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Decision Support

Global sensitivity measures from given data

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ABSTRACT

Simulation models support managers in the solution of complex problems. International agencies recommend uncertainty and global sensitivity methods as best practice in the audit, validation and application of scientific codes. However, numerical complexity, especially in the presence of a high number of factors, induces analysts to employ less informative but numerically cheaper methods. This work introduces a design for estimating global sensitivity indices from given data (including simulation input–output data), at the minimum computational cost. We address the problem starting with a statistic based on the L^1-norm. A formal definition of the estimators is provided and corresponding consistency theorems are proved. The determination of confidence intervals through a bias-reducing bootstrap estimator is investigated. The strategy is applied in the identification of the key drivers of uncertainty for the complex computer code developed at the National Aeronautics and Space Administration (NASA) assessing the risk of lunar space missions. We also introduce a symmetry result that enables the estimation of global sensitivity measures to datasets produced outside a conventional input–output functional framework.

1. Introduction

Simulation and decision support models accompany managers in the solution of operational problems (Dillon et al., 2003). Theoretical advances as well as the steady increase in computing power allow analysts to build sophisticated codes that capture detailed facets of the problems under investigation. However, because of model complexity the structure of the input–output mapping becomes a black-box exposing analysts and decision makers to the risk of overconfidence in model predictions (Kleijnen, 2005).

Agencies such as the US Environmental Protection Agency (US EPA, 2009, p. vii), the National Aeronautics and Space Administration (Borgonovo and Smith, 2011), the Florida Commission Hurricane Loss Projection Methodology (Iman et al., 2005) and the European Commission (Saisana et al., 2005; Saltelli, 2009), recommend the use of uncertainty analysis and global sensitivity analysis (SA) as part of best practices for model application, validation and audit. On the role of uncertainty analysis in the context of modelling, we also refer to Kleijnen (2001). When model parameters are not known with certainty, uncertainty analysis is essential for modellers to obtain a representation of model predictions consistent with their state-of-knowledge, hedging the risk of overconfidence in model results (see Kleijnen and Helton (1999), Helton (2004) for a thorough discussion).

Global sensitivity analysis (SA) allows decision makers to sharpen their view of the problem. As underlined in Helton (2004), *SA should be a fundamental part of any analysis that involves the assessment and propagation of uncertainty*. By a global SA, we gain several insights concerning the input–output mapping, and the key drivers of uncertainty (Saltelli et al., 2000). When the number of model inputs is large, recognising the factors on which to focus resources in data collection and/or in further modelling efforts becomes crucial for most effectively managing uncertainty. However, a high number of model input factors increases the computational burden (the so-called *curse of dimensionality* (Rabitz and Alış, 1999)). In such a case, analysts tend to use computationally convenient methods (non-global) to the detriment of rigour (see the surveys in Saltelli and Annoni (2010), Saltelli et al. (2011)).

In operations research (OR), the first work addressing global sensitivity analysis is Wagner (1995), where variance-based sensitivity measures are introduced and discussed. The literature has, since then, produced several results on the twofold side of ameliorating variance-based measures estimation and of proposing new sensitivity measures. Among the recently introduced sensitivity measures, the class of density-based is attracting increasing attention (Borgonovo, 2007; Liu and Homma, 2009; Caniou and Sudret, 2010) for their ability to overcome certain limitations associated with the interpretation of variance-based measures in the presence of dependencies among the model inputs. However, their estimation runs the risk of becoming infeasible when the number of model inputs is large or when the computing time of the model takes longer than a few minutes.

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In this work, we introduce a novel approach that enables to estimate density-based sensitivity measures directly from the dataset generated by an uncertainty analysis. Thus, the computational burden is the same as in a traditional Monte Carlo uncertainty propagation. Furthermore, the method is independent of the sampling generation method (Latin hypercube, quasi-Monte Carlo, etc.).

We show that the proposed method yields also variance-based sensitivity measures or measures based on alternative separation metrics (e.g., Kullback–Leibler, Kolmogorov–Smirnov). Our first step is a formal definition of the estimators for density-based measures. We rely on the notion of class-conditional densities where a class is a sub-sample stemming from a suitable partition of the dataset. We prove consistency theorems that ensure asymptotic convergence. Numerical experiments reveal a low-sample bias for density-based methods. This bias is intrinsic to designs based on replicates or partitioning of the same dataset (Morris et al., 2008). Our goal is to control numerical noise while keeping the approach independent of the way the dataset is generated and without requiring additional model runs. We analyse two strategies. For the class of models in which large sample sizes are within reach of computational time, we propose a bias-controlling filter based on the Kolmogorov–Smirnov (KS) test controlled by a dummy variable. For computationally intensive models, at finite or small sample sizes, we discuss a different strategy, namely, the robust determination of confidence intervals through the bias reducing bootstrap approach of Efron and Gong (1983), see also Hall (1992). A numerically demanding test case with analytically known values of the sensitivity statistics is employed to demonstrate the strategy.

In developing the designs, we introduce new properties of density-based sensitivity statistics. In particular, suppose that X and Y are two random variables. (In a model input/output framework X is called the independent or input variable while Y is the dependent or output variable). For the moment-independent measure δ introduced by Borgonovo (2007) we show that $\delta(X,Y) = \delta(Y,X)$. By this symmetry, X or Y can indifferently play the role of dependent (or independent) variable. This finding extends the estimation of global sensitivity statistics beyond the traditional model input/output frame. We discuss a non-functional case study (involving an alphabet-letter B shape). Results show that by $\delta(X,Y)$ one unveils a statistical dependence that would not be appraised by a variance-based method.

We then challenge the approach by application to the output of a complex computational code. The code is the simulation model utilised by NASA and the US Idaho National Laboratory for safety assessment in the design phase of the next generation of lunar space missions (Borgonovo and Smith, 2011). The model is computationally intensive, with 872 uncertain input factors. This high number often rules out the direct estimation of global sensitivity measures. However, the proposed strategy enables the estimation of both density-and variance-based statistics by post-processing the dataset generated by Monte Carlo simulation of the original code. One fully exploits the advantage of the proposed design: computational burden is independent of the number of factors. Confidence intervals indicate that the sensitivity measures are accurately estimated, providing analysts with a reliable identification of the key drivers of uncertainty. Results also show that uncertainty drivers do not coincide with the key drivers obtained through a deterministic sensitivity method applied to the same model. By the simultaneous estimation of variance-based measures, one also realises that interactions play a notable role in the input–output mapping (Borgonovo and Smith, 2011).

This paper is organised as follows. Section 2 gives a concise review of global sensitivity analysis. Section 3 proposes some new results and examples for variance-based sensitivity measures. Section 4 defines density-based sensitivity measures and presents new properties. Section 5 introduces the estimators and proves convergence and consistency results. Section 6 describes the computational algorithm and introduces a bias-controlling filter. Section 7 discusses numerical results for analytical test cases and the determination of confidence intervals of the sensitivity measures. Section 8 presents extensions to alternative sensitivity measures. Section 9 discusses the extension to a non-input–output setting. A full-scale application is studied in Section 10. Section 11 offers conclusions.

2. Estimating global sensitivity statistics: A review

This section offers a review of uncertainty and global sensitivity analysis (SA), with focus on numerical aspects. Uncertainty analysis (sometimes referred to as probabilistic sensitivity (Hazen and Huang, 2006)) consists of the steps discussed in Helton (2004). These steps can be synthesised in the assignment of distributions to the model input factors followed by propagation into the simulation code via Monte Carlo simulation (see also Helton and Davis, 2003). The first task, distribution assignment, is the crucial step in ensuring the quality and consistency of results (see Chick, 2001; Helton, 2004).

Several ways for generating random inputs that follow a given joint distributions are available, ranging from crude Monte Carlo to Latin hypercube sampling and quasi-random low-discrepancy sequences (e.g., Halton, Sobol', Niederreiter) (Wang, 2006). The input sample is fed into the model to obtain the output distribution. Global SA is performed after the uncertainty analysis and allows analysts to obtain additional information about the input–output mapping (Saltelli and Tarantola, 2002; Oakley and O'Hagan, 2004). Let us introduce the global SA frame. In accordance with the classical assumptions of Gelfand and Smith (1990), we assume to have information about the factors probability distribution, either joint or marginal, with or without correlation, and that this knowledge comes from measurements, estimates, expert opinion, physical bounds, output from simulations, analogy with factors for similar species, and so forth (Saltelli and Tarantola, 2002, p. 704). Consider $\mathbf{x} = [x_1, x_2, \ldots, x_k] \in \mathcal{X} \subseteq \mathbb{R}^k$ and $y \in \mathcal{Y} \subseteq \mathbb{R}$ related through the function

$$g : \mathcal{X} \to \mathcal{Y}, \quad \mathbf{x} \mapsto y = g(\mathbf{x}). \tag{1}$$

The function $g(\mathbf{x})$ is not necessarily known analytically and is generally the output of a computer code performing a numerical simulation. In a global SA, $\mathbf{x}$ is a realisation of the random vector $\mathbf{X} = [X_1, X_2, \ldots, X_k]$ on a measurable space $(\mathcal{X}, \mathcal{A})$, with X_i on space $(\mathcal{X}^i, \mathcal{A}^i)$. The probability distribution of X_i is denoted by $P_{X_i}(A) = \mathbb{P}(X_i \in A), A \in \mathcal{A}^i$, and its distribution function by $F_{X_i}(x) = \mathbb{P}(X_i \leqslant x), x \in \mathcal{X}^i$. For Y, similar notations apply. Here, $\mathbb{P}(X_i \leqslant x)$ is the probability measure that reflects the decision maker's view about X_i. As mentioned, it can correspond to a given probability model or to a mixture of models. Because in this work we are interested on estimation algorithms, we shall assume, for simplicity, that the probabilistic distributions are fully specified. The model output y becomes a random variable Y on $(\mathcal{Y}, \mathcal{B})$. Let us recall that the conditional probability of Y given X_i is a map

$$P_{Y|X_i} : \mathcal{B} \times \mathcal{X}^i \ni (Y, x) \mapsto P_{Y|X_i = x}(Y) \in [0, 1], \tag{2}$$

satisfying the following properties: $P_{Y|X_i=x}(\cdot)$ is a probability measure on $\mathcal{B}$, $P_{Y|X_i=x}(Y)$ is measurable in $\mathcal{A}^i$. Associated with $P_{Y|X_i}$ are the conditional cumulative distribution $F_{Y|X_i}(y) = P_{Y|X_i}(Y \leqslant y)$ and the conditional density of Y given X_i which is defined using the marginal density functions $f_Y(y), f_{X_i}(x)$ and the joint density function $f_{X_iY}(x, y)$ by

$$f_{Y|X_i=x}(y) = \begin{cases} \frac{f_{X_i Y}(x,y)}{f_{X_i}(x)}, & f_{X_i}(x) > 0, \\ f_Y(y), & \text{otherwise.} \end{cases} \quad (3)$$

Before discussing global sensitivity methods, it is useful to recall the concept of sensitivity analysis setting. A setting is a *way of framing the sensitivity analysis quest in such a way that the answer can be confidently entrusted to a given method* (Saltelli et al., 2008, p. 24). The two main settings are *factor prioritisation* and *factor fixing*. They correspond to the identification of the most and least relevant factors, respectively.

Several global methods have been developed since the 1990s to address these two settings: screening methods (including the randomised one-at-a-time design of Morris (1991) and sequential bifurcation techniques (Bettonvil and Kleijnen, 1997; Wan et al., 2010), see also Kleijnen (2009a) for an overview), non-parametric or regression-based (Saltelli and Marivoet, 1990; Helton, 1993), variance-based methods (Sobol', 1993; Oakley and O'Hagan, 2004), density-based (Park and Ahn, 1994; Chun et al., 2000; Borgonovo, 2007; Liu and Homma, 2009) and expected-value-of-information (EVI) based methods (Oakley et al., 2010). The common feature of the last three classes of methods is that they are, on the one hand, the most informative in terms of uncertainty appraisal and, on the other hand, the most computationally intensive. Let γ_i be a global sensitivity measure (variance-, density- or EVI-based). Then, γ_i is obtained by (i) defining an appropriate inner statistic (say $\gamma|x_i$) conditional on $X_i = x_i$ and (ii) averaging $\gamma|x_i$ over X_i. The corresponding brute force computational cost is

$$C = k \cdot n_{int} \cdot n_{ext} + n, \quad (4)$$

where k is the number of factors, n_{int} the sample size necessary for estimating the inner statistic, n_{ext} the sample size used for the external expectation, and n the size of the uncertainty analysis sample, if needed. For instance, C in Eq. (4) is the cost for estimating EVI sensitivity measures following the algorithm in Oakley et al. (2010). It is also the cost for a brute-force estimation of variance-based statistics. These statistics are defined as

$$\eta_i^2 = \frac{\mathrm{Var}[\mathrm{E}[Y|X_i]]}{\mathrm{Var}[Y]} = 1 - \frac{\mathrm{E}[\mathrm{Var}[Y|X_i]]}{\mathrm{Var}[Y]}, \quad i = 1, \ldots, k. \quad (5)$$

Pearson (1905) named η_i^2 *correlation ratio*. Sensitivity measures of the form of Eq. (5) have been independently introduced as global sensitivity measures in the 1990s by Sobol' (1993) in high-dimensional integration, and by Wagner (1995) in operations research. The difference between the definitions proposed by these two authors lies in the independence assumption invoked by Sobol' (1993), and not by Wagner (1995). Both authors, in addition to first order sensitivity indices introduce the total order indices

$$\eta_i^T = \frac{\mathrm{E}[\mathrm{Var}[Y|\mathbf{X}_{\sim i}]]}{\mathrm{Var}[Y]} = 1 - \frac{\mathrm{Var}[\mathrm{E}[Y|\mathbf{X}_{\sim i}]]}{\mathrm{Var}[Y]}, \quad i = 1, \ldots, k \quad (6)$$

where $\mathbf{X}_{\sim i} = (X_1, \ldots, X_{i-1}, X_{i+1}, \ldots, X_k)$ is the random vector where all factors are fixed but X_i. Under the condition $F_{\mathbf{X}}(\mathbf{x}) = \prod_{i=1}^k F_{X_i}(x_i)$ (independence assumption), η_i^T coincides with the fraction of the model output variance that persists if all factors are fixed but X_i. The independence assumption also enables a reduction in computational burden proven in Sobol' (1993). Refining results of (Homma and Saltelli, 1996; Saltelli, 2002), Saltelli et al. (2010) introduce a design for estimating first and total order variance-based sensitivity measures at $C = k(n + 2)$ model runs. In the presence of input dependencies, the computational cost increases (Kucherenko et al., 2012). Researchers have also explored ways for estimating sensitivity measures at $C = n$ runs of the original model. A first set of strategies consists of utilising model reduction through emulators (also called metamodels or surrogates). A first review of the literature in design and analysis of computer experiments is offered in the seminal work of Sacks et al. (1989b), where contributions as O'Hagan (1978), McKay et al. (1979), Iman and Helton (1988), and Sacks et al. (1989a) are analysed. These works have paved the way to subsequent research in the area of metamodelling (or model emulation, surrogate modelling). We also recall the monograph by Santner et al. (2003); for recent developments, we refer to the thematic issue edited by Bayarri et al. (2009). For a review on Bayesian approaches to model emulation we refer to Oakley and O'Hagan (2004); on smoothing splines ANOVA models, to Gu (2002) and Ratto et al. (2007); on kriging, to Kleijnen (2008) and Kleijnen (2009b); on metamodelling through polynomial chaos expansion to Sudret (2008). In metamodelling, n model runs are used to train the emulator. The remaining runs of a double-loop design are performed using the emulator in place of the original model. This strategy is investigated in the estimation of variance-based sensitivity indices by Oakley and O'Hagan (2004), Sudret (2008), Ratto et al. (2007), and Ziehn and Tomlin (2009), which use Gaussian emulation, polynomial chaos expansion, smoothing splines and functional ANOVA with orthogonal polynomials, respectively. It is used in the estimation of density-based sensitivity measures in Ratto et al. (2009) and Borgonovo et al. (2011). In Ratto et al. (2009) the model output density is approximated by an Edgeworth series, exploiting estimates of the first four order moments obtained via the emulator of Ratto et al. (2007). In Borgonovo et al. (2011), the statistics are estimated by substitution of the metamodel for the original model. A notable computational burden reduction can be achieved, if the emulator fits the original model. However, if training requires a high number of model runs, the potential advantage diminishes.

The Fourier Amplitude Sensitivity Test (FAST) (Cukier et al., 1973; Tarantola et al., 2006; Xu and Gertner, 2007) lowers computational burden at around n model runs for estimating η_i^2 for each factor i, without passing through an emulator. The EASI approach by Plischke (2010) reduces the overall costs C for all factors to n model runs. The main difference between FAST and EASI is that FAST requires evaluation of the model according to a specific design, while EASI is independent of the way in which the dataset is produced.

3. Some new results on variance-based sensitivity measures

The literature has shown that η_i^2 is a robust measure of functional dependence. However, some types of functional dependence are not captured by η_i^2 as the next result shows (the proof is in Appendix A).

Proposition 1. *Consider a multivariate function of the form*

$$y = f(x_1, \ldots, x_k) = a(x_J) g(x_j) + b(x_{J'}), \quad J \oplus \{j\} \oplus J' = \{1, \ldots, k\}, \quad (7)$$

where $g(x_j)$ is a function of x_j, J and J' are groups of indices such that $j \notin J \cup J'$, $J \cap J' = \emptyset$, $a(\cdot)$ is a function of the factors in J and $b(\cdot)$ is a function depending on the remaining factors in J'. Let $\mathbf{X} = (X_1, \ldots, X_k)$ be a random vector such that (X_j), $\mathbf{X}_J = (X_i; i \in J)$ and $\mathbf{X}_{J'} = (X_i; i \in J')$ are stochastically independent groups of random variables. Then, if $E[g(X_j)] = 0$, the first order effect of $Y = f(\mathbf{X})$ satisfies $\eta_i^2 = 0$ for all $i \in J$.

Proposition 1 states the following. If a set of factors, J, is paired with one factor j which is independent of the remaining factors and such that $\mathrm{E}[g(X_j)] = 0$, then η_i^2 are zero for all $i \in J$. Thus, Y is statistically dependent on X_J, but the influence of any factor i in J is not revealed by η_i^2. Proposition 1 holds independently of the functional forms assigned to $a(\cdot)$, $b(\cdot)$, $g(\cdot)$ and of the choice of the distributions $F_j(\cdot)$, $F_J(\cdot)$ and $F_{J'}(\cdot)$.

In the global SA literature, a widely studied example of the form of Eq. (7) is the Ishigami function (Saltelli et al., 2004),

$$Y = \sin X_1 + 7\sin^2 X_2 + 0.1X_3^4 \sin X_1$$
$$= (1 + 0.1X_3^4)\sin X_1 + 7\sin^2 X_2, \quad (8)$$

with $\mathbf{X} = [X_1, X_2, X_3, X_4], \mathcal{X} = (-\pi, \pi)^4$ and $X_i \sim U(-\pi, \pi)$ (independently uniformly distributed). Here, we have $J = \{3\}$, $j = 1$ and $J' = \{2\}$. X_4 is an additional dummy model input.

The first four plots (a)–(d) in Fig. 1 show estimates of $f_Y(y)$ (thick lines) and $f_{Y|X_i=x_i}(y)$ for $i = 1, 2, 3, 4$ given a quasi-Monte Carlo sample of size 8192. We will discuss the method behind these plots in Section 5. One notes that X_1, X_2 and X_3 lead to evident modifications in $f_Y(y)$. However, if an analyst quantifies the contribution of X_3 to uncertainty by individual contribution to variance, she would consider X_3 as non-influential. In fact, $\eta_3^2 = 0$ by Proposition 1. However, as Fig. 1c shows, knowing $X_3 = x_3$ modifies $f_Y(y)$. In the case of the Ishigami function, the influence of X_3 can be inferred by estimation of the total order sensitivity measure η_i^T. (The estimation of η_i^T from given data is an open issue).

Proposition 1 contains as a particular case the following result found in Borgonovo and Baucells (2011). That is, for any product function

$$y = \prod_{i=1}^{k} g_i(x_i) + K, \quad (9)$$

where K is a constant and $g_i(\cdot)$ is such that $\mathrm{E}[g_i(X_i)] = 0$ and $(X_1, \ldots, X_k)$ are independent, the first and total order effects are non-informative as for all $i, \eta_i^2 = 0$ and $\eta_i^T = 1$. Thus, for functions modelled after Eq. (9), one cannot prioritise factors using variance-based measures (both η_i^2 and η_i^T provide degenerate answers). However, the issue is solved by complementing variance-based measures with density-based measures, whose rationale is explained in the next section.

4. Density-based sensitivity methods: Generalisations and new results

Let $X : (\Omega, \mathcal{F}) \to (\mathcal{X}, \mathcal{A})$ and $Y : (\Omega, \mathcal{F}) \to (\mathcal{Y}, \mathcal{B})$ be two continuous random variables on probability space $(\Omega, \mathcal{F}, \mathbb{P})$, where X and Y are not necessarily the input and output of a computer code. For discrete random variables, we refer to the last paragraph of Section 5.

If $X = x$, then $F_{Y|X=x}(y)$ represents the decision maker's new degree-of-belief about Y. Measuring the separation between $F_Y(y)$ and $F_{Y|X=x}(y)$ or between $f_Y(y)$ and $f_{Y|X=x}(y)$ is a way to quantify the effect of fixing X at x on the decision maker's degree-of-belief. A wide literature is available on the subject of distribution separation measurements, whose complete review is outside the purpose of the present article. We refer to Csiszár (1963) and Glick (1975) and to the review of Gibbs and Su (2002). We utilise the L^1-norm between densities for the reasons we are to discuss. The separation is written as

$$s(x) = \int_{\mathcal{Y}} |f_Y(y) - f_{Y|X=x}(y)|\, \mathrm{d}y \quad \text{or, with factor } i \text{ of interest,}$$
$$s_i(x) = \int_{\mathcal{Y}} |f_Y(y) - f_{Y|X_i=x}(y)|\, \mathrm{d}y. \quad (10)$$

In Eq. (10) the operator $\int_{\mathcal{Y}} |\cdot|$ is a separation measurement in the sense of Glick (1975). By Scheffé's theorem (Scheffé, 1947; Devroye and Györfi, 1985)

$$s(x) = \int_{\mathcal{Y}} |f_Y(y) - f_{Y|X=x}(y)|\, \mathrm{d}y = 2 \sup_{B \in \mathcal{B}} |P_Y(B) - P_{Y|X=x}(B)|, \quad (11)$$

where the sup operation is extended to all sets B in the algebra $\mathcal{B}$ of $\mathcal{Y}$. Eq. (11) implies that instead of measuring the separation of two distributions utilising the L^1-norm (left hand side) one can equivalently use the variational distance (Strasser, 1985). More specifically, the variational distance in the right-hand side of Eq. (11) is a generalisation of the Kolmogorov–Smirnov distance d_{KS} and the discrepancy metric d_D (Gibbs and Su, 2002, pp. 420–424). We have

$$d_{KS} = \sup_{y \in \mathcal{Y}} |F_Y(y) - F_{Y|X}(y)| \leqslant$$
$$d_D = \sup_{\text{all closed balls } A} |P_Y(A) - P_{Y|X}(A)| \leqslant$$
$$d_\delta = \sup_{B \in \mathcal{B}} |P_Y(B) - P_{Y|X}(B)|. \quad (12)$$

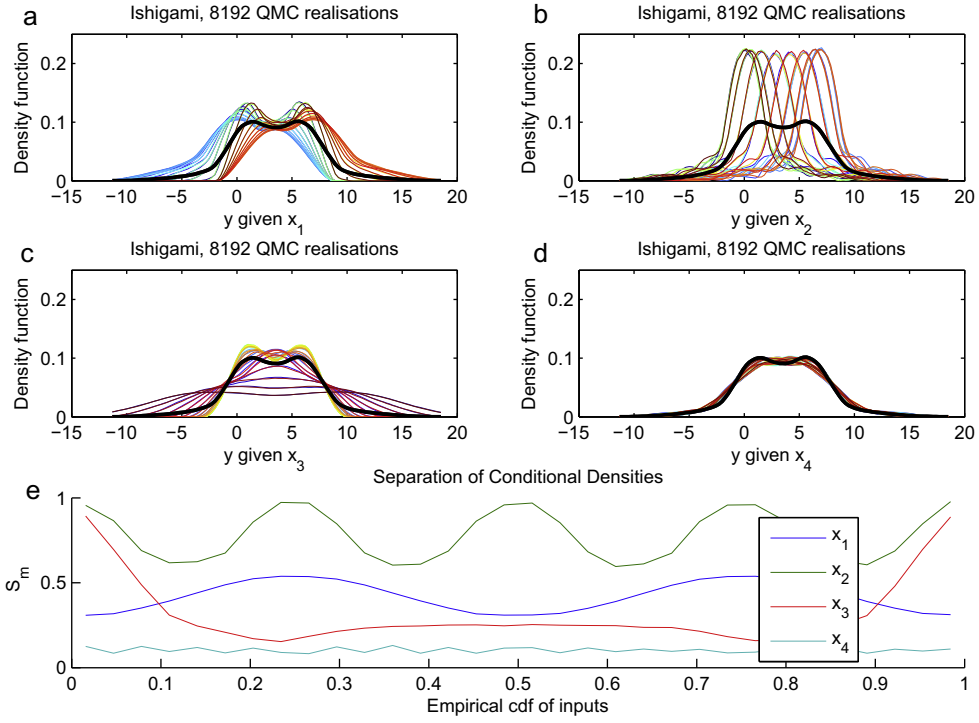

Fig. 1. Ishigami test function: (a)–(d) conditional and unconditional densities, and (e) separation measures.

The Kolmogorov–Smirnov distance inspects discrepancy over all half-rays in $\mathcal{Y}$, the discrepancy metric over all closed balls in $\mathcal{B}$, while the variational distance in d_δ considers all sets in $\mathcal{B}$.

In a global SA context, $s_i(x)$ is conditional on $X_i = x$. Averaging over the possible values of s_i attained by X_i leads us to the following definition.

Definition 1. Given two random variables X and Y on measurable spaces $(\mathcal{X},\mathcal{A})$ and $(\mathcal{Y},\mathcal{B})$, we define the importance of X on Y as

$$\delta(Y,X) = \frac{1}{2}\mathrm{E}[s(X)] = \int_{\mathcal{X}} f_X(x)s(x)\mathrm{d}x = \int_{\mathcal{X}} f_X(x)\cdot \sup_{B\in\mathcal{B}}|P_Y(B) - P_{Y|X=x}(B)|\mathrm{d}x. \tag{13}$$

Note that, by Scheffé's theorem, it is

$$\delta(Y,X) = \frac{1}{2}\int_{\mathcal{X}} f_X(x)\int_{\mathcal{Y}} |f_Y(y) - f_{Y|X=x}(y)|\mathrm{d}y\mathrm{d}x. \tag{14}$$

We can now prove the following symmetry relationship (see Appendix A).

Proposition 2. *For any X and Y on measurable spaces $(\mathcal{X},\mathcal{A})$ and $(\mathcal{Y},\mathcal{B})$, it holds that*

$$\delta(Y,X) = \delta(X,Y) = \frac{1}{2}\int_{\mathcal{X}\times\mathcal{Y}} |f_X(x)f_Y(y) - f_{XY}(x,y)|\mathrm{d}y\ \mathrm{d}x. \tag{15}$$

Eq. (15) suggests that δ is symmetric in X and Y, so that one can exchange their roles. Therefore, the roles of *explanans* and *explanandum* are not necessarily fixed for δ. In a global SA of model output, where we distinguish between input factors and model output, this change of viewpoint is not viable. However, when processing given data exchanging X and Y is possible and may lead to an increased confidence in the obtained results (we discuss an example in Section 9). Furthermore, Proposition 2 has the following implication.

Corollary 1. *$\delta(Y,X) = 0$ if and only if Y and X are independent.*

Thus, $\delta(Y,X) = 0$ provides an indication of the strength of the dependence between Y and X, avoiding type I errors.

In the remainder of this section, we explicitly consider Y as the model output in Eq. (1) and $\mathbf{X}$ as the vector of input factors. We fix one input variable X_i of interest. Then, the importance of factor X_i on Y is given by

$$\delta_i = \delta(Y,X_i) = \frac{1}{2}\mathrm{E}[s(X_i)] = \frac{1}{2}\int_{\mathcal{X}^i} f_{X_i}(x)\int_{\mathcal{Y}} |f_Y(y) - f_{Y|X_i=x}(y)|\mathrm{d}y\ \mathrm{d}x. \tag{16}$$

It can be shown that δ_i possesses additional properties (Borgonovo, 2007; Borgonovo et al., 2011). A first property is normalisation: $0 \leqslant \delta_i \leqslant 1$. A second is invariance to monotonic transformation: Suppose that $z(y)$ is a monotonic function of Y. Then, it can be proven that $\delta(Y,X_i) = \delta(z(Y),X_i)$ (Borgonovo et al., 2011). By Proposition 2, we even have $\delta(Y,X_i) = \delta(z_1(Y),z_2(X_i))$ for monotonic maps z_1, z_2.

Invariance to monotonic transformation has both numerical (*i*) and decision-theoretical implications (ii):

(i) If the model output is sparse or ranges over several orders of magnitude then analysts might resort to scale-transformations for improving numerical processing. However, transferring back results obtained on the transformed data to the original data is usually not straightforward (Saltelli and Sobol', 1995). This problem is circumvented if the sensitivity statistic is monotonic-transformation invariant.

(ii) Consider a decision maker who is assessing a von Neumann–Morgenstern utility function U over $\mathcal{Y}$. Monotonicity of U is a standard requirement in Economics (Baucells and Sarin, 2007). Any monotonic transformation of Y or of $U(Y)$ preserves the preference structure. Thus, if and only if a sensitivity measure is scale invariant then sensitivity analysis results hold for all equivalent preference structures (Borgonovo and Baucells, 2011). That is, results obtained using Y hold for any $U(Y)$. Additionally, in many situations assigning a precise form to U is a cumbersome task (Lichtendahl and Bodily, 2010). However, when U is assumed monotonic then sensitivity analysis results are unaffected by imprecisions in the assessment of U, if one selects a scale invariant sensitivity measure. Finally, we observe that any sensitivity measure based upon an f-divergence (Csiszár, 1963) is comprised within our framework. This is achieved by replacing the L^1-norm with alternative metrics. Among these, an important class is represented by the symmetric Kullback–Leibler divergence,

$$s_{\mathrm{KL}}(x) = \frac{1}{2}\left(\int_{\mathcal{Y}} f_Y(y)\log\frac{f_Y(y)}{f_{Y|X=x}(y)}\ \mathrm{d}y + \int_{\mathcal{Y}} f_{Y|X=x}(y)\log\frac{f_{Y|X=x}(y)}{f_Y(y)}\ \mathrm{d}y\right) = \frac{1}{2}\int_{\mathcal{Y}} (f_{Y|X=x}(y) - f_Y(y))\log\frac{f_{XY}(x,y)}{f_X(x)f_Y(y)}\ \mathrm{d}y. \tag{17}$$

Averaging over X yields the following variant of Shannon's information,

$$\delta_{\mathrm{KL}} = \mathrm{E}[s_{\mathrm{KL}}(X)] = \frac{1}{2}\int_{\mathcal{X}\times\mathcal{Y}} (f_{XY}(x,y) - f_X(x)f_Y(y))\log\frac{f_{XY}(x,y)}{f_X(x)f_Y(y)}\,\mathrm{d}y\,\mathrm{d}x, \tag{18}$$

which is symmetric in X and Y, scale invariant and bears close resemblance to Eq. (15). However, when used for global SA, δ_{KL} encounters some limitations. It has been shown in Borgonovo et al. (2011) that the ratios in Eq. (18) are not always well-defined, because in global SA we are frequently faced with a support problem. δ_{KL} is originally conceived within Bayes' theorem framework (Soofi, 1994), where the support is always invariant. Furthermore, analytical case studies have not been developed for Eq. (18) yet. For these reasons, we focus on the estimation of Eq. (15) in the remainder of our work.

5. Estimators

In this section, we define an estimator for δ_i. We collect the realisations of n i.i.d. copies of the pair $(\mathbf{X},Y)$ in the sample matrix $Z = ((x_{j,1}\ldots x_{j,k}\ y_j)) \in \mathbb{R}^{n\times(k+1)}$. Most of the time we consider a fixed factor $i \in \{1,\ldots,k\}$ so that only the n-vectors $x_i = (x_{j,i})$ and $y = (y_j)$ are used in the following discussion. After fixing this generic factor i we form the scatterplot of x_i and y. Next, we partition the x_i-axis of the scatterplot into M classes. The key intuition of our approach is the following. Instead of considering the density conditional on $X_i = x$ we consider the conditional density generated by X_i belonging to this class-interval of a suitably chosen partition of $\mathcal{X}^i$ to obtain any observations conditional to this class. Formally, let $\mathcal{P} = \{\mathcal{C}_m; m = 1,\ldots,M\}$ with $\bigcup_{m=1}^{M}\mathcal{C}_m = \mathcal{X}^i$, $\mathcal{C}_m \cap \mathcal{C}_{m'} = \emptyset, m \neq m'$ denote a partition of $\mathcal{X}^i$ into M classes. The probability of X_i belonging to class $\mathcal{C}_m$ is given by

$$P_{X_i}(\mathcal{C}_m) = \int_{\mathcal{C}_m} f_{X_i}(x)\ \mathrm{d}x. \tag{19}$$

By the total probability theorem, the class-conditional density of Y given $\mathcal{C}_m \subset \mathcal{X}^i$ is given by

$$f_{Y|\mathcal{C}_m}(y) = \frac{\int_{\mathcal{C}_m} f_{Y|X_i=x}(y) f_{X_i}(x)\mathrm{d}x}{\int_{\mathcal{C}_m} f_{X_i}(x)\mathrm{d}x} = \frac{1}{P_{X_i}(\mathcal{C}_m)} \int_{\mathcal{C}_m} f_{X_i Y}(x,y)\mathrm{d}x. \tag{20}$$

Then, we call the quantity

$$S_m = S(\mathcal{C}_m) = \int_{\mathcal{Y}} |f_Y(y) - f_{Y|\mathcal{C}_m}(y)|\mathrm{d}y, \tag{21}$$

the class separation induced by $\mathcal{C}_m \subset \mathcal{X}^i$. Correspondingly, we define an approximation of the distributional-importance of X_i for partition $\mathcal{P}$ as

$$\delta_i^{\mathcal{P}} = \frac{1}{2}\sum\nolimits_{\mathcal{C}\in\mathcal{P}} S(\mathcal{C}) P_{X_i}(\mathcal{C}) = \frac{1}{2}\sum\nolimits_{m=1}^{M} S_m P_{X_i}(\mathcal{C}_m). \tag{22}$$

We have the following result (the proof is in the Appendix).

Theorem 1. *Suppose that X_i has a continuous density on $\mathcal{X}^i$. Consider a refining family of partitions $\mathcal{P}_j = \left\{\mathcal{C}_1^j, \ldots, \mathcal{C}_M^j\right\}, M = 2^j$, of $\mathcal{X}^i$ with $\mathcal{C}_1^0 = \mathcal{X}^i, \mathcal{C}_{2m-1}^j \cup \mathcal{C}_{2m}^j = \mathcal{C}_m^{j-1}$ for $j > 0$, which is finely grained such that $\lim_{j\to\infty} \max_{m=1,\ldots,M} P_{X_i}\left(\mathcal{C}_m^j\right) = 0$ and which has positive mass in each class such that for all j and $m, P_{X_i}\left(\mathcal{C}_m^j\right) > 0$. Then $\lim_{j\to\infty} \delta_i^{\mathcal{P}_j} = \delta_i$.*

Theorem 1 ensures that, as the number of partition classes increases, the class approximation $\delta_i^{\mathcal{P}}$ of a density-based sensitivity measure tends to δ_i. Intuitively, one can explain this result as follows. For $M \to \infty$, the partition size decreases and, eventually, $\mathcal{C}_m$ collapses to an individual point, which we can call x_m. Thus, $S(\mathcal{C}_m) \to S(\{x_m\}) = s_i(x_m)$ as M tends to infinity.

Theorem 1 and Eq. (21) lead us to the problem of estimating f_Y and $f_{Y|\mathcal{C}_m}$. We use kernel-density (Parzen, 1962; Devroye and Györfi, 1985). Assume that $\{(x_j, y_j); j = 1, \ldots, n\}$ is a sample of n pairs of realisations of X_i and Y. The estimate $\hat{f}_Y(\cdot)$ is obtained from a kernel-density estimation of all realisations $\{y_j; j = 1, \ldots, n\}$ while $\hat{f}_{Y|\mathcal{C}_m}(\cdot)$ is obtained from a kernel-density estimation of the subset $\{y_j; x_j \in \mathcal{C}_m\}$. For a given kernel $K(\cdot)$ and given bandwidths α, α_m, $m = 1, \ldots, M$ these kernel-density estimates are

$$\begin{aligned} \hat{f}_Y(y) &= \frac{1}{n}\sum\nolimits_{j=1}^{n} \frac{1}{\alpha} K\left(\frac{y - y_j}{\alpha}\right), \\ \hat{f}_{Y|\mathcal{C}_m}(y) &= \frac{1}{n_m}\sum\nolimits_{j:x_j\in\mathcal{C}_m} \frac{1}{\alpha_m} K\left(\frac{y - y_j}{\alpha_m}\right). \end{aligned} \tag{23}$$

Here, $n_m = \sum_{j:x_j\in\mathcal{C}_m} 1$ counts the number of realisations in class $\mathcal{C}_m$ of $\mathcal{P}$. With a given set of ℓ quadrature points $\{\tilde{y}_j; j = 1, \ldots, \ell\}$, Eq. (23) allows us define the point-wise separation of the estimated densities,

$$s_{m,j} = \hat{f}_Y(\tilde{y}_j) - \hat{f}_{Y|\mathcal{C}_m}(\tilde{y}_j), \quad j = 1, \ldots, \ell, \quad m = 1, \ldots, M. \tag{24}$$

The numerical integration of $s_{m,j}$ may be performed using the trapezoidal rule, yielding class separation estimates

$$\widehat{S}_m = \frac{1}{2}\sum\nolimits_{j=1}^{\ell-1} (|s_{m,j+1}| + |s_{m,j}|)(\tilde{y}_{j+1} - \tilde{y}_j), \quad m = 1, \ldots, M. \tag{25}$$

As an example, Fig. 1e) shows estimates $\widehat{S}_m$ for all $k = 4$ factors of the Ishigami model using $M = 32$ partitions.

Definition 2. We call the quantity

$$\hat{\delta}_i = \frac{1}{2n}\sum\nolimits_{m=1}^{M} n_m \widehat{S}_m \tag{26}$$

an estimator of δ_i on the partition $\mathcal{P} = \{\mathcal{C}_m; m = 1, \ldots, M\}$ with quadrature points $\{\tilde{y}_j; j = 1, \ldots, \ell\}$ for sample size $n = \sum_{m=1}^{M} n_m$.

It is now necessary to prove that $\hat{\delta}_i$ is a consistent estimator of δ_i for two reasons. First, if the model allows the adoption of an estimation strategy based on increasing sample sizes, then we need to be ensured that $\hat{\delta}_i$ tends to δ_i as the sample size increases. Second, if the model allows only a fixed budget of model runs, then we need to assess confidence intervals around $\hat{\delta}_i$ at finite or small sample sizes. Suppose that we use bootstrap. We need to prove that $\hat{\delta}_i$ is consistent for ensuring that the bootstrap estimator is also consistent. The following holds (see Appendix A).

Theorem 2. *$\hat{\delta}_i$ is a consistent estimator of δ_i, i.e., $\lim_{n,M,\ell\to\infty} \hat{\delta}_i = \delta_i$.*

We note the complementarity of Theorems 1 and 2. The former states that a strategy based on partitions leads to a consistent estimator of δ_i provided that class densities are consistently estimated. The latter ensures that this is the case if one combines the trapezoidal rule and kernel-density, under the assumptions of convergence of the kernel-density estimators (see Appendix A; we also refer to Devroye and Györfi (1985); Härdle (1990)).

Definition 2 can be turned into an estimation strategy. Fixing a factor i, we follow the procedure described below for estimating $\delta_i = \delta(Y, X_i)$.

1. (a) Performing a traditional uncertainty analysis (with any sample generation method), if one is investigating the output Y of a computer code; or
   (b) setting the dependent variable Y among the variables of a given dataset, if one is not in a model input/output framework.
2. Partitioning the dataset to form the classes $\mathcal{C}_m, m = 1, 2, \ldots, M$.
3. Approximating the densities conditional to these classes via kernel smoothing, Eq. (23).
4. Estimating δ_i in accordance with Eq. (26).

We observe:

About Step 1: no restrictions apply on the sampling procedure (simple random, quasi-Monte Carlo or Latin hypercube sampling) used for obtaining the realisations from the random vector $\mathbf{X}$.

About Step 2: several partition strategies are available (Plischke, 2012). A way which has been proven effective for the authors is partitioning the data by factor ranks, forming classes of nearly the same size. Numerical experiments have shown that increasing such equally sized partitions beyond 50 classes has negligible effect on the estimation accuracy.

About Step 3: knowledge of the conditional distributions can be used for extracting additional information from the code. In fact, plotting the unconditional model output density against the conditional densities provides a direct way for assessing whether and how fixing a factor modifies the model output density, see also Section 2.

Finally, a remark on the presence of discrete random variables. If X_i is continuous then the partition into classes can always be chosen in such way that $nP_{X_i}(\mathcal{C}_m) = n_m$. If X_i is discrete then one can exploit knowledge of the values assumed by X_i to set the proper partitions by having the class $\mathcal{C}_m$ coinciding with the mth realisation of X_i. Then, we are in the particular case in which conditioning on $X_i \in \mathcal{C}_m$ is equivalent to conditioning on $X_i = x_i^m$. As far as the continuity of Y is concerned, using the Dirac-δ density symbol the symbolic definitions stated so far can also be extended to the case of discrete Y. However, if Y is discrete then the probability density function is replaced by a probability mass function and there is no need for kernel smoothing (one can use a simple absolute value difference between the conditional and unconditional probability mass functions). Of course, estimation accuracy is then dependent on the accuracy of the corresponding histograms. A detailed discussion is out of the scope of the present work. Because many realistic computer codes have continuous output, and for the sake of simplicity, we shall retain focus on continuous random variables in the remainder.

6. Point estimation: A bias reduction filter

Consider a strategy based on estimating $\hat{\delta}_i$ at increasing sample sizes and stopping the algorithm when the difference in point estimates at two next sample sizes is smaller than a predetermined $\epsilon > 0$. Applying the steps described in Section 5 to the Ishigami example in Eq. (8), we obtain the conditional densities and separations which have been presented in Fig. 1 and the following values for $\hat{\delta}_1 = 0.208, \hat{\delta}_2 = 0.391, \hat{\delta}_3 = 0.156, \hat{\delta}_4 = 0.060$. X_2 is the most influential factor, followed by X_1, X_3 and X_4. This result is in agreement with the intuition generated by Fig. 1. However, δ_4 is not equal to zero. In fact, when applied to Eq. (8), a strategy based on increasing sample sizes produces the results in Fig. 2 (continuous lines) for estimating δ_4. To study the numerical variability of the estimates, 4 repetitions are used, each with a partition size of $M = 10$ and $\ell = 110$ quadrature points for evaluating the inner integral.

Because $\delta_4 = 0$, we would expect $\hat{\delta}_4$ to tend to zero as n increases (Theorem 2). However, while this is the case, convergence is slow and, at any finite $n, \hat{\delta}_4 \neq 0$. There are two reasons for this bias in uninfluential factors: the use of kernel-density estimates and the partitioning of the dataset. Kernel-density introduces numerical noise due to its intrinsic numerical approximation. For a dummy parameter, partitioning of the $X|Y$ scatterplot and conditioning leads to the removal of a number of randomly chosen realisations. This removal creates residuals that do not cancel out when forming $\widehat{S}_m$ which leads to a spurious contribution to terms in the addition of Eq. (26). These spurious additions generate a non-null (albeit small) $\hat{\delta}$. This problem is intrinsic to designs based on replicates and is also observed for variance-based methods (Morris et al., 2006, 2008; Plischke, 2010). Morris et al. (2008) obtain a non-biased estimator of η_i^2 by a sampling plan based on orthogonal arrays. However, the bias is unavoidable if the estimation design stays independent of the sample generation method (Plischke, 2010). Because we require independence of the sampling generation method and no additional model runs (this requirement is the main difference between our approach and the one of Oakley et al. (2010)), we propose a different approach to control unwanted numerical influences in a point estimation strategy. The rationale is to profit by information about the conditional and unconditional distributions of Y, yielded by Step 3 of Section 5 and to utilise a statistical test to check whether the difference in $F_Y(y)$ and $F_{Y|\mathcal{C}_m}(y)$ is significant. Because its statistic can be related to $\hat{\delta}_i$, the (asymptotic) two-sample Kolmogorov–Smirnov (KS) test (Conover, 1999) appears as a natural selection for this approach. Let $\widehat{F}_Y(y)$ denote the empirical distribution functions of Y and $\widehat{F}_{Y|\mathcal{C}_m}(y)$ the class-based empirical conditional distribution function. Then, the contribution of class $\mathcal{C}_m$ to $\hat{\delta}_i$ is insignificant at level α if

$$\max_{y\in\mathcal{Y}} |\widehat{F}_Y(y) - \widehat{F}_{Y|\mathcal{C}_m}(y)| \leqslant K_\alpha \sqrt{\frac{1}{n} + \frac{1}{n_m}}, \tag{27}$$

holds where K_α is the upper α-quantile of the Kolmogorov distribution, n is the overall sample size and n_m the subsample size of class $\mathcal{C}_m$. The fact that subsamples are used for describing $Y|\mathcal{C}_m$ introduces ties into the pooled sample. In the presence of ties the K_α statistic is conservative (Nikiforov, 1994). This problem can be avoided as follows. Instead of using the observations directly, we use the available kernel density estimates of Eq. (24) to resample from smooth approximations of the cumulative distributions. This adds one additional calculation in Step 4. Using the trapezoidal quadrature rule for integrating the difference of the densities, Eq. (27) is then replaced by

$$\max_{\kappa=1,\ldots,\ell-1} \left| \sum_{j=1}^{\kappa} (s_{m,j} + s_{m,j+1})(\tilde{y}_{j+1} - \tilde{y}_j) \right| \leqslant 2K_\alpha \sqrt{\frac{1}{n} + \frac{1}{n_m}}. \tag{28}$$

This test statistic may be further simplified. For empirical densities and empirical cumulative distributions Eq. (12) immediately yields $2\max_{y\in\mathcal{Y}}|\widehat{F}_Y(y) - \widehat{F}_{Y|\mathcal{C}_m}(y)| \leqslant \widehat{S}_m$. Hence if

$$\widehat{S}_m \leqslant 2K_\alpha \sqrt{\frac{1}{n} + \frac{1}{n_m}} \tag{29}$$

then the Kolmogorov–Smirnov test in Eq. (27) is satisfied. Note that Eq. (29) is conservative compared to Eq. (27), but it requires no additional calculations. If the contribution of class $\mathcal{C}_m$ is deemed insignificant by either of the tests in Eq. (28) or (29), we can replace $\widehat{S}_m$ with 0 avoiding the summation of a spurious term in Eq. (26). To set a rejection level α in Eq. (27) or Eq. (29), we can utilise a dummy variable and exploit our knowledge of the fact that it is uninfluential. Or, we can even do more, and compute for each factor the significance level at which the KS test would reject the conditional contributions of all the classes $\mathcal{C}_m$ deeming it uninfluential. Thus, the significance of the KS test can be endogenously set. For example, in the Ishigami function of Fig. 1 at $n = 8192$ quasi MC realisations, using Eq. (29) the dummy factor has an acceptance level of 0.759 while the other three parameters have at least 0.995. Hence a threshold greater then or equal to $1 - \alpha = 0.76$ will effectively eliminate the influence of the dummy parameter. Fig. 2 displays the results for the Ishigami function, with the test implemented in accordance with Eq. (29) (dash-dotted lines) and with the test implemented by Eq. (28) (dashed lines). Both variants of the KS test effectively eliminate numerical noise and produce a null line. An alternative bias-removal method through bootstrapping is discussed in the next section.

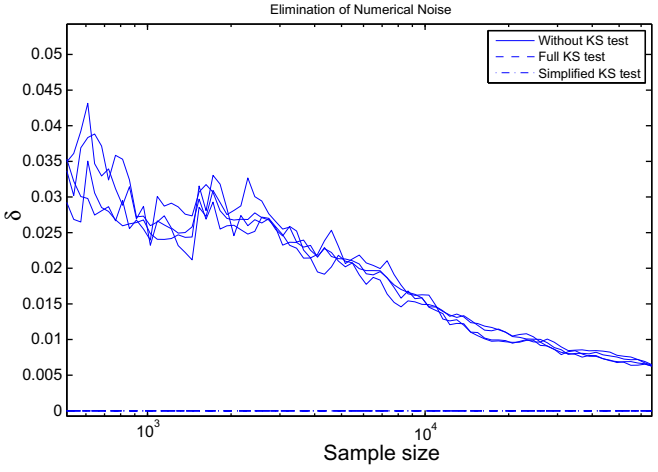

Fig. 2. Computation of δ with acceptance level for factor X_4 of the Ishigami function.

7. Confidence bounds at finite sample sizes: Estimators and numerical experiments

When models require virtually no time to run (much like metamodels), the strategy of estimating δ (and also η_i^2) by application of the steps in Section 5 and controlling the bias through the KS test as sample sizes increases is within computational reach. This is often the case of models used in business planning, decision analysis (in Oakley et al. (2010) a sample of size 250,000 is used) and, frequently, in reliability analysis (Borgonovo and Smith, 2011).

For other models, especially the ones utilised in the physical and environmental sciences, the total budget of model executions might be limited by a long execution time. At small sample sizes, one needs to account for imprecision in the estimates. In this respect, we note that determining the degree of confidence in the

estimation of global sensitivity measures has not been subject of extensive research so far, with practically all works addressing strategies based on increasing sample sizes.

For maintaining the confidence assessment in a post-processing mode, the literature offers us two main methods: the bootstrap and the jackknife (Shao and Tu, 1995; Hall, 1992; Efron and Tibshirani, 1993). The authors have performed several experiments for the assessment of confidence intervals with both methods. To our purposes, the bias-reducing bootstrap estimator of Efron and Gong (1983) has revealed as the most efficient one and it is subject of this section. For further information on the utilisation of the bootstrap in simulation, we refer to Kleijnen and Deflandre (2006) and van Beers and Kleijnen (2008).

Let $\bar{\delta}^*$ be the average of the moment-independent measure estimates derived from B bootstrap replicates of the given observations. Here, each replicate is obtained by drawing a sample of n realisations from the n available observations, with replacement. B is also called bootstrap sample size (Efron and Tibshirani, 1993). A bootstrap estimate of the bias of $\hat{\delta}$ is given by $\widehat{\text{bias}}(\hat{\delta}) = \bar{\delta}^* - \hat{\delta}$. Then, one obtains the bias-reducing bootstrap estimate of δ:

$$\hat{\hat{\delta}} = \hat{\delta} - \widehat{\text{bias}}(\hat{\delta}) = 2\hat{\delta} - \bar{\delta}^*. \tag{30}$$

By the theory of bootstrap, one knows that $\hat{\hat{\delta}}$ is a consistent estimator of δ, provided that $\hat{\delta}$ is. Consistency of $\hat{\delta}$ is ensured by Theorem 2. By construction (Efron and Gong, 1983), an approach based on the statistic in Eq. (30) is bias-reducing, see also Hall (1992). Thus, the statistic in Eq. (30) represents an alternative bias-reducing strategy with respect to the strategy in Section 6. Furthermore, we can utilise the distribution of $2\hat{\delta} - \bar{\delta}^*$ for assessing confidence in the estimates. This is particularly relevant at small sample sizes.

All numerical experiments in the remainder of this section are performed without any KS cut-off threshold. We start with the Ishigami function example, Eq. (8), considering the inactive variable X_4. Results at increasing sample sizes are displayed in Fig. 3. Here, the squares represent the point estimates $\hat{\delta}_4$, the whiskers the bootstrap distribution of $2\hat{\delta}_4 - \delta_4^*$, and the circles the corresponding $\hat{\hat{\delta}}_4$. The bootstrap sample size is $B = 500$. One observes that the point estimates $\hat{\delta}_4$ slowly decrease from 0.04 to 0.02, as the sample size increases from 512 to 16,384. Conversely, $\hat{\hat{\delta}}_4$ is comprised within −0.01 and +0.01 at all sample sizes, i.e., it is at least one order of magnitude lower than $\hat{\delta}_4$. To conduct further analyses, we implement an analytical albeit computationally intensive example constituted by a product model. We offer first

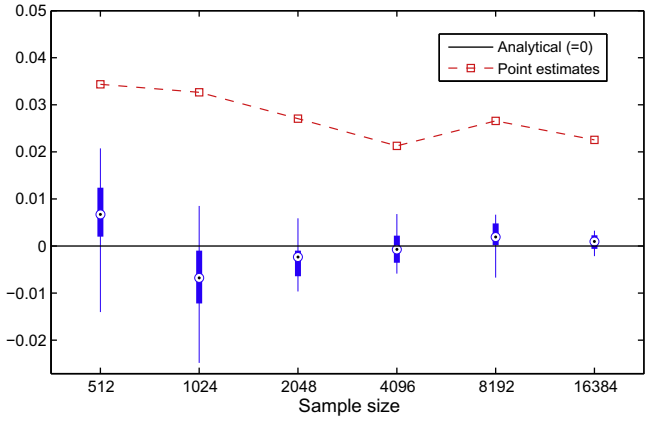

Fig. 3. $\hat{\delta}_4$ Point estimates (squares) and corresponding bootstrap distribution using the estimator in Eq. (30) (boxplots), for the inactive variable of the Ishigami function.

a general result for variance-based measures for this class of functions (see Appendix for the proof).

Proposition 3. *Suppose that* $\mathbf{X} = (X_1, \ldots, X_k)$ *is a random vector with* k *independently distributed components. Then the first order effects of* $Y = \prod_{i=1}^{k} g_i(X_i)$ *with* $g_i : \mathcal{X}_i \to \mathbb{R}$ *such that* $E[g_i(X_i)] \neq 0$ *are given by*

$$\eta_i^2 = \frac{E[Y]^2}{\text{Var}[Y]} \cdot \frac{\text{Var}[g_i(X_i)]}{E[g_i(X_i)]^2}. \tag{31}$$

From a historical viewpoint, Proposition 3 generalises results in Goodman (1962). It is also related to results in Owen (2003). In the remainder of this section, we consider the input–output mapping

$$Y = \prod_{i=1}^{k} X_i^{a_i}, \tag{32}$$

where $\mathbf{X} = (X_1, \ldots, X_k)$ is a random vector of independently log-normally distributed factors with densities

$$f_i(x_i; \omega_i, \xi_i) = \frac{1}{\sqrt{2\pi}\xi_i x_i} \exp -\frac{1}{2}\left[\frac{\log(x_i) - \omega_i}{\xi_i}\right]^2, \quad i = 1, \ldots, k. \tag{33}$$

We utilise $k = 21$ factors with $\omega_i = 1$ and $\xi_i = 1$, $i = 1, 2, \ldots, 21$, and $a_{1\ldots7} = 4$, $a_{8\ldots14} = 2$, $a_{15\ldots21} = 1$. The 21 factors are then divided into three groups of high, moderate and low importance. Analytical values are obtained by implementing Proposition 5 of Borgonovo et al. (2011) in a symbolic mathematical software (Mathcad in our case). This yields $\delta_{1\ldots7} = 0.112$, $\delta_{8\ldots14} = 0.053$ and $\delta_{15\ldots21} = 0.026$.

By these parameter choices, one obtains the following analytical values of the relevant moments for Eq. (31): $E[Y]^2 = 2.52 \cdot 10^{106}$, $\text{Var}[Y] = 6.37 \cdot 10^{212}$, $E[X_1^4]^2 = 2.649 \cdot 10^{10}$, $\text{Var}[X_1^4] = 2.35 \cdot 10^{17}$. Note the extremely large value of $\text{Var}[Y]$, which leads to $\hat{\eta}_i^2 = 0, i = 1, 2, \ldots, 21$, for all practical purposes. The reason is readily explained. The map $\mathbf{X} \mapsto Y$ in Eq. (32) is highly non-additive. Hence, individual contributions are negligible in the functional ANOVA decomposition of Y. Under independence assumption, the first terms of this decomposition are given by the correlation ratios η_i^2 (Bedford, 1998).

Let us now come to numerical results. We generate samples by the quasi-Monte Carlo subroutine of SimLab (2011) of varying sizes, from $n = 512$ to $n = 65{,}536$. By propagating the sample through the model, we obtain the corresponding model output values, y. As a consequence of the extremely large value of $\text{Var}[Y]$, y is sparse. For instance, at $n = 65{,}536$, the values of y span 42 orders of magnitude (from 15 to $3.4 \cdot 10^{43}$). Such a sparsity impairs a direct application of any global sensitivity estimation procedure, unless one resorts to monotonic transformations to reduce numerical noise. (The use of transformations in sensitivity analysis is discussed in Saltelli and Sobol' (1995) and Ratto et al. (2009)). Computing δ_i on Y in Eq. (32), on $\log_a(Y)$ (logarithmic transformation) or on the cumulative distribution of Y (rank transformation) leaves δ_i invariant. However, such a transformation is not applicable for estimating η_i^2. By the log-transformation the model structure changes from multiplicative – $\prod_{i=1}^{21} X_i^{a_i}$ – to additive – $\sum_{i=1}^{21} a_i \log X_i$ – and η_i^2 becomes

$$\eta_i^2 = \frac{a_i^2}{\sum_{i=1}^{21} a_i^2}. \tag{34}$$

Eqs. (31) and (34) imply the following: any estimator of η_i^2 applied to log-transformed data for the model in Eq. (32) is distorted.

By steps 2–4 in Section 5, we obtain the following results for the point estimates $\hat{\delta}_i$ of δ_i. Fig. 4 shows that $\hat{\delta}_i$ tends to the respective analytical value δ_i (marked by dashed lines) for all factor groups as n increases. This is consistent with the results of Section 5. Figs. 5 and 6 report the results of bootstrapping the model in Eq. (32) with $B = 1000$ replicates. To highlight the variation within the bootstrap

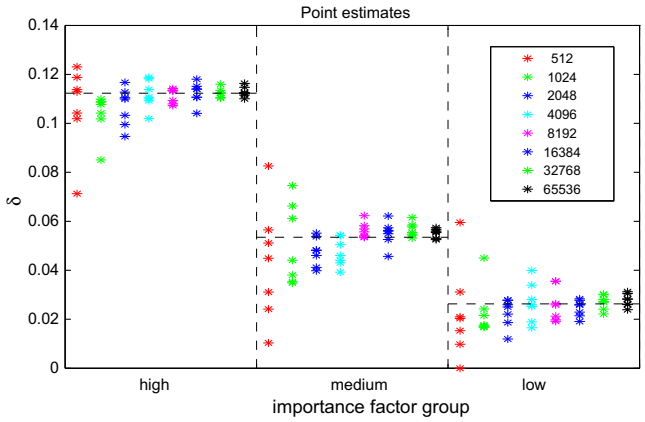

Fig. 4. Point estimates ($*$) at different sample sizes for $n = 512$ to $n = 65536$.

estimates, the data used to create the box-plots are based on all bootstrap replicates of $2\hat{\delta} - \delta^*$.

Fig. 5 reports results at sample sizes from 512 to 2048. It shows that the analytical values are always comprised within the bootstrap distributions. Especially at the lowest sample sizes ($n = 512$), $\hat{\delta}_i$ are less sparse around the analytical value than the corresponding $\widehat{\delta_i}$ shown in Fig. 4. Fig. 6 displays results for the distributions of $\hat{\delta}$ of the three factor groups obtained when n varies from 512 to 65,536. It shows that the confidence intervals shrink towards the analytical value as n increases. Note that, at $n = 2048$ there is no more overlapping among the distributions of the importance measures of most and least relevant factors. Thus, this sample size is sufficient for the *factor prioritisation* setting, even in the presence of such computationally challenging model. Starting at $n = 16{,}384$, the importance measures of the three factor groups are neatly separated.

8. Extensions: Estimating alternative sensitivity measures

The sensitivity measures presented in Section 5 are based on the estimation of the conditional densities of Y given X_i. Then, it is readily observed that knowledge of $f_{Y|X_i=x_i}(y)$ yields knowledge of all conditional moments of Y given X_i. Here, the expectation of Y conditioned on X_i is given by

$$\mathrm{E}[Y|X_i = x] = \int_{\mathcal{Y}} y f_{Y|X_i=x}(y)\mathrm{d}y. \tag{35}$$

Now, if we consider the weighted L^2-distance of $\mathrm{E}[Y|\ X_i = x]$ from $\mathrm{E}[Y]$ then we obtain the numerator of Eq. (5):

$$\int \left(\int (y f_{Y|X_i=x}(y) - y f_Y(y))\mathrm{d}y \right)^2 f_{X_i}(x)\mathrm{d}x = \int (\mathrm{E}[Y|X_i = x] - \mathrm{E}[Y])^2 f_{X_i}(x)\mathrm{d}x = \mathrm{Var}[\mathrm{E}[Y|X_i]]. \tag{36}$$

Instead of estimating η_i from the knowledge of the conditional first central moment using kernel density estimates of Eq. (23) via Eq. (36), we can also estimate Eq. (5) via correlation ratios (Pearson, 1905; Plischke, 2012) by directly counting out the values. In this case, we rely on the same partition as for $\hat{\delta}_i$. The correlation ratio estimator is then obtained by using the variance between classes,

$$\bar{y}_m = \frac{1}{n_m} \sum_{j:x_j \in \mathcal{C}_m} y_j, \quad \hat{\eta}_i^2 = \frac{\sum_{m=1}^{M} n_m (\bar{y}_m - \bar{y})^2}{\sum_{j=1}^{n} (y_j - \bar{y})^2}. \tag{37}$$

Finally, as discussed in Section 4, knowledge of the conditional densities also allows one to estimate any sensitivity measure based on alternative metrics to quantify the separation between $f_Y(y)$ and $f_{Y|X_i=x_i}(y)$ (see Eq. (18)). Hence, also the importance measures introduced in Park and Ahn (1994) based on the Kullback–Leibler divergence, or in Chun et al. (2000) based on Minkowski's distance of order 2 are subsumed within the present framework. Note that Eq. (28) may also serve as a sensitivity measure based on the Kolmogorov–Smirnov distance (Borgonovo and Baucells, 2011). Moreover, the expected-value-of-information statistic falls within the present framework. Ongoing research is addressing its estimation through a single loop (Strong et al., 2012).

9. Letter B: A non-functional relation

Section 4 has discussed that the sensitivity measures proposed in this work can be estimated in a non-input–output framework. The general intuition is that a sensitivity index can be associated with a scatterplot, as an indicator coding information about the

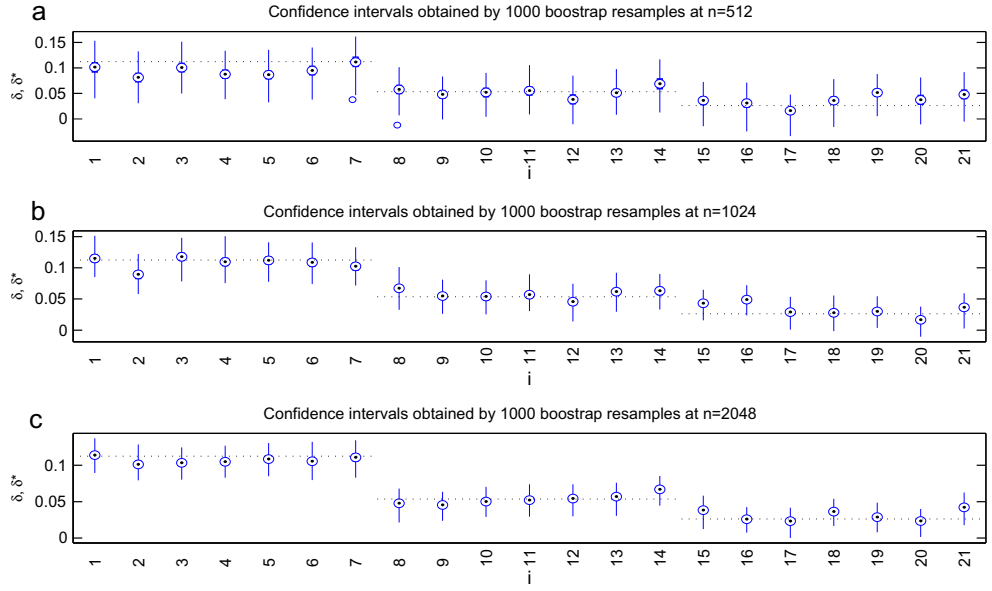

Fig. 5. Distributions of $\hat{\delta}$ obtained with 1000 bootstrap replicates at sample sizes (a) $n = 512$, (b) $n = 1024$, and (c) $n = 2048$.

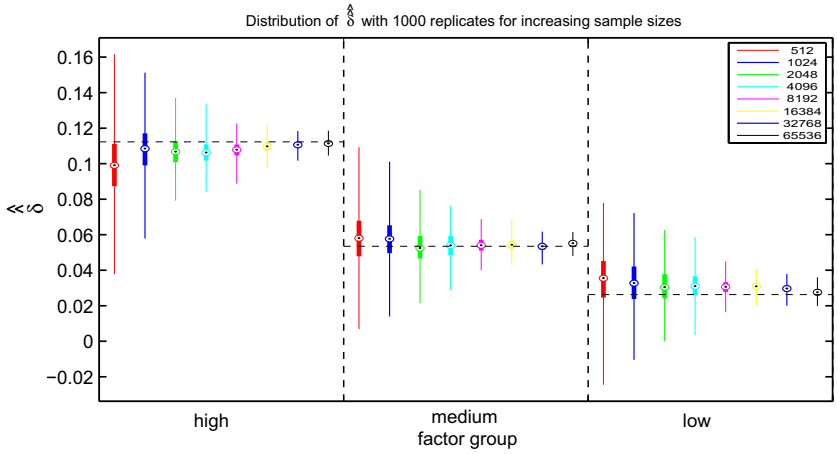

Fig. 6. Bootstrap distributions of $2\hat{\delta} - \delta^*$ for the three factor groups with $B = 1000$ replicates for $n = 512$ to 65536. In the whiskers-plots, $\odot$ denotes the median.

dependence of the associated random variables, see also Ratto et al. (2009). Suppose that one is provided with the scatterplot of Fig. 7a which resembles Latin alphabet letter B. It is generated by a sampling-rejection method. Thus, there is no functional input–output relationship between the random variables on the X–Y axis. Fig. 7b shows the product of the marginals obtained by partitioning the graph in Fig. 7a with horizontal and vertical stripes (see Section 5). One notes that this product of marginals differs from the original plot, signalling a statistical dependence between X and Y. In fact, by partitioning the X-axis and estimating the conditional densities, we obtain $\hat{\delta}(X,Y) = 0.288$. We now perform a further test, switching the roles of X and Y. Then also $\hat{\delta}(Y,X) = 0.288$ holds. Indeed, by Proposition 2 theses values should coincide. The discontinuities of the densities associated with letter B were dealt with by manually selecting a bandwidth. For the scatterplot in Fig. 7, one can also compute Pearson's correlation ratio η_i^2 using Eq. (37), see Section 8. We obtain $\eta_X^2 \approx 0$. Because the acceptance area is symmetric in Y, the data yield an almost constant conditional expectation. Note that by $\eta_X^2 \approx 0$ the decision maker would (erroneously) infer that there is no dependence between X and Y (type-I error). Conversely, a dependence is present because the joint density is different from the product of the marginals, what is captured by the non-null value of $\delta(X,Y)$ (This result is similar to the one obtained in the case of factor X_3 of the Ishigami test function, where, however, a traditional input/output functional relationship exists, see Section 2).

10. Application: Uncertainty management in the design phase of a lunar space mission

In this section, we discuss the application of the previous findings in a realistic decision support application. The model under investigation has been developed by a team of NASA's and Idaho National Laboratories risk experts to corroborate the risk assessment of lunar space missions in accordance with NASA's Risk Assessment Procedures (Stamatelatos et al., 2002).

The mission is modelled as an 8-phase process (see Fig. 8), from launch to orbit around the moon, to astronauts activity on lunar soil to return to earth. For a detailed description of the phases, we refer to Borgonovo and Smith (2011). For each phase, the model provides an accurate description of all engineering systems and activities involved in accordance with the prescriptions of NASA (2005). To our purposes, let us assume that the model is a black-box processing $k = 872$ uncertain input factors. This high number of factors makes it crucial to determine which factors analysts need to focus resources in data collection and further modelling efforts (areas where to intervene when). We then investigate whether this information can be gathered from a dataset generated by quasi-Monte Carlo uncertainty propagation through the model. The sample of the dataset is of size $65{,}536 \times 873$, where $n = 65{,}536$ is the number of realisations and 873 is split into $k = 872$ input factors plus the model output.

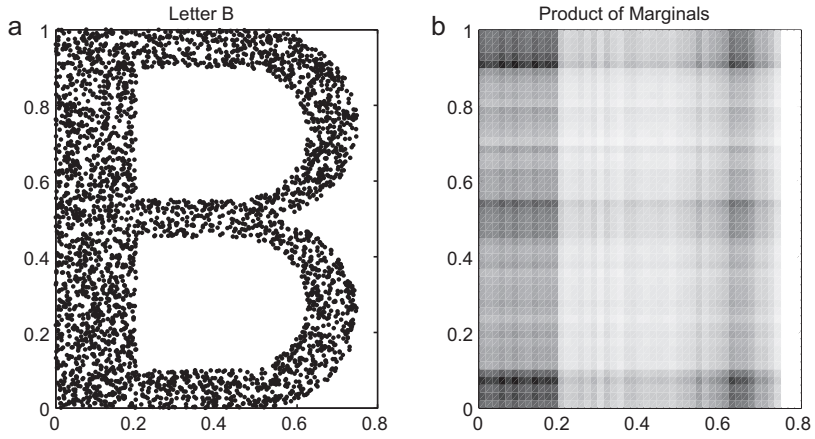

Fig. 7. A non-functional example for use with δ.

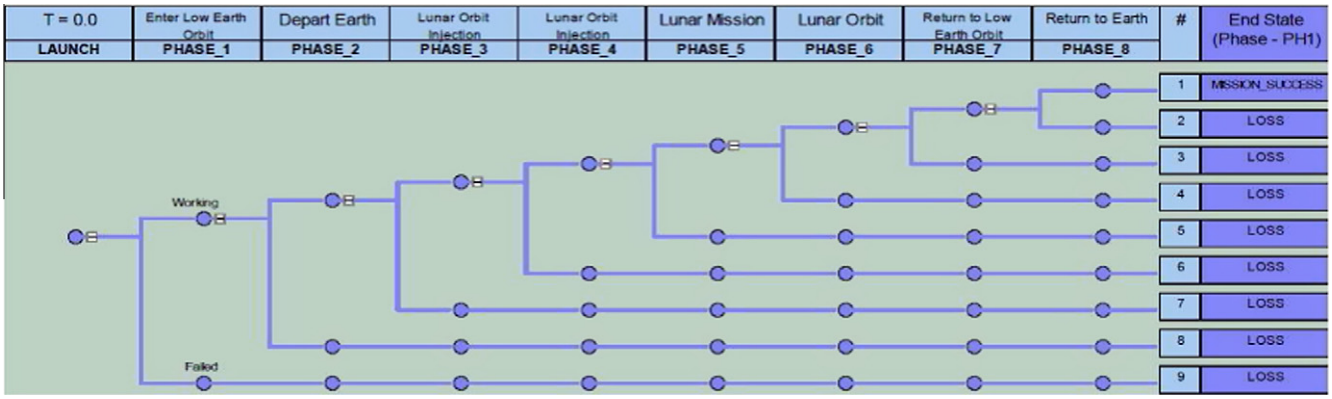

Fig. 8. Phases of the lunar space mission as simulated in the model.

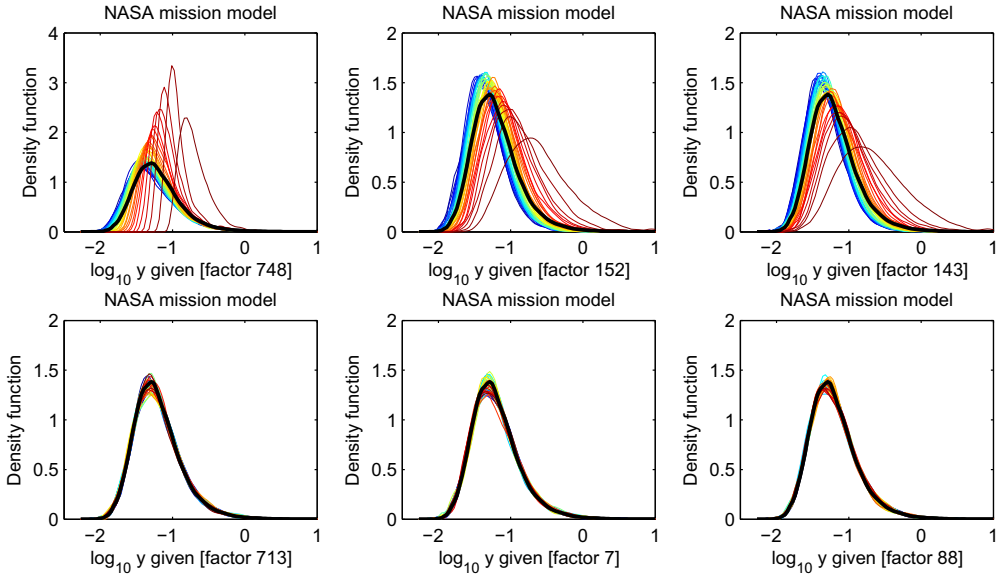

Fig. 9. $f_Y(y)$ and $f_{Y|X_{748}}(y)$, $f_{Y|X_{152}}(y)$, $f_{Y|X_{143}}(y)$, $f_{Y|X_{713}}(y)$, $f_{Y|X_7}(y)$, $f_{Y|X_{88}}(y)$ for the output of the NASA space mission model.

Note that, for this model the cost of appraising δ_i through a double-design is $872 \cdot n_{int} \cdot n_{ext} + n$ (Castaings et al., 2012). Even if a low value of n_{ext} was used (say 4 as in Castaings et al. (2012)), the cost would rapidly become prohibitive. As a reference, at $n_{int} = 65{,}536$, $C \approx 230{,}000{,}000$ model runs are required. Similarly, for η_i^2, if one assumes independence and utilises the result in Saltelli et al. (2010) one obtains $C \approx 57{,}000{,}000$ model runs at $n_{int} = 65{,}536$. Such high C, which is determined by the high number of factors, would impair the identification of key drivers of uncertainty, because of the long computational time and of memory limitations. Conversely, by the proposed approach it is $C = 65{,}536$. The total time required to process the dataset is around 600 s on a personal computer. Fig. 9 displays the results of Step 3 of the algorithm proposed in Section 5. It reports the distributions of the model output obtained by conditioning on X_{748}, X_{152}, X_{143}, X_{713}, X_7 and X_{88} (this is a subset of the 872 factors).

Fig. 9 allows us to visually appreciate that Y is statistically influenced by factors X_{748}, X_{152} and X_{143} in a stronger fashion than by factors X_{713}, X_7, and X_{88}.

In Step 4, (see Section 5), $\hat{\delta}_i$ and $\hat{\eta}_i^2$ are determined. We discuss these results in conjunction with the assessment of confidence intervals through the estimator in Eq. (30). Fig. 10 shows that at $n = 65{,}536$ the confidence intervals are non-overlapping for both the most important and least relevant factors. Thus, information on the key drivers of uncertainty is reliable. At the lowest sample size of $n = 512$ these factors are still identified as the most important ones, although there is a slight overlapping among the distribution of $\hat{\delta}$ of X_{152} and both X_{713}, X_7. However, at $n = 1024$ there is no overlapping. Thus, in a factor fixing setting, already at $n = 1024$ one can conclude that factors X_{713}, X_7 and X_{88} do not deserve priority when compared to factors X_{748}, X_{152}, X_{143}. The simultaneous estimation of δ_i and $\eta_i^2, i = 1, 2, \ldots, 872$ provides analysts with additional crucial insights. Fig. 11 displays $\hat{\delta}_i$ and $\hat{\eta}_i^2, i = 1, 2, \ldots, 872$ Overall, the agreement about the key drivers of uncertainty is high, although not perfectly coincident. In particular, the value of the correlation coefficient on ranks is $\rho_{\delta,\eta}^{\text{Rank}} = 0.86$, while the value on the corresponding Savage scores (SS) (Iman and Conover, 1987) is $\rho_{\delta,\eta}^{\text{SS}} = 0.89$. By construction, these values indicate that the disagreement concentrates mostly on the non-relevant factors. Also, results reveal that *479* variables are associated with null values of both $\hat{\delta}_i$ and $\hat{\eta}_i^2$. To further corroborate this finding, one has available (and can examine) the results of the KS-test filter for all partitions and all factors. The KS-test systematically shows that these factors have no influence on the model output. This result is in agreement with the findings in Borgonovo and Smith (2011), where a deterministic method is applied to the present model.

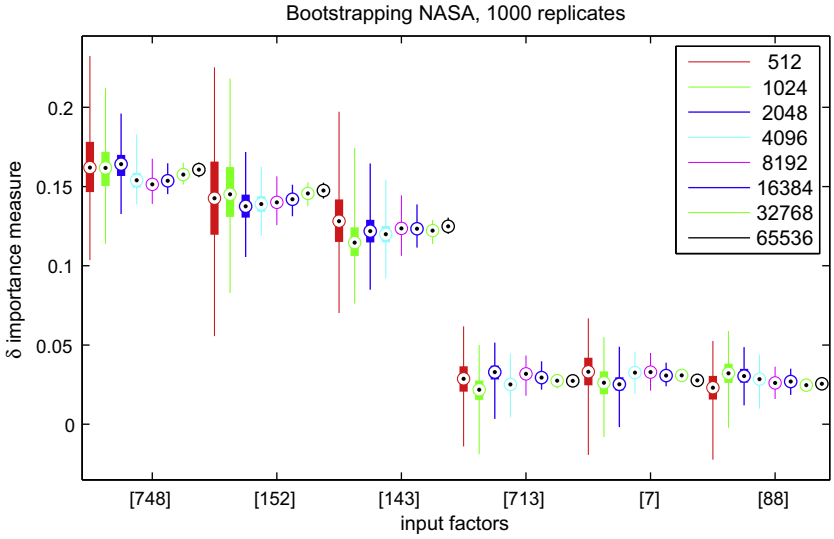

Fig. 10. Bootstrapping results for $\hat{\delta}$ of X_{748}, X_{152}, X_{143}, X_{713}, X_7 and X_{88}.

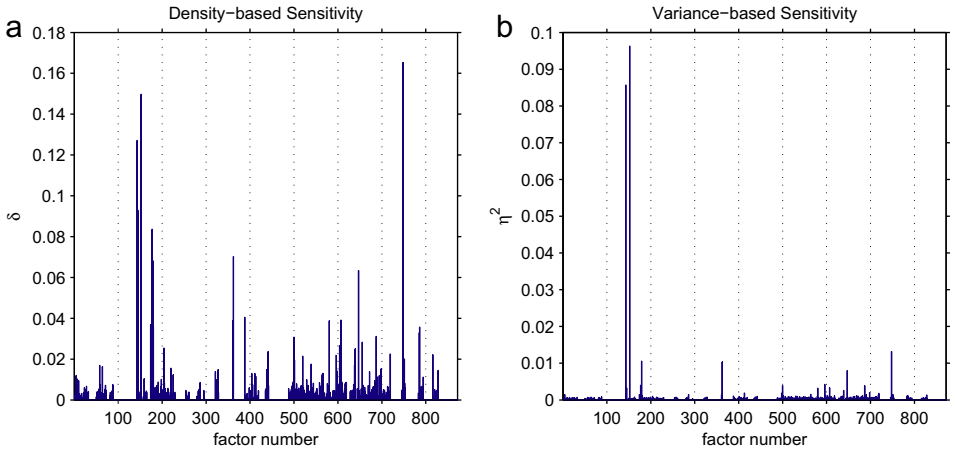

Fig. 11. Results of density (a) and variance (b) based sensitivity measures for the NASA space mission model.

Fig. 11 shows that factors X_{143}, X_{152} and X_{748} are associated with global sensitivity measures outstanding over the remaining ones both according to δ_i and η_i^2. However, X_{748} ranks third with variance-based sensitivity measures, while ranking first with δ_i. The reason is functional dependence and, in particular, the presence of interactions. By computing $\sum_{i=1}^{k} \hat{\eta}_i^2$ one understands whether interactions matter in the model response. In our case, it is $\sum_{i=1}^{872} \hat{\eta}_i^2 \approx 0.42$. Thus, individual effects account for around 42% of the model output variance. This difference highlights the active role of interactions in determining the model behaviour. We know that interaction effects are not captured by η_i^2. η_i^2 does not account for the importance of X_{782} associated with its interactions with the remaining factors. This finding is in agreement with the analysis of interactions performed by Borgonovo and Smith (2011) for the same model employing a deterministic design (finite change sensitivity indices). Such design delivers useful information on maintenance and inspection policies, but does not aim at producing information on uncertainty drivers. Indeed, the very low value (0.08) of Savage score correlation between the ranking induced by δ_i and finite change sensitivity indices confirms the intuition that deterministic methods ought not to be utilised as surrogates of global methods for uncertainty analysis purposes. However, factor X_{152} represents a notable exception. It is ranked among the three most important factors by all methods ($\hat{\delta}, \hat{\eta}_i^2$ and the finite change sensitivity indices). This fact suggests that X_{152} indeed deserves priority in further data collection and modelling efforts.

11. Conclusions

This work has presented a new strategy for estimating global sensitivity measures from given data. We have defined new estimators for density-based statistics and proved their consistency. Numerical aspects have been analysed in detail, with the introduction of a bias-reduction strategy as well as the determination of confidence bounds through bootstrapping. The method has the following advantages. It allows a notable reduction in computational burden, making the estimation cost independent of the number of factors. Thus, it is appropriate in the factor prioritisation and factor fixing settings for models with a high number of inputs. It allows for the estimation of both distribution-based sensitivity measures and of sensitivity measures that look at contributions to a specific moment. Besides being equipped with a wide range of information, analysts avoid type-I errors, because δ unveils statistical dependencies that would not be captured using variance-based statistics.

The strategy has been applied to the dataset generated by an *872*-factor model developed for NASA's risk assessment of lunar space missions. A reliable determination of the key drivers of uncertainty is obtained. Given the high number of factors, such information is particularly relevant in helping analysts redirect attention and resources in information collection and further modelling.

Finally, a note on future research. Because our approach is based on given data, the effect of the choice of the input factor distribution can be tested by mixing our approach with the input sample reshaping method of Beckman and McKay (1987).

Disclaimer

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Appendix A. Mathematical proofs

In this appendix we gather the proofs of the presented mathematical results.

Proof of Proposition 1. Consider $i \in J$ and Eq. (7). By additivity of the expectation, it is

$$\mathrm{E}[Y|X_i] = \mathrm{E}[a(\mathbf{X}_J)g(X_j)|X_i] + \mathrm{E}[b(\mathbf{X}_{J'})|X_i]. \tag{A.1}$$

Then, as X_i is independent of X_j and $\mathbf{X}_{J'}$,

$$\mathrm{E}[Y \mid X_i] = \mathrm{E}[a(\mathbf{X}_J) \mid X_i]\mathrm{E}[g(X_j)] + \mathrm{E}[b(\mathbf{X}_{J'})]. \tag{A.2}$$

Because $\mathrm{E}[g(X_j)] = 0$, Eq. (A.2) becomes $\mathrm{E}[Y \mid X_i] = \mathrm{E}[b(\mathbf{X}_{J'})]$. Thus, $\mathrm{Var}\{\mathrm{E}[Y|X_i]\} = 0$. Hence, we have $\eta_i^2 = 0$ for all $i \in J$. □

Proof of Proposition 2. By Eq. (14), and by the properties of integrals one gets:

$$\delta(Y,X) = \frac{1}{2}\int_{\mathcal{X}\times\mathcal{Y}} |f_Y(y)f_X(x) - f_X(x)f_{Y|X=x}(y)|\mathrm{d}y\ \mathrm{d}x. \tag{A.3}$$

By Eq. (3), one can write:

$$\delta(Y,X) = \frac{1}{2}\int_{\mathcal{X}\times\mathcal{Y}} |f_X(x)f_Y(y) - f_{XY}(x,y)|\mathrm{d}y\ \mathrm{d}x. \tag{A.4}$$

Eq. (A.4) is symmetric in X and Y, so that $\delta(Y,X) = \delta(X,Y)$. □

Proof of Corollary 1. By definition of independence between random variables we have $f_{XY}(x,y) = f_X(x)f_Y(y)$. Hence, if Y is independent of X then $\delta(X,Y) = 0$ follows straightforwardly. Conversely, assume that $\delta(X,Y) = 0$. Then, we get by Eq. (15), $\int_{\mathcal{X}\times\mathcal{Y}} |f_Y(y)f_X(x) - f_X(x)f_{Y|X=x}(y)|\ \mathrm{d}y\ \mathrm{d}x = 0$. Note that the following equalities are meant in an almost everywhere sense, as it is usual in measure theory. Because of the absolute value, the integral is null if the integrand is, i.e., $|f_Y(y)f_X(x) - f_X(x)f_{Y|X=x}(y)| = 0$. Thus, $f_Y(y)f_X(x) = f_X(x)f_{Y|X=x}(y) = 0$. Hence, $\delta = 0$ implies independence, since the product of the marginal densities almost surely equals the joint density and densities are almost surely uniquely determined (Schürger, 1998). □

Proof of Theorem 1. The main idea of the proof is already used for Eqs. (A.3) and (15). For ease of notation, we set $X = X_i, \mathcal{X} = \mathcal{X}^i$ and $\delta = \delta_i$ for a given factor i of interest. We first note the following auxiliary result. For disjoint sets $\mathcal{C}, \mathcal{C}' \in \mathcal{X}$ we have for $\mathcal{C}^0 = \mathcal{C} \cup \mathcal{C}'$

$$\begin{aligned} f_{Y|\mathcal{C}^0}(y) = f_{Y|\mathcal{C}\cup\mathcal{C}'}(y) &= \frac{P_X(\mathcal{C})f_{Y|\mathcal{C}}(y) + P_X(\mathcal{C}')f_{Y|\mathcal{C}'}(y)}{P_X(\mathcal{C}) + P_X(\mathcal{C}')} \\ &= \theta f_{Y|\mathcal{C}}(y) + (1-\theta)f_{Y|\mathcal{C}'}(y), \end{aligned} \tag{A.5}$$

which is a weighted average with $\theta = \frac{P_X(\mathcal{C})}{P_X(\mathcal{C}^0)}$. We now consider the class-conditional separation $S_m^j = \int_{\mathcal{Y}} |f_Y(y) - f_{Y|\mathcal{C}_m^j}(y)|\mathrm{d}y$. Using Eq. (A.5), the refinement strategy and the triangle inequality, yields

$$\begin{aligned} S_m^j &= \int_{\mathcal{Y}} |f_Y(y) - f_{Y|\mathcal{C}_{2m-1}^{j+1}\cup\mathcal{C}_{2m}^{j+1}}(y)|\mathrm{d}y \\ &= \int_{\mathcal{Y}} |\theta_m^j\left(f_Y(y) - f_{Y|\mathcal{C}_{2m-1}^{j+1}}(y)\right) \\ &\quad + \left(1-\theta_m^j\right)\left(f_Y(y) - f_{Y|\mathcal{C}_{2m-1}^{j+1}}(y)\right)|\mathrm{d}y \\ &\leqslant \int_{\mathcal{Y}} \left(\theta_m^j|f_Y(y) - f_{Y|\mathcal{C}_{2m-1}^{j+1}}(y)| + \left(1-\theta_m^j\right)|f_Y(y) - f_{Y|\mathcal{C}_{2m-1}^{j+1}}(y)|\right)\mathrm{d}y \\ &= \theta_m^j S_{2m-1}^{j+1} + \left(1-\theta_m^j\right)S_{2m}^{j+1}, \end{aligned} \tag{A.6}$$

with $\theta_m^j = \frac{P_X\left(\mathcal{C}_{2m-1}^{j+1}\right)}{P_X\left(\mathcal{C}_m^j\right)}$. Hence we obtain for the discrepancy measure

$$\begin{aligned} 2\delta_{j+1} &= \sum_{m=1}^{2^{j+1}} P_X\left(\mathcal{C}_m^{j+1}\right)S_m^{j+1} \\ &= \sum_{m=1}^{2^j} P_X\left(\mathcal{C}_m^j\right)\left(\theta_m^j S_{2m-1}^{j+1} + \left(1-\theta_m^j\right)S_{2m}^{j+1}\right) \\ &\geqslant \sum_{m=1}^{2^j} P_X\left(\mathcal{C}_m^j\right)S_m^j = 2\delta_j. \end{aligned} \tag{A.7}$$

As $S_m^j \leqslant 2$ for all m and j, the sequence (δ_j) is bounded by 1 and monotonically increasing. Therefore it converges to a limit. Consider an arbitrary partition $\mathcal{P}$ of M classes,

$$\begin{aligned} \delta_{\mathcal{P}} &= \frac{1}{2}\sum_{m=1}^{M}\int_{\mathcal{Y}} |f_Y(y) - f_{Y|\mathcal{C}_m}(y)|\mathrm{d}y \int_{\mathcal{C}_m} f_X(x)\mathrm{d}x \\ &= \frac{1}{2}\sum_{m=1}^{M}\int_{\mathcal{Y}} \left|\int_{\mathcal{C}_m} f_X(x)f_Y(y) - f_{XY}(x,y)\mathrm{d}x\right|\mathrm{d}y \\ &= \frac{1}{2}\sum_{m=1}^{M}\int_{\mathcal{Y}} f_Y(y)|\int_{\mathcal{C}_m} f_X(x) - f_{X|Y=y}(x)\mathrm{d}x|\mathrm{d}y. \end{aligned} \tag{A.8}$$

If $f_X(\cdot) - f_{X|Y=y}(\cdot)$ is continuous on $\mathcal{C}_m$ the mean value theorem shows that there exists a sequence $x_m \in \mathcal{C}_m, m = 1,\ldots,M$ such that

$$\delta_{\mathcal{P}} = \frac{1}{2}\int_{\mathcal{Y}} f_Y(y)\sum_{m=1}^{M}|f_X(x_m) - f_{X|Y=y}(x_m)|\int_{\mathcal{C}_m} f_X(x)\mathrm{d}x\mathrm{d}y. \tag{A.9}$$

This is a Riemann sum approximating δ. We have already shown that the sequence (δ_j) converges. □

Proof of Theorem 2. We have to show that all terms in the error expression are under control. Let us therefore consider the difference of Eqs. (26) and (13),

$$
\begin{aligned}
2(\hat{\delta}-\delta) &= \left(\sum_{m=1}^{M}\frac{n_m}{n}\widehat{S}_m\right) - \int_{\mathcal{X}} f_X(x)s(x)\mathrm{d}x \\
&= \sum_{m=1}^{M}\left(\frac{n_m}{n}\widehat{S}_m - \int_{\mathcal{C}_m} f_X(x)s(x)\mathrm{d}x\right) \\
&= \sum_{m=1}^{M}\widehat{S}_m\left(\frac{n_m}{n} - \int_{\mathcal{C}_m} f_X(x)\mathrm{d}x\right) \\
&\quad + \left(\widehat{S}_m - S_m\right)\int_{\mathcal{C}_m} f_X(x)\mathrm{d}x + \int_{\mathcal{C}_m}(S_m \\
&\quad - s(x))f_X(x)\mathrm{d}x. \qquad \text{(A.10)}
\end{aligned}
$$

Now, $\frac{n_m}{n}$ is the Monte Carlo estimate for $P_X(\mathcal{C}_m) = \int_{\mathcal{C}_m} f_X(x)\mathrm{d}x$. The separation estimate $\widehat{S}_m$ is obtained from numerical integration of the absolute difference of the kernel density estimators. Its convergence is driven by the quadrature rule, for a trapezoidal rule with ℓ equidistant quadrature points as of Eq. (25) we have

$$
\widehat{S}_m = \int |\hat{f}_Y(y) - \hat{f}_{Y|\mathcal{C}_m}(y)|\mathrm{d}y + O(\ell^{-2}). \qquad \text{(A.11)}
$$

In Devroye and Györfi (1985) it is shown that kernel estimators satisfy a consistency condition: For increasing sample size n there exists a bandwidth choice $h = h_n > 0$ such that the L_1 distance satisfies $\int |\hat{f}^n(y) - f(y)|\mathrm{d}y \to 0$ for the density $f(y)$ and its kernel density approximations $\hat{f}_n(y) = (nh_n)^{-1}\sum_{i=1}^{n} K\left(\frac{y-y_i}{h_n}\right)$, provided that the standard deviation is approximated by reasonable data-based estimator $\hat{\sigma}$. For instance, this is the case if the following $\hat{\sigma} = \min\left\{(n-1)^{-1}\sum_{i=1}^{n}(y_i-\bar{y})^2, 0.675^{-1}iqr(y)\right\}, h = \hat{\sigma}\left(\frac{3n}{4}\right)^{-\frac{1}{5}}$ are used with kernels $K(\cdot)$ with $\int K(x)\mathrm{d}x = 1, \int xK(x)\mathrm{d}x = 0$ and $\int x^2K(x)\mathrm{d}x = 1$, including Gaussian, boxed (uniform) and Epanechnikov kernels. (These alternative shapes are implemented in a Matlab script available upon request). Denoting $\widetilde{S}_m = \int |\hat{f}_Y(y) - \hat{f}_{Y|\mathcal{C}_m}(y)|\mathrm{d}y$ we have $\widehat{S}_m \approx \widetilde{S}_m$ and the approximation of the class separation satisfies

$$
\begin{aligned}
|\widetilde{S}_m - S_m| &\leqslant \int_{\mathcal{Y}} \left||\hat{f}_Y(y) - \hat{f}_{Y|\mathcal{C}_m}(y)| - |f_Y(y) - f_{Y|\mathcal{C}_m}(y)|\right|\mathrm{d}y \\
&\leqslant \int |\hat{f}_Y(y) - \hat{f}_{Y|\mathcal{C}_m}(y) - f_Y(y) + f_{Y|\mathcal{C}_m}(y)|\mathrm{d}y \\
&= \int_{\mathcal{Y}} |(\hat{f}_Y(y) - f_Y(y)) - (\hat{f}_{Y|\mathcal{C}_m}(y) - f_{Y|\mathcal{C}_m}(y))|\mathrm{d}y \\
&\leqslant \int_{\mathcal{Y}} |\hat{f}_Y(y) - f_Y(y)|\mathrm{d}y + \int_{\mathcal{Y}} |\hat{f}_{Y|\mathcal{C}_m}(y) - f_{Y|\mathcal{C}_m}(y)|\mathrm{d}y \\
&\to 0 \text{ as } n \to \infty. \qquad \text{(A.12)}
\end{aligned}
$$

Hence for n and ℓ approaching infinity, we obtain in the limit

$$
2(\hat{\delta}-\delta) \to \sum_{m=1}^{M}\int_{\mathcal{C}_m}(S_m - s(x))f_X(x)\mathrm{d}x. \qquad \text{(A.13)}
$$

Theorem 1 shows that for $M \to \infty$, this limit vanishes. □

Proof of Proposition 3. From the properties of the expectation and the variance and by independence we obtain for the product terms

$$
\mathrm{E}[Y] = \mathrm{E}\left[\prod_{i=1}^{k} g_i(X_i)\right] = \prod_{i=1}^{k}\mathrm{E}[g_i(X_i)], \qquad \text{(A.14)}
$$

$$
\begin{aligned}
\mathrm{E}[Y|X_i] &= g_i(X_i)\prod_{j\neq i}\mathrm{E}[g_j(X_j)], \quad \mathrm{Var}[\mathrm{E}[Y|X_i]] \\
&= \left(\mathrm{E}[g_i(X_i)^2] - \mathrm{E}[g_i(X_i)]^2\right)\prod_{j\neq i}\mathrm{E}[g_j(X_j)]^2. \qquad \text{(A.15)}
\end{aligned}
$$

Hence, if $\mathrm{E}[g_i(X_i)] \neq 0$,

$$
\eta_i^2 = \frac{\mathrm{Var}[\mathrm{E}[Y|X_i]]}{\mathrm{Var}[Y]} = \frac{\mathrm{Var}[g_i(X_i)]}{\mathrm{Var}[Y]}\cdot\frac{\mathrm{E}[Y]^2}{\mathrm{E}[g_i(X_i)]^2}. \quad \square \qquad \text{(A.16)}
$$

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