Discrepancy measures for sensitivity analysis in mathematical modeling

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Abstract

While Sensitivity Analysis (SA) improves the transparency and reliability of mathematical models, its uptake by modelers is still scarce. This is partially explained by its technical requirements, which may be hard to decipher and interpret for the non-specialist. Here we draw on the concept of discrepancy and propose a sensitivity measure that is as easy to understand as the visual inspection of input-output scatterplots. Numerical experiments on classic SA functions and on meta-models suggest that the symmetric $L_2$ discrepancy measure is able to rank the most influential parameters almost as accurately as the variance-based total sensitivity index, one of the most established global sensitivity measures.
Sensitivity analysis (SA), the study of how the uncertainty in a model output can be apportioned to uncertainty in the model inputs [1], is a cornerstone of responsible mathematical modeling and a recommended practice in the modeling guidelines of the European Commission, the Intergovernmental Panel on Climate Change or the US Environmental Protection Agency [2–4]. Modelers dispose of several SA methods: Variance-based methods, for instance, are well embedded in statistical theory (ANOVA), can treat sets of factors and can be used in problem settings such as “factor fixing” or “factor prioritization” [5]. Moment-independent methods may be preferred over variance-based ones when the output has a long-tailed distribution [6], while VARS is especially suited to inform about the local structure of the output variance [7]. If the inputs are correlated, the use of Shapley coefficients may be a good alternative [8]. Other methods are also available and a rich literature informs on which are the most efficient estimators in each of the SA approaches available to the analyst [9, 10].

Despite this abundance, there is still a scarce uptake of uncertainty quantification techniques and SA in mathematical modeling. When performed, the SA is often conducted by moving one variable-at-a-time (OAT) to determine its influence on the output, an approach that is only guaranteed to work in low-dimensional, linear models [11]. One of the reasons behind this neglect is that proper SA methods are grounded on statistical theory and may be hard to implement and understand by the non-specialist [12].

Here we propose an SA measure whose use and interpretation requires little statistical training and that is as intuitive as the visual inspection of input–output scatterplots. Given a model of the form \( y = f(x) \), \( x = (x_1, x_2, \ldots, x_i, \ldots, x_d) \in \mathbb{R}^d \), where \( y \) is the model output and \( x_1, \ldots, x_d \) are \( d \) model inputs described by probability distributions, a scatterplot of \( x_i \) against \( y \) with the points displaying a trend is a safe indicator of \( x_i \) influencing the model output. The sharper the trend or the larger the area without points, the stronger the influence of \( x_i \) [5]. In contrast, a scatterplot where the dots are uniformly distributed across the space formed by \( x_i \) and \( y \) evidences a totally non-influential parameter (Fig. 1a–c). Scatterplots are a well-established qualitative approach in SA to rank influential parameters and often precede a quantitative assessment of influence by means of the sensitivity methods mentioned above [13].

We turn the visual assessment of scatterplots into a specific sensitivity index by drawing on the concept of discrepancy, a term associated with the design of numerical experiments [16]. Discrepancy measures quantify the deviation of the distribution of points in a multi-dimensional space from the uniform distribution. If the space of the input factors is represented as the unit cube in \( d \) dimensions, a uniform distribution would correspond to a density of points in an arbitrary portion of the hypercube identical to the volume of the portion itself, i.e., a portion corresponding to 10% of the cube should also contain 10% of the design points. Several measures have been proposed to compute discrepancy and here we explore the potential of \( L_2 \) discrepancy measures given their higher computational affordability [17]. Specifically, we focus on the “modified” [18], the star [19], the classic \( L_2 \), the centered [17], the wrap-around [20] and the symmetric [17] \( L_2 \) discrepancy measures.

To check how these measures perform in an SA framework, we compare their capacity to properly rank the most influential model inputs with that of the total-order index (\( T_i \)) [21] computed with the Jansen estimator [22]. This is one of the most accurate variance-based SA estimators and the litmus test against which new SA measures tend to be compared [9, 23]. We focus on this setting because most often, and especially for high-dimensional models such as those in the environmental sciences/climate domains, the interest lies in properly identifying the top ranks only [24]. Firstly, and in order to relax the dependency of the results on the benchmarking design, we compare the discrepancy measures and the Jansen estimator on a meta-model based on the Becker [10] metafunction. Our meta-model randomizes the model functional form over 13 different univariate functions representing common responses in physical systems, from linear to cubic and trigonometric (Fig. ??) [10]. It also randomizes over the model dimensionality \( d \), the sampling method, the underlying (continuous) input distributions and the strength of higher-
Fig. 1: Scatterplots and discrepancy measures as sensitivity proxies. a), b), c): Scatterplots of $x_i$ against $y$ for three different two-dimensional functions. The red dots show the running mean. The functions are F1, F2 and F3 respectively in Azzini and Rosati [14]. In a), $y$ is totally determined by $x_1$ while $x_2$ is non-influential. In b), $x_1$ is more influential than $x_2$ given its sharper trend. In c), $x_1$ is more influential than $x_2$ given the presence of larger areas where points are more rarefied. d) Pearson correlation ($r$) between the vector of Savage-transformed ranks of the model inputs produced by the Jansen estimator and the different discrepancy measures. Each dot is a simulation conducted with the meta-model, for a total of $2^{10}$ simulations, and the $y$-axis denotes the number of model inputs in each simulation. The greener (lighter) the color, the better the match between $T_i$ (Jansen estimator) and the discrepancy measure. The exploration is done in a non-rectangular domain because the total number of runs required by the Jansen estimator is $C = n(d + 1)$, where $n$ is the sample size of the base sample matrix. We have fixed the total number of runs for the discrepancy measures in each simulation at $C$ to ensure that the comparison with the Jansen estimator is done on the same number of model runs. e) Boxplots summarizing the results for both the meta-model approach and the Bratley et al. function [15] (centre line, median; box limits, upper and lower quartiles; whiskers, 1.5x interquartile range; points, outliers). f) Scatterplots and $T_i$ indices of the Bratley et al. function [15]. g) Example of the scatterplots and their $T_i$ values after randomly discretizating inputs of the Bratley et al. function.
order effects active in the function. This approach allows to conduct the comparison on a very wide range of SA settings [9] (Fig. ??). Secondly, we extend the analysis towards inputs with discrete distributions by randomly discretizing the Bratley et al. function [15], a $d$-dimensional Type A function (few influential inputs and minor interactions [25]). Discrete inputs are also common in models either as variables or triggers and the Bratley et al. functions permits to observe how discrepancy measures respond when both continuous and discrete inputs coexist in the same model.

Several $L_2$ discrepancy measures nicely match the ranking of the most important parameters by the Jansen estimator, especially the symmetric, the wrap-around and the centered. With our meta-model experiment, the median correlation ($r$) between the ranks produced by the Jansen and these discrepancy measures is 0.85, 0.8 and 0.75 respectively, with the symmetric showing the narrowest spread. With the Bratley et al. function, $r$ equals 0.82, 0.77 and 0.73 for the wrap-around, the symmetric and the centered measure respectively (Fig. 1d–e). The star and the modified discrepancy measure lag significantly behind (median of $\sim 0.55$ and $\sim 0.66$ in the meta-model and the Bratley et al. approach respectively) and they overturn the ranks in several simulations, producing negative $r$ values.

These results open up a potentially fertile research path on the use of discrepancy measures as sensitivity indices in mathematical modeling. In this brief report we have used the Pearson correlation as a measure to check the correspondence between the ranks provided by the Jansen estimator and the discrepancy measures selected, but other measures of fit may also be used. Different discrepancy algorithms may fit better different definitions of importance corresponding to different SA methods. More work is needed to investigate the structure of the fit between discrepancy measures and measures of importance.

Acknowledgements

We thank Bertrand Iooss and Art Owen for their insights into discrepancy measures. This work has been funded by the European Commission (Marie Sklodowska-Curie Global Fellowship, grant number 792178 to AP).

Code availability

The R code to replicate our results is available in Puy [26] and in https://github.com/arnaldpuy/discrepancy.

Author contributions

AS conceptualized the paper. AP ran the simulations. AP and AS wrote the paper and revised the final version.

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Supplementary Materials

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1 Figures

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Figure S1: Univariate functions included in the meta-model, based on Becker's meta-function [1].

![Space images](image)

Figure S2: Examples of the $x_i, y$ spaces created by the meta-model. a) Three-dimensional function. b) Twelve-dimensional function.
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