mathematically a broad range of sensitivity measures which make as few assumptions as possible on the model at hand, while remaining flexible enough to be adapted to many particular situations.

To provide dedicated tools for target and conditional sensitivity analysis, we focus our attention on the popular sensitivity indices based on correlation ratio, namely Sobol' indices, and on dependence measures which seem to us particularly well-adapted to our problematic. More particularly, we consider two dependence measures: the kernel quadratic dependence measure also called Hilbert–Schmidt independence criterion and the Csiszár divergence dependence measure, the mutual information being a particular case of the latter. For these different selected sensitivity measures, we propose adapted versions for target and conditional analysis, by considering transformation of the output using hard or smooth weight functions. We also propose an hybrid version for correlation ratio.

The proposed tools are illustrated and compared on analytical test cases. These experiments on synthetic data clearly illustrate the interest of target and conditional sensitivity analysis which can differ from global one. They also show that dependence

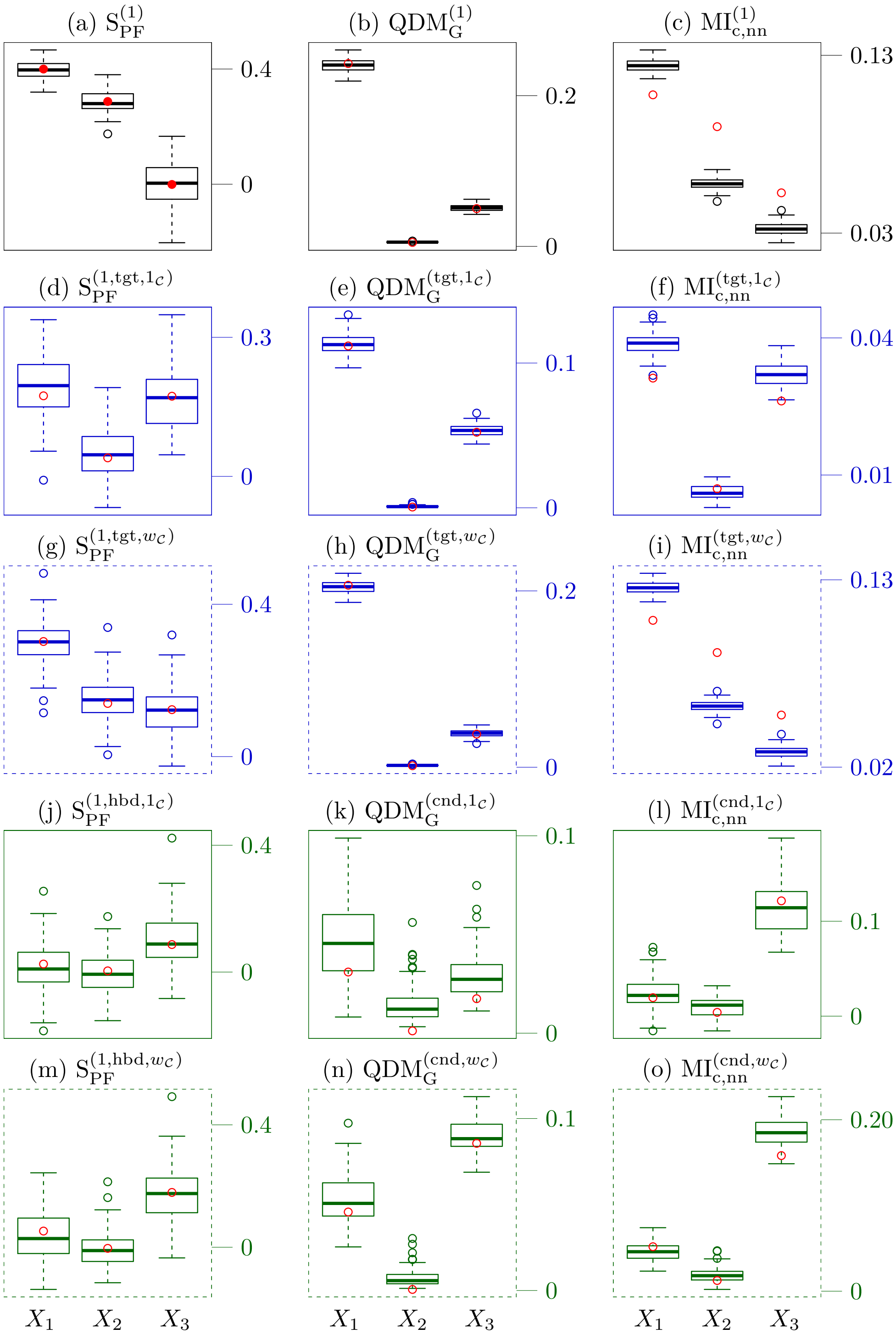

Figure 5.2: Global (black), target (blue) and conditional (green) sensitivity analysis of Ishigami–Homma model on samples of size $n \overset{\text{set}}{=} 1\,000$. Filled red dots are analytical values, hollow red circles are asymptotic values estimated on samples of size $n \overset{\text{set}}{=} 10\,000$.

measures are well suited for this task and are more precise than the correlation ratio. Our preliminary results favor the use of kernel quadratic dependence measures rather than correlation ratio. The mutual information with truncated nearest-neighbors copula density estimation is also relevant (low variability and good capacity to capture influence), but more adjustments should be required to reduce its bias. Furthermore, even if more numerical explorations are necessary before drawing further conclusions, the proposed smooth versions of estimators seem clearly suited for conditional estimators, especially when the number of available observations in the critical domain is low. However, their use for target sensitivity analysis remains questionable yet.

Altogether, this work is a good starting point towards sensitivity measures which are more powerful and more adapted to questions raised by experimenters. There is still much to do before actually establishing good practice. Naturally, we do not pretend to exhaustiveness, since we cannot evaluate in this work all existing dependence measures. Other popular approaches of global sensitivity analysis could be adapted to target or conditional sensitivity analysis. We voluntarily set those aside for brevity, but other approaches such as the regional sensitivity analysis ought to be more deeply studied; e.g. by considering other measures of discrepancy between probability distributions rather than Kolmogorov distance.

Then, it is important to test the target and conditional sensitivity measures in more challenging situations, it particular where the critical probability is low, or to put it otherwise, where less critical observations are available. In that respect, we believe that the smoothing technique is promising, if correctly tuned. Last but not least, all these sensitivity measures can only be completely assessed through confrontation to real data.

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