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Highlights

- Sample-based estimators for the total sensitivity index are compared
- Avenues to improve the existing best practices (design and estimators) are explored
- The convergence to the analytical values of test functions is adopted as benchmark
- The two-matrices design outperforms other multiple-matrices based designs
- Distributing model evaluations on the most important factors yields improvements

Variance-based sensitivity analysis: The quest for better estimators and designs between explorativity and economy

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Abstract

Variance-based sensitivity indices have established themselves as a reference among practitioners of sensitivity analysis of model outputs. A variance-based sensitivity analysis typically produces the first-order sensitivity indices S_i and the so-called total-effect sensitivity indices S_{Ti} for the uncertain factors of the mathematical model under analysis.

Computational cost is critical in sensitivity analysis. This cost depends upon the number of model evaluations needed to obtain stable and accurate values of the estimates. While efficient estimation procedures are available for S_i (Tarantola et al., 2006), this availability is less the case for S_{Ti} (Iooss and Lemaître, 2015). When estimating these indices, one can either use a sample-based approach whose computational cost depends on the number of factors or use approaches based on meta-modelling/emulators (e.g., Gaussian processes).

The present work focuses on sample-based estimation procedures for S_{T_i} for independent inputs and tests different avenues to achieve an algorithmic improvement over the existing best practices. To improve the exploration of the space of the input factors (design) and the formula to compute the indices (estimator), we propose strategies based on the concepts of *economy* and *explorativity*. We then discuss how several existing estimators perform along these characteristics.

Numerical results are presented for a set of seven test functions corresponding to different settings (few important factors with low cross-factor interactions, all factors equally important with low cross-factor interactions, and all factors equally important with high cross-factor interactions). We conclude the following from these experiments: a) sample-based approaches based on the use of multiple matrices to enhance the economy are outperformed by designs using fewer matrices but with better explorativity; b) among the latter, asymmetric designs perform the best and outperform symmetric designs having corrective terms for spurious correlations; c) improving on the existing best practices is fraught with difficulties; and d) ameliorating the results comes at the cost of introducing extra design parameters.

***Table 1** - Legend*

$A, B, C, \dots$	Sample matrices
$A_B^{(i)}$	Sample matrix where all columns are from A except for column i, which is from B; likewise for other sample matrices C, D and so forth
$a_j, b_j, c_j, \dots$	j-th row of matrices A, B, C, etc., respectively
$a_{B,j}^{(i)}$	j-th row of matrix $A_B^{(i)}$
η	Economy of a given design, defined as the number of elementary effects useful to compute S_{T_i} ($\eta \leq N_t$)
EE	Generic elementary effect
N_t	Total number of elementary effects
$E_{X_i}(\cdot), V_{X_i}(\cdot)$	Expected value and variance of argument $(\cdot)$ taken over factor X_i
$E_{X_{\sim i}}(\cdot), V_{X_{\sim i}}(\cdot)$	Expected value and variance of argument $(\cdot)$ taken over all factors but X_i
X	Generic sample matrix $A, B, C, \dots$
j	Running index for the rows of a sample matrix $j = 1, 2, \dots, N$
i	Running index for factor $i = 1, 2, \dots, k$
k	Number of factors
l	Running index over factor *j;* $l = 1, 2, \dots, k$

ά ή	Running indices for the pool of sample-matrices (e.g., Ὀ ὂ ÁÎÄ Ὀ ὂ)
ὲ	Number of sample matrices
ΰ	Column-dimension (length) of a single sample matrix
ΰ	Total number of points in the design
p	Running index for the block on which the algorithm is executed (each block has column length ΰ ς
ὶ	Running index for the repetition ὶ ρ ς 8 υπ
ί	Running index for the block with a power of two ί ρ ς 8 Ὠ ρ
Ὑ	First-order effect sensitivity index for a generic factor Ὠ
Ὑ	Total-effect sensitivity index for a generic factor Ὠ
…	Explorativity, the fraction of non-repeated coordinates in the design

1. Introduction

The sensitivity analysis of mathematical models aims to ‘apportion the output uncertainty to the uncertainty in the input factors’ (Saltelli and Sobol’, 1995). Uses of sensitivity analysis are found in quality assurance, model calibration, model validation, uncertainty reduction, and model simplification, which are just a few among the possible applications.

Over the last three decades, sensitivity analysis (SA) has made steps to establish itself as a self-standing discipline with a community of practitioners gathering around the SAMO (Sensitivity Analysis of Modelling Output) international conferences since 1995. Special issues have been devoted to SA (Borgonovo and Tarantola, 2012; Ginsbourger et al., 2015; Helton et al., 2006; Saltelli, 2009; Tarantola and Saint-Geours, 2015; Tarantola and Saltelli, 2003; Turányi, 2008), mostly in relation to the SAMO events. Available textbooks for sensitivity analysis include Borgonovo (2017), Cacuci (2003), de Rocquigny et al. (2008), Fang et al. (2005), and Saltelli et al. (2008, 2004, 2000). SA is acknowledged as a useful practice in model development and applications. Its use in regulatory settings (e.g., in impact assessment studies) is prescribed in guidelines both in Europe and the United States (European Commission, 2015; Office of Management and Budget, 2006; US EPA, 2015). SA is also an ingredient of sensitivity auditing (Saltelli et al., 2013; Saltelli and Funtowicz, 2014), a procedure to investigate the relevance and plausibility of model-based inference as an input to policy (European Commission, 2015; Science Advice for Policy by European Academies, 2019).

Tools such as sensitivity analysis and sensitivity auditing are particularly needed at this point in time when the accuracy, relevance and plausibility of the statistical and mathematical models used to support policy are often the subject of controversy (Jakeman et al., 2006; Padilla et al., 2018; Pilkey and Pilkey-Jarvis, 2007; Saltelli and Funtowicz, 2017; Saltelli and Giampietro, 2017), including at the time of submitting the present article, the COVID-19 pandemic (Saltelli et al., 2020; Steinmann et al., 2020). As highlighted elsewhere (Lo Piano and Robinson, 2019; Saltelli et al., 2019; Saltelli and Annoni, 2010), part of the problem in the validation of models is that the quality of the accompanying SA is often wanting. Most SA applications still favour the use of a method known as OAT, where the sensitivity of factors is gauged by moving One-factor-At-a-Time (Ferretti et al., 2016; Saltelli et al., 2019). When a sensitivity analysis is run in this fashion, it results in a perfunctory test of the robustness of the model predictions. While different methods exist for sensitivity analysis (see recent reviews in Becker and Saltelli (2015), Borgonovo and Plischke (2016), Iooss and Lemaître (2015), Neumann (2012), Norton (2015), Pianosi et al. (2016), Saltelli et al. (2012), and Wei et al. (2015)), the so-called 'variance-based' methods are considered to be a reference among practitioners. To make an example, when a new method for SA is introduced, its performance is investigated against variance-based measure (see, e.g., Mara et al. (2017)). At present, the most widely used variance-based measures are Sobol' indices (Sobol′, 1993), particularly the Sobol' first-order sensitivity measures S_i and the so-called total sensitivity indices T_i (Homma and Saltelli, 1996). In the following, we take the suggestion from Glen and Isaacs (2012) and for simplicity adopt the symbol T_i, rather than S_{Ti} or S_i^T, for the total sensitivity indices, although these notations are also commonly found in the literature.

In the next section, we briefly describe how S_i and T_i are defined and computed for the case of independent input factors (Sections 2.1-2.2). Then, we present the set of estimators used (Section 2.3) and define the concepts of economy and explorativity in the estimation procedures for T_i (Saltelli et al., 2010) (Section 2.4). The experimental set up, including the test functions, is outlined in Section 3. Section 4 is dedicated to presenting and discussing our findings, while the general conclusions on the lessons learned are drawn in Section 5.

2 Variance-based sensitivity analysis

2.1 Variance-based sensitivity measures

For a scalar model output $Y = f(X_1, X_2, \ldots, X_k)$, where X_1 to X_k are k uncertain factors, the first-order sensitivity index S_i can be written as

$$S_i = \frac{V_{X_i}\left(E_{\mathbf{X}_{\sim i}}(Y \mid X_i)\right)}{V(Y)} \qquad (1)$$

Figure 6 - MAE vs cost (N_T) on a logarithmic scale for the Šaltenis asymmetric estimator (circle, continuous line), two-matrix-based symmetric estimator (triangle, dashed line), Lamboni three-matrix-based estimator (square, dot-dashed-dotted line), Lamboni four-matrix-based estimator (cross, dash-dotted line) and. Lamboni six-matrix-based estimator (empty square, cross-dotted line). Functions: A1, A2, B1, B2, B3, C1, and C2 (Eq. 24-30). Python implementation.

As shown above, the trade-off between Ω and … demonstrates that ἐ ς is not a convenient design choice. Another way to look at these results is to assess them in terms of stars, which are computationally equivalent to the Saltelli asymmetric design (Saltelli et al., 2010), as seen in section 2.4. The basic design is the one where each star is made of *k+1* points using *2k* coordinates. To increase Ω, one must increase the number of points in the stars, although this results in decreasing … since one uses more coordinates of the core. The cases where the number of matrices is greater than 2 fall into this class. This approach led to worse results. In other words, increasing Ω does not seem to pay off.

We have also tried to compute ˝Ɣ using matrix ═ alone, i.e., instead of computing ˝Ɣ from ˝Ω ╪ and ˝Ω ╪ we used ˝Ω ╪ and ˝Ω ╪ . In this approach, when the last N-th row is reached, one uses ˝Ω ╪ and ˝Ω ╪ for ˝Ɣ, i.e., the system closes on itself. However, this approach did not lead to improvements.

Another sampling procedure we have tested to improve the Šaltenis asymmetric estimator consisted of variably investing the computational budget by improving ˝Ɣ's estimation for the subset of the most important factors while devoting less computational resources to the least important ones for each subsequent model execution. In this adaptive sampling strategy, the choices of the factor to estimate are made using increasing blocks of power of two to fully take advantage of the properties of the low-discrepancy Sobol' sequence.

The number of design parameters of the adaptive sampling strategy is reduced to a modicum. Let one assume that one has ὒ Ω ρ ς model runs available.

- The algorithm is run as per the Šaltenis asymmetric estimator (Saltelli et al., 2010) to 'warm up' to a sample size ὒ=ς at a cost of Ω ρ ς.
- The Ω factors are then ordered in decreasing order of the standard deviation of the elementary effect ίὸΩ.
- At every following block of rows ὒ=ς (with ί in the range ρ Ω ρ), it is decided whether the computation of the elementary effect can be stopped at the Ω ί factor per order of decreasing importance, thus saving runs.
- The condition upon which this decision is made is the ratio between ίὸΩ-s. It is assumed that ίὸΩ would be reduced by a factor of Ὦς by doubling the sample size.

- Hence, the main assumption of the computation is that if íȯΩ$^{ᶦ ᵗ ᶦ ᵒ}$ Ӥς íȯΩ, this latter factor (and all those having lower íȯΩs) can be removed from the calculation in the following block.

The computational details are available from [the dedicated Jupyter notebook](). The results are here presented for test functions A1 and A2, for which "Ɣ differs across parameters. Another type of function G has also been tested in this experiment, where A3 ὤ ρ ς τ ψ ρφ σς corresponds to various degrees of importance across parameters.

In Figure 7, one can appreciate how our method outperforms the â D O W H Q L V D V \ P P H W U L F H V W by up to a factor of two for functions A2 and A3. In this context, the importance of input variables on the output uncertainty can be easily disentangled due to the difference in magnitude across factors' "Ɣ. This is the setting of a typical real-world model, where the importance of the input factors on the output uncertainty obeys the Pareto principle (Pareto, 1906) with few factors responsible for most of the output variance. However, the case where the sensitivity indices of the input factors are closer in magnitude is more challenging. This adaptive sampling strategy does not outperform the â D O W H Q L V *asymmetric estimator* in the case of function A1 (Figure 7).

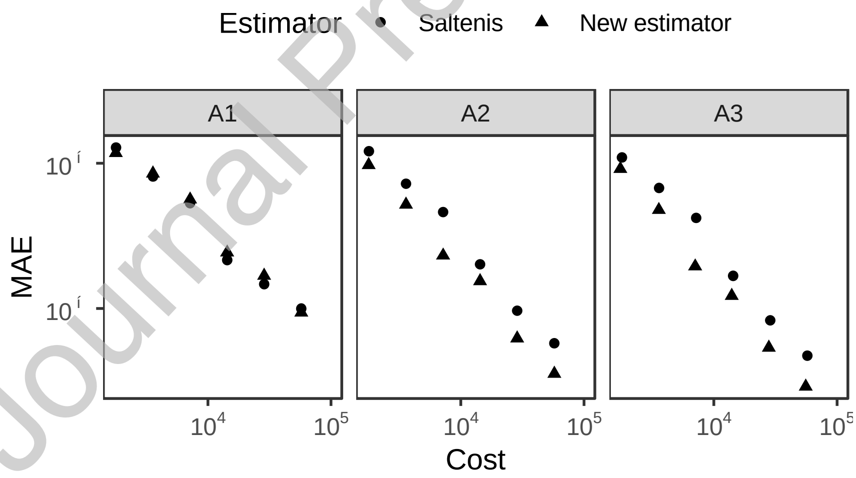

Figure 7 - MAE vs cost (N_T) on a logarithmic scale for the â D O W H Q L V D V \ P P H W U L F H V W (circle) and the proposed adaptive sampling strategy (triangle). Each point corresponds to the MAE reported at full cost ΰ ΐ ρ ς. Functions: A1 and A2 (Eqs. 24-25, respectively) and A3.

5 Conclusions

Taking the works of Glen and Isaacs (2012), Lamboni (2018), and Saltelli et al. (2010) as our points of departure, we have explored different estimators to improve the computation of the total-effect index "Ɣ for independent factors using a taxonomy of test functions proposed by Kucherenko (2011).

We have seen that the estimator of Glen and Isaacs (2012) is outperformed by Šaltenis and Dzemyda (1982) and the Saltelli asymmetric design (Saltelli et al., 2010). Furthermore, we did not observe improvements in the computational results by extending the symmetric matrix arrangement to values ὲ ς. The larger number of effects obtained with ὲ ς does not compensate for the loss of explorativity, as is also evidenced by our discrepancy calculation. The increase in economy by using more matrices is offset by the loss of explorativity due to the higher share of repeated coordinates.

To increase the explorativity, one would need to rely on a 'stars' design with centres having less than *k* rays, which decreases the economy. The latter approach has led to an improvement in the setting of factors receiving a number of estimates proportional to their importance. However, this comes at the cost of introducing an extra design parameter.

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Author statement

Samuele Lo Piano: Formal analysis, Investigation, Methodology, Software, Validation, Visualisation, Writing.

Federico Ferretti: Formal analysis, Investigation, Methodology, Software, Validation.

Arnald Puy: Funding acquisition, Software, Validation, Visualisation, Writing.

Daniel Albrecht: Investigation, Methodology, Writing.

Andrea Saltelli: Conceptualisation, Formal analysis, Funding acquisition, Supervision, Writing.

Declaration of interests

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

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A Appendix

Table A1 *±Terms composing the Glen & Isaacs (2012) estimator D3*

Term	Explicit formula
[illegible]	[illegible]
[illegible]	[illegible]
[illegible]	[illegible]
[illegible]	[illegible]
[illegible]	[illegible]