



Innovative Applications of O.R.

Screening: From tornado diagrams to effective dimensions

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ABSTRACT

Popular sensitivity analysis techniques such as Tornado Diagrams or the Morris method are based on one-at-a-time input variations (local main effects, henceforth). We evidence a link between local main effects of screening methods and global sensitivity measures. The link allows analysts to obtain insights on interactions on the local and global scales simultaneously. We evidence a mirroring effect according to which a local main effect calculated from the base case to the sensitivity case is equal in magnitude to the local total effect in the opposite direction, and their difference yields an overall local interaction index. We then obtain the exact relationship between Morris sensitivity measures and Sobol' total indices and discuss its implications on the choice of the sampling scheme. We show that the non-diagonal elements of the variance-covariance matrix of main effects computed at randomized locations yield Liu and Owen's global interaction indices. Asymptotic results are derived with particular reference to confidence intervals for the mean dimension. We illustrate findings and insights through numerical experiments on two well known simulators.

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1. Introduction

Computer simulations support decision-makers in a wide range of applications (Nelson, 2013). In several instances, analysts are asked to derive insights on the robustness of the simulator response, on the direction of change in its predictions, on the factors on which to focus managerial attention during implementation or on the areas on which to recommend further modelling efforts (Pesenti, Millossovich, & Tsanakas, 2019; Saltelli et al., 2008; Tsanakas & Millossovich, 2016). Commercial software easily generates a bar-chart, usually a Tornado diagram (Eschenbach, 1992; Howard, 1988), that orders the inputs according to the magnitude of one-at-a-time sensitivities. While simple and intuitive, this approach does not take uncertainty into account and provides a too limited exploration of the simulator input space to make an informed decision about robustness, trend or importance (Saltelli & Annoni, 2010). On the other side, best practice recommends the use of global approaches (Wagner, 1995), with indicators such as the mean dimension and total variance-based sensitivity indices (Owen, 2003; Wang, 2006). These indicators require a thorough exploration of the input space and are computationally more demanding than one-at-a-time sensitivities.

Screening methods represent an ideal bridge between global and one-at-a-time approaches; they aim at the identification of the most important inputs while employing a limited number of model evaluations. This has created considerable interest in finding a link between screening sensitivity measures and their global counterparts. Moreover, recently, in their work concerning the use of the mean dimension in machine learning, Owen & Hoyt (2021) suggest an implicit path between one-way-at-a-time sensitivity and total indices. Of particular interest is the relationship between the sensitivity measures of the popular Morris method (Morris, 1991) and the so-called Sobol' total-indices (Kucherenko, Rodríguez-Fernandez, Pantelides, & Shah, 2009). Works such as Campolongo, Cariboni, & Saltelli (2007); Campolongo, Saltelli, & Cariboni (2011); Kucherenko et al. (2009); Saltelli, Campolongo, & Cariboni (2009); Shi & Chen (2019) – see the literature review in Supplementary Section 1 – show that a path for connecting Morris and Sobol' sensitivity measures can be found in the evaluation of Morris elementary effects at several locations in the simulator input space. These works also suggest that Morris squared sensitivity measure ($\hat{\sigma}_{EE_i}^2$, henceforth) delivers indications about interaction and non-linearity. However, while the link has been argued in several works, the formal expression that ties these indices has not been established to date.

In this work, we revisit designs based on one-at-a-time sensitivities. We characterize a new property of local main effects. Considering the forward and backward one-at-a-time input changes

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across two locations in the input space, we show that a local main effect computed in the forward direction equals the opposite of the local total effect computed in the backward direction. Their difference yields an overall local interaction index whose value is independent of the direction of change.

When uncertainty in the inputs is taken into account, we address the statistical properties of the population of local main effects¹ computed at randomized locations of the simulator input space. We show that they have zero mean, that the diagonal terms of their variance-covariance matrix are proportional to the total Sobol' indices, while the non-diagonal elements correspond to the superset interaction indices of Liu & Owen (2006). We connect these estimators to the local main, interaction and total effects discussed above. Specifically, total global indices can be seen as variances of total local indices and the nullity of local overall interaction indices implies the nullity of global interaction indices. We then study the properties of these indices when the Morris design is used to generate local main effects deriving the exact relationship between Morris quadratic sensitivity measures ($\hat{\sigma}_{EE_i}^2$) and Sobol' total indices. It appears that, while Morris $\hat{\sigma}_{EE_i}^2$ indeed contains information on interactions as previously argued, its information is distorted. The reason is that in the Morris design all local main effects are calculated at a constant Δ step. However, exploiting the connection an analyst can recover the exact value of the total Sobol' indices from Morris $\hat{\sigma}_{EE_i}^2$.

We then carry out an asymptotic analysis to quantify uncertainty in the estimates of total order Sobol' indices, mean dimension, first order Sobol' indices and Morris sensitivity measures. The upper bound of the confidence interval about total indices leads to a screening criterion that takes uncertainty in the estimates into consideration.

We carry out numerical experiments on two well known simulators: the Asian option model of Nelson (2013), and the NASA space probabilistic safety assessment code of Borgonovo & Smith (2011). The design is exploited to obtain insights regarding the most influential inputs, as well as regarding interaction quantification and direction of change.

The remainder of the paper is organized as follows. Section 2 introduces screening designs offering a novel link between finite difference operators and scenario analysis. Section 3 presents the connection between local main effects and global sensitivity indices. In this section we also introduce a new sensitivity index for interactions which differ from the superset importance measure of Liu & Owen (2006).

Section 4 presents the intuition of a fold-over design. Section 5 establishes the formal relationship between Morris and Sobol' sensitivity indices. Section 6 presents the asymptotic analysis of the global sensitivity indices based on randomized local main effects and constructs a conservative screening criterion.

Section 7 presents two relevant simulation applications. Section 8 offers final remarks and discussion. The electronic complement contains all proof and additional discussion.

2. Finite change indices

Let $\mathbf{X}$ and Y be random vectors on $(\Omega, \mathcal{F}, \mathbb{P})$ with ranges given by $\mathcal{X} \subseteq \mathbb{R}^d$, $\mathcal{Y} \subseteq \mathbb{R}$ respectively. Let also $g: \mathcal{X} \rightarrow \mathcal{Y}$ denote an input-output mapping that links Y to $\mathbf{X}$, and let $\epsilon: \Omega \rightarrow \mathbb{R}$ be a noise random variable. In the traditional setup of computer experiments, g is a simulator created by the analyst to forecast a quantity of interest Y (output, henceforth) from knowledge of one or more independent variables $\mathbf{X} = \{X_1, X_2, \dots, X_d\}$ (inputs henceforth). One

writes the relationship in the form

$$Y = g(\mathbf{X}) + \epsilon, \quad (1)$$

where ϵ is independent of $\mathbf{X} \in \mathcal{X}$ and has the meaning of a stochastic error term. Usually, one assumes that the stochastic error term has null mean. Results in the reminder then hold either for $g(\mathbf{x})$ if the simulator is deterministic, or for its expected value if the simulator is stochastic.

Consider now two possible simulator input levels $\mathbf{x}^0, \mathbf{x}^1 \in \mathcal{X}$ and the corresponding simulator output responses $g(\mathbf{x}^0)$ and $g(\mathbf{x}^1)$. We can regard $\mathbf{x}^0$ and $\mathbf{x}^1$ as base-case and sensitivity-case, respectively. When the simulator inputs vary from the base to the sensitivity case ($0 \rightarrow 1$, henceforth) the change in model output is $\Delta^{0 \rightarrow 1}g = g(\mathbf{x}^1) - g(\mathbf{x}^0)$.

This change can be dissected in $2^d - 1$ orthogonal effects as follows. Let $U = (1, 2, \dots, d)$ and $\mathcal{U} = 2^U$ denote the corresponding power set and let $u \in \mathcal{U}$ be any subset of indices. It is then possible to prove that (see Li, Wang, Rosenthal, & Rabitz, 2001 among others):

$$\Delta^{0 \rightarrow 1}g = \sum_{u \in \mathcal{U}, u \neq \emptyset} \phi_u^{0 \rightarrow 1}, \quad (2)$$

where

$$\phi_u^{0 \rightarrow 1} = g(\mathbf{x}_u^1; \mathbf{x}_{-u}^0) - \sum_{v \subset u} \phi_v^{0 \rightarrow 1}, \quad (3)$$

and where $(\mathbf{x}_u^1; \mathbf{x}_{-u}^0)$ is the point obtained shifting all inputs with indices in u at the sensitivity-case and keeping the remaining inputs at the base-case. With a little abuse of notation, when $u = \emptyset$, we let $\sum_{v \subset \emptyset} \phi_v^{0 \rightarrow 1} = g(\mathbf{x}_0)$. To illustrate, these expressions are equivalent to

$$\Delta^{0 \rightarrow 1}g = \sum_{i=1}^d \phi_i^{0 \rightarrow 1} + \sum_{i < j} \phi_{i,j}^{0 \rightarrow 1} + \sum_{i < j < k} \phi_{i,j,k}^{0 \rightarrow 1} + \dots + \phi_{1,2,\dots,d}^{0 \rightarrow 1}, \quad (4)$$

where

$$\begin{cases} \phi_i^{0 \rightarrow 1} = g(\mathbf{x}_i^1; \mathbf{x}_{-i}^0) - g(\mathbf{x}^0) \\ \phi_{i,j}^{0 \rightarrow 1} = g(\mathbf{x}_{i,j}^1; \mathbf{x}_{-[i,j]}^0) - g(\mathbf{x}^0) - \phi_i^{0 \rightarrow 1} - \phi_j^{0 \rightarrow 1} \\ \phi_{i,j,k}^{0 \rightarrow 1} = g(\mathbf{x}_{i,j,k}^1; \mathbf{x}_{-[i,j,k]}^0) - g(\mathbf{x}^0) - \phi_i^{0 \rightarrow 1} - \phi_j^{0 \rightarrow 1} - \phi_k^{0 \rightarrow 1} \\ \dots \end{cases} \quad (5)$$

In the above equation, $(\mathbf{x}_i^1; \mathbf{x}_{-i}^0)$ denotes the point in $\mathcal{X}$ in which all inputs are at the base case with the exception of x_i . The quantities $\phi_i^{0 \rightarrow 1}$ are the local main effects of the inputs related to the shift $\mathbf{x}^0 \rightarrow \mathbf{x}^1$.

Similarly, $(\mathbf{x}_{i,j}^1; \mathbf{x}_{-[i,j]}^0)$ denotes the point in which all inputs are at the base case, but for the pair x_i and x_j . The second order effect $\phi_{i,j}^{0 \rightarrow 1}$ quantifies the residual interaction given that x_i and x_j are simultaneously shifted to the sensitivity case.

The quantity $\phi_u^{0 \rightarrow 1}$ is a measure of the contribution of the residual interaction of the indices in u to the finite change $\Delta^{0 \rightarrow 1}g$. To illustrate the notation in (4), consider the case of four inputs labelled $\{1, 2, 3, 4\}$. The sum $\sum_{i < j < k} \phi_{i,j,k}^{0 \rightarrow 1}$ stands for $\phi_{1,2,3}^{0 \rightarrow 1} + \phi_{1,2,4}^{0 \rightarrow 1} + \phi_{1,3,4}^{0 \rightarrow 1} + \phi_{2,3,4}^{0 \rightarrow 1}$.

One can then define the total contribution of x_i to $\Delta^{0 \rightarrow 1}g$ as Borgonovo, Plischke, & Rabitti (2021)

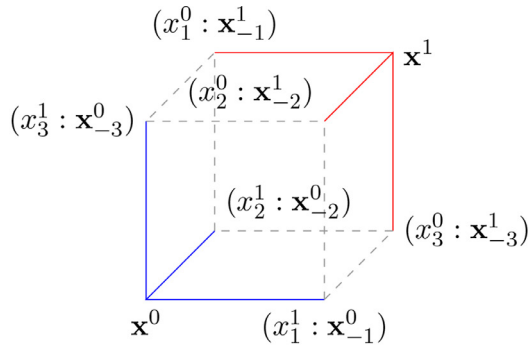
$$\tau_i^{0 \rightarrow 1} = \sum_{u \in \mathcal{U}_i} \phi_u^{0 \rightarrow 1}, \quad (6)$$

where $\mathcal{U}_i = \{u \subseteq \{1, 2, \dots, d\} | i \in u\}$, and the total interaction contribution by

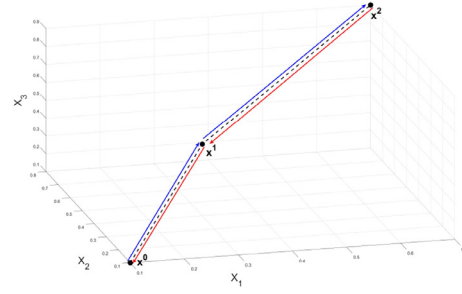
$$\Lambda_i^{0 \rightarrow 1} = \tau_i^{0 \rightarrow 1} - \phi_i^{0 \rightarrow 1}. \quad (7)$$

The triplet of indices $\phi_i^{0 \rightarrow 1}$, $\tau_i^{0 \rightarrow 1}$, and $\Lambda_i^{0 \rightarrow 1}$ can be represented in the form of a Generalized Tornado Diagram (Borgonovo & Smith,

¹ We shall use the term one-at-a-time sensitivity and local main effect as synonyms in the reminder.



(a) Zoom into $\mathbf{x}^0 \rightarrow \mathbf{x}^1$ and $\mathbf{x}^0 \leftarrow \mathbf{x}^1$. Blue: changes in the forward pass. Red: changes in the backward pass.



(b) Forward (blue) and backward (red) passes for a three point trajectory. The points are $\mathbf{x}^0 = (0.1, 0.1, 0.1)$, $\mathbf{x}^1 = (0.3, 0.4, 0.5)$ and $\mathbf{x}^2 = (0.7, 0.8, 0.9)$.

Fig. 1. Three-dimensional illustration of forward and backwards passes in a trajectory of a fold-over design.

2011). Determining all the $\phi_u^{0 \rightarrow 1}$ effects in (5) requires a full factorial design. As underlined already in Jacoby & Harrison (1962) a full factorial design becomes rapidly infeasible. Therefore, the literature has proposed designs to reduce computational burden (Barton, 2015; Lin, 2000).

We consider the fold-over design of Cotter (1979), which is based on one-at-a-time changes from $\mathbf{x}^0$ to $\mathbf{x}^1$ (forward-pass) and their mirror-changes from $\mathbf{x}^1$ to $\mathbf{x}^0$ (backward-pass). Fig. 1a proposes a three dimensional visualization. The one-at-a-time variations from $\mathbf{x}^0$ to $\mathbf{x}^1$ (forward-pass, henceforth) are marked in blue, the ones from $\mathbf{x}^1$ to $\mathbf{x}^0$ (backward-pass, henceforth) in red.

The next result summarizes two properties of fold-over designs (All proofs are contained in the Supplementary material).

Proposition 1. Consider a forward and a backward pass in a fold-over design between $\mathbf{x}^0$ and $\mathbf{x}^1$. It is $\phi_i^{0 \rightarrow 1} = -\tau_i^{1 \rightarrow 0}$ and $\Lambda_i^{0 \rightarrow 1} = \Lambda_i^{1 \rightarrow 0}$ for all i .

Proposition 1 suggests that a forward-pass main effect $\phi_i^{0 \rightarrow 1}$ equals the opposite of the corresponding backward-pass total effect $\tau_i^{1 \rightarrow 0}$. Note that the equality also holds for the change from the backward-pass to the forward-pass, that is, $\phi_i^{1 \rightarrow 0} = -\tau_i^{0 \rightarrow 1}$. Also, $\tau_i^{0 \rightarrow 1} = 0$ doesn't imply $\phi_i^{0 \rightarrow 1}$, since $\phi_i^{0 \rightarrow 1} = -\tau_i^{1 \rightarrow 0}$ can be non-zero. Thus, both first and total indices should be considered for local screening.

Moreover, Proposition 1 shows that the total interaction contributions $\Lambda_i^{0 \rightarrow 1}$ and $\Lambda_i^{1 \rightarrow 0}$ coincide: While the local main and total effects are opposite between the two passes, the interaction effect is the same regardless of the direction of the pass. Proposition 1 also says that the triplet of indices $\phi_i^{0 \rightarrow 1}$, $\Lambda_i^{0 \rightarrow 1}$ and $\tau_i^{0 \rightarrow 1}$ can be estimated from $2d + 2$ simulator evaluations. To illustrate, for $d = 3$ (see Fig. 1a), we have a first evaluation of the model at $\mathbf{x}^0$, a second at $\mathbf{x}^1$, then 3 evaluations for moving the inputs one-at-a-time from $\mathbf{x}^0$ to $\mathbf{x}^1$ (forward-pass) and 3 evaluations for moving the inputs one-at-a-time from $\mathbf{x}^1$ to $\mathbf{x}^0$ (backward pass), for 8 evaluations overall.

The total interaction index $\Lambda_i^{0 \rightarrow 1}$ is connected to well-known interaction measures. Let

$$A^{i,-i}(\mathbf{x}^0, \mathbf{x}^1) = \frac{1}{2} [g(\mathbf{x}^0) - g(\mathbf{x}_{-i}^0 : x_i^1) + g(\mathbf{x}^1) - g(x_i^0 : \mathbf{x}_{-i}^1)] \quad (8)$$

denote the two-factor interaction of Design of Experiments (Wu, 2015) – see also the interaction measure: $E^{i,-i} = |A^{i,-i}|$ proposed by Campolongo et al. (2011). We have:

$$A^{i,-i}(\mathbf{x}^0, \mathbf{x}^1) = -\frac{1}{2} [\phi_i^{0 \rightarrow 1} + \phi_i^{1 \rightarrow 0}] = -\frac{1}{2} [\phi_i^{0 \rightarrow 1} - \tau_i^{0 \rightarrow 1}] = \frac{1}{2} \Lambda_i^{0 \rightarrow 1}.$$

Note the symmetry of the interaction measures: $A^{i,-i}(\mathbf{x}^0, \mathbf{x}^1) = \frac{1}{2} \Lambda_i^{0 \rightarrow 1} = \frac{1}{2} \Lambda_i^{1 \rightarrow 0} = A^{i,-i}(\mathbf{x}^1, \mathbf{x}^0)$.

Consider now repeating these calculations at several locations in the input space. Denote these locations with $\mathbf{x}^r$ in $\mathcal{X}$, $r = 0, 1, \dots, N$. These locations can be selected using alternative sampling designs (Campolongo et al., 2007; Le Guiban, Rimmel, Weisser, & Tomasik, 2018). We call trajectory a sequence of points $\mathcal{T} = \{\mathbf{x}^0 \rightarrow \mathbf{x}^1 \rightarrow \dots \rightarrow \mathbf{x}^N\}$. A trajectory can be sampled using crude, quasi Monte Carlo, Latin Hypercube or any other sample generation mechanism (see Pronzato & Müller (2012) for a review). Thus, in general trajectories are sequences of points randomly sampled in $\mathcal{X}$.

Evaluating the simulator at $\mathcal{T}$ allows the analyst to obtain a set of N output changes $\Delta^{k \rightarrow k+1}g$ from point k to $k + 1$, with $k = 0, 1, \dots, N - 1$, that we denote with $(\Delta^{0 \rightarrow 1}g)_{(k)}$ to highlight the initial and final evaluation points. Because each of these changes can be decomposed via (4), one obtains a population of $N \cdot (2^d - 1)$ main and interaction effects $(\phi_u^{0 \rightarrow 1})_{(k)}$. However, this quantification is equivalent to repeatedly performing full factorial designs and becomes rapidly impractical. If, instead, one considers computing only local main effects, she can run the code $(d + 1) \cdot N$ times to obtain N replicates of d local main effects.

Now, suppose we extend the fold-over intuition to a trajectory: For a forward-pass $\mathbf{x}^0 \rightarrow \mathbf{x}^1 \rightarrow \dots \rightarrow \mathbf{x}^N$ (forward-pass) one also calculates local main effects in the backward-pass $\mathbf{x}^N \rightarrow \mathbf{x}^{N-1} \rightarrow \dots \rightarrow \mathbf{x}^0$ (backward-pass). Fig. 1b offers a three dimensional visualization. This design yields:

- $2N$ local main effects of which N are forward effects $(\phi_i^{0 \rightarrow 1})_{(k)}$ and N are backward effects $(\phi_i^{1 \rightarrow 0})_{(k)}$;
- $2N$ total effects $(\tau_i^{0 \rightarrow 1})_{(k)} = -(\phi_i^{0 \rightarrow 1})_{(k)}$, by Proposition 1;
- N interaction effects $(\Lambda_i^{0 \rightarrow 1})_{(k)}$.

Then, the total cost for obtaining these sensitivity measures is $N(2d + 2)$ simulator runs. This information would be represented in $2N - 2$ Tornado diagrams. Note that the strategy of estimating backward passes is compatible with any one-at-a-time design (Chan, Saltelli, & Tarantola, 2000; Owen & Hoyt, 2021).

Example 2. Let $y = x_1 \cdot x_2 \cdot x_3$, and consider on the sequence of $N = 3$ points $\mathbf{x}^0 = (0.1, 0.1, 0.1)$, $\mathbf{x}^1 = (0.3, 0.4, 0.5)$ and $\mathbf{x}^2 = (0.7, 0.8, 0.9)$. In Fig. 1b, the forward-pass across these three points is marked in blue, the backward-pass in red.

Table 1 presents results for the first input x_1 (the local effects of x_2 and x_3 can be similarly found although they have different values). First, one computes the local main effects for the

Table 1
Finite change indices for the Example 2.

	Forward-pass		Backward-pass	
	$\mathbf{x}^0 \rightarrow \mathbf{x}^1$	$\mathbf{x}^1 \rightarrow \mathbf{x}^2$	$\mathbf{x}^2 \rightarrow \mathbf{x}^1$	$\mathbf{x}^1 \rightarrow \mathbf{x}^0$
$\phi_1^{0 \rightarrow 1}$	0.002	0.08	−0.288	−0.04
$\Lambda_1^{0 \rightarrow 1}$	0.038	0.208	0.208	0.038
$\tau_1^{0 \rightarrow 1}$	0.04	0.288	−0.08	−0.002

forward-passes $\mathbf{x}^0 \rightarrow \mathbf{x}^1$ and $\mathbf{x}^1 \rightarrow \mathbf{x}^2$ obtaining $\phi_1^{0 \rightarrow 1} = 0.002$ and $\phi_1^{1 \rightarrow 2} = 0.08$ (columns 2 and 3 in Table 1). Then, one computes the local main effects for the backward-passes $\mathbf{x}^2 \rightarrow \mathbf{x}^1$ and $\mathbf{x}^1 \rightarrow \mathbf{x}^0$, obtaining $\phi_1^{2 \rightarrow 1} = -0.288$ and $\phi_1^{1 \rightarrow 0} = -0.04$ respectively (columns 4 and 5 in Table 1). By Proposition 1 we can then immediately find the total effects $\tau_1^{0 \rightarrow 1}$, $\tau_1^{1 \rightarrow 2}$ and the total interaction effects $\Lambda_1^{0 \rightarrow 1}$ and $\Lambda_1^{1 \rightarrow 2}$ without additional model runs. For instance, the total effects for the forward-passes can be found changing the sign of the local main effects for the backward-passes, yielding $\tau_1^{0 \rightarrow 1} = 0.04$ and $\tau_1^{1 \rightarrow 2} = 0.288$. Then, the total interaction effects for the forward-passes are given by $\Lambda_1^{0 \rightarrow 1} = \tau_1^{0 \rightarrow 1} - \phi_1^{0 \rightarrow 1} = 0.038$ and $\Lambda_1^{1 \rightarrow 2} = 0.208$. The backward-pass indices can be found with a similar procedure. Note that the total interaction effects remain the same in agreement with Proposition 1.

In the next sections, we further explore how to use this information efficiently starting with the connection to global sensitivity indices.

3. From local main effects to Sobol' total indices

In this section, we present a formal link between finite change indices and global sensitivity indicators. Given $\mathbf{X} = (X_1, X_2, \dots, X_d)$ with cumulative distribution function $F_{\mathbf{X}}$, we denote with $F_{\mathbf{X}_u}$ the cumulative distribution function of the vector $\mathbf{X}_u$ made of the components of $\mathbf{X}$ indexed by u . With $F_{\mathbf{X}_{-u}}$ we denote the distribution function of the vector $\mathbf{X}_{-u}$, whose components are taken from the complementary set $\{1, 2, \dots, d\} \setminus u$.

Henceforth, we assume that g is a square integrable function and that the inputs are independent, so that $F_{\mathbf{X}} = \prod_{i=1}^d F_{X_i}(x_i)$.

The classical result of Efron & Stein (1981); Sobol' (1993) allows us to expand the variance of Y in $2^d - 1$ terms as:

$$\sigma_Y^2 = \sum_{u \in \mathcal{U}} \sigma_u^2, \quad (9)$$

where $\sigma_u^2 = \int [g_u(\mathbf{x}_u)]^2 dF_{\mathbf{X}_u}(\mathbf{x}_u)$, with

$$g_u(\mathbf{x}_u) = \int g(\mathbf{x}_u : \mathbf{s}_{-u}) dF_{\mathbf{X}_{-u}}(\mathbf{s}_{-u}) - \sum_{v \subset u} g_v(\mathbf{x}_v). \quad (10)$$

In (9), the first order terms σ_i^2 and the higher order terms σ_u^2 represent, respectively, the individual contribution and the contribution of the residual interaction among the inputs whose indices are in subset u . In the literature one often finds the normalized version of these indices. They are called Sobol' indices and denoted by $S_u = \frac{\sigma_u^2}{\sigma_Y^2}$. We observe that the term $h_u(\mathbf{x}_u) = \int g(\mathbf{x}_u : \mathbf{s}_{-u}) dF_{\mathbf{X}_{-u}}(\mathbf{s}_{-u})$ in (10) corresponds to the partial dependence function of $\mathbf{x}_u$ introduced by Friedman (2001), and widely used in the machine learning literature – see Goldstein, Kapelner, Bleich, & Pitkin (2015); Zhao & Hastie (2019) for additional details.

From (9) one defines the global sensitivity indices (Homma & Saltelli, 1996; Liu & Owen, 2006; Wagner, 1995):

$$\bar{\tau}_i^2 = \sigma_i^2, \quad (11)$$

$$\bar{\tau}_i^2 = \sum_{i \in v} \sigma_v^2, \quad (12)$$

$$\Lambda_i^2 = \bar{\tau}_i^2 - \tau_i^2, \quad (13)$$

and

$$\Upsilon_u^2 = \sum_{v \supseteq u} \sigma_v^2. \quad (14)$$

where τ_i^2 is the first order variance based index of X_i and $\bar{\tau}_i^2$ is Homma & Saltelli (1996)'s total index and Υ_u^2 is Liu & Owen (2006)'s superset importance. Note that $\bar{\tau}_i^2$ is the sum of all terms in the right hand side of (9) that contain a contribution from X_i , while Λ_i^2 contains only the contributions from subsets of cardinality greater than 1, thus stemming from the interactions of X_i with the remaining inputs. In this respect, Λ_i^2 is different from Υ_i^2 . For instance, if $u = \{i\}$, Υ_i^2 coincides with $\bar{\tau}_i^2$, while Λ_i^2 conveys solely the importance of interactions, excluding τ_i^2 .

Owen (2003) shows that the sum of the total order indices equals the mean dimension in the superimposition sense of g (mean dimension, henceforth). This quantity is defined as

$$D_g = \frac{\sum_{u \in \mathcal{U}} |u| \sigma_u^2}{\sigma_Y^2}, \quad (15)$$

where $|u|$ is the cardinality of u . The higher the value of D_g , the more relevant the presence of interactions. The mean dimension has been originally introduced in Cafisch, Morokoff, & Owen (1997) in association with the notion of dimension distribution to characterize the size of interactions in g , and has found notable applications for dimension reduction in financial engineering (Wang, 2006; 2016; Wang & Sloan, 2011) as well as high-dimensional integration.

When uncertainty in the inputs is considered, the local main effects in (5) become random quantities defined as

$$\Phi_i = g(X_i^1; \mathbf{X}^0) - g(\mathbf{X}^0), \quad (16)$$

where $\mathbf{X}^0, \mathbf{X}^1$ are iid random variables distributed according to $F_{\mathbf{X}}$ and X_i^1 is the i th coordinate of $\mathbf{X}^1$. The collection of these indices $\Phi = \{\Phi_1, \Phi_2, \dots, \Phi_d\}$ is a random vector on $(\Omega, \mathcal{B}(\Omega), \mathbb{P})$ with push-forward measure $\mathbb{P}_{\Phi}$ induced by (16) (We shall use the notation $\Phi^{\mathbf{x}^0 \rightarrow \mathbf{x}^1}$ when it is necessary to evidence the base case and the sensitivity case).

Theorem 3. Given the above setup, Φ is a random vector, with expectation

$$\mathbb{E}[\Phi_i] = 0, \quad (17)$$

for all i , and variance-covariance matrix

$$\mathbb{C}(\Phi) = \begin{pmatrix} 2\bar{\tau}_1^2 & \Upsilon_{12}^2 & \dots & \Upsilon_{1d}^2 \\ \Upsilon_{12}^2 & 2\bar{\tau}_2^2 & \dots & \Upsilon_{2d}^2 \\ \vdots & \vdots & \ddots & \vdots \\ \Upsilon_{1d}^2 & \Upsilon_{2d}^2 & \dots & 2\bar{\tau}_d^2 \end{pmatrix}. \quad (18)$$

Theorem 3 implies that the mean of a local main effect Φ_i is zero, and its variance equals twice the Sobol' total index of X_i , that is:

$$\bar{\tau}_i^2 = \frac{\mathbb{V}[\Phi_i]}{2}. \quad (19)$$

Eq. (19) suggests that the most important inputs are those for which the first order effects show greater variability. Thus, given a sample of local main effects, analysts can gain a rough idea of the relative input importance by visualizing their distribution and considering their dispersion around zero.

Another way to compute the total Sobol' index is given by

$$\bar{\tau}_i^2 = \frac{1}{2} \mathbb{E}[(\Phi_i)^2]. \quad (20)$$

The empirical version of (20) is the so called *Jansen estimator* of the Sobol' total index. Because the local main effects have null mean, the formulations in (19) and (20) are equivalent.

Remark 4. Proposition 1 allows us to rewrite (20) as

$$\bar{\tau}_i^2 = \frac{1}{2} \mathbb{E}[(\Phi_i^{\mathbf{X}^0 \rightarrow \mathbf{X}^1})^2] = \frac{1}{2} \mathbb{E}[(\tau_i^{\mathbf{X}^1 \rightarrow \mathbf{X}^0})^2]. \quad (21)$$

Thus, global total indices $\bar{\tau}_i^2$ can also be regarded as an average of local total indices $\tau_i^{\mathbf{X}^1 \rightarrow \mathbf{X}^0}$, highlighting a direct connection of total effects from the local to the global scale.

The non-diagonal entries in Equation (18) equal the superset importance $\Upsilon_{i,j}^2$ of X_i and X_j . This leads to a computational saving: we obtain the superset indices and the total indices at a cost of $N(d+1)$ model runs. Using, for instance, a dedicated estimator based on the Sobol' design would call for $\binom{d}{2} + d + 1$ evaluations (the cost remains lower also with respect to the other dedicated designs in Fruth, Roustant, & Kuhnt, 2014). The index $\Upsilon_{i,j}^2$ is null when g is additive and a value different from zero signals the presence of interactions in g that involve both X_i and X_j .

Example 5. Consider the input-output mapping $g(\mathbf{X}) = X_1 X_2 X_3$ with X_1, X_2 and X_3 iid $\mathcal{N}(1, 1)$. The model output variance is $\sigma_Y^2 = 7$ and the local main effect variance-covariance matrix is $\mathbb{C}(\Phi) = \begin{pmatrix} 8 & 2 & 2 \\ 2 & 8 & 2 \\ 2 & 2 & 8 \end{pmatrix}$, from which we obtain $\tau_i^2 = 1$, $\Lambda_i^2 = 3$ and $\bar{\tau}_i^2 = 4$ for $i = 1, 2, 3$, $\Upsilon_{i,j}^2 = 2$ for $i, j = 1, 2, 3, i \neq j$ and $D_g = \frac{12}{7} = 1.71$.

From the knowledge of first order effects one can estimate also first order variance-based indices from (see Owen & Hoyt, 2021)

$$\tau_i^2 = \mathbb{E}[g(\mathbf{X}^0) \cdot \Phi_i^{\mathbf{X}^1 \rightarrow \mathbf{X}^0}]. \quad (22)$$

In analogy to Remark 4, the following information holds.

Remark 6. The first order variance-based indices in (22) can be written as

$$\tau_i^2 = \mathbb{E}[g(\mathbf{X}^1) \cdot \Phi_i^{\mathbf{X}^0 \rightarrow \mathbf{X}^1}], \quad (23)$$

where $\Phi_i^{\mathbf{X}^1 \rightarrow \mathbf{X}^0}$ denotes the population of local main effects computed setting $\mathbf{X}^1$ as base case and $\mathbf{X}^0$ as sensitivity case (backward-pass).

Remark 6 implies that we can estimate the first order indices adopting first order effects for both forward and backward pass. The only requirement is that the first order effects from the base case to the sensitivity case are multiplied by the value of the model at the sensitivity case.

Regarding the relevance of interactions consider the sum $\sum_{i=1}^d \Lambda_i^2$. This quantity is null if g is additive. Combining (13) and $\sum_{u \in \mathcal{U}} |u| \sigma_u^2 = \sum_{i=1}^d \bar{\tau}_i^2$, the following holds:

$$\sum_{u \in \mathcal{U}} |u| \sigma_u^2 = \sum_{i=1}^d \Lambda_i^2 + \sum_{i=1}^d \tau_i^2, \quad (24)$$

that is the sum of the interaction indices Λ_i^2 exceeds the sum of all the first order indices by the numerator of the mean dimension. Since $\sum_u |u| \sigma_u^2 = \sum_{i=1}^d \tau_i^2 + \sum_{|u|>1} |u| \sigma_u^2$, it follows $\sum_{i=1}^d \Lambda_i^2 = \sum_{|u|>1} |u| \sigma_u^2$. If we divide (24) by σ_Y^2 , we obtain

$$D_g = D_g^{\text{Add}} + D_g^{\text{Int}}, \quad \text{where} \quad D_g^{\text{Add}} = \frac{\sum_{i=1}^d \tau_i^2}{\sigma_Y^2}, \quad D_g^{\text{Int}} = \frac{\sum_{i=1}^d \Lambda_i^2}{\sigma_Y^2}, \quad (25)$$

so that the mean dimension is decomposed into the sum of two terms, D_g^{Add} and D_g^{Int} . We recall works such as Wang (2006) and

Wang & Tan (2013) that regard D_g^{Add} as a measure of the degree of additivity of g . In fact, if and only if g is additive, $D_g^{\text{Int}} = 0$, and $D_g = D_g^{\text{Add}}$, and $\sum_{i=1}^d \tau_i^2 = \sigma_Y^2$, so that $D_g = 1$. Conversely, if $D_g^{\text{Int}} \gg 1$, then g is dominated by interaction effects.

We can then connect local and global interaction measures.

Proposition 7. We have

$$\Lambda_i^2 = \mathbb{E}[g(\mathbf{X}^0) \cdot \Lambda_i^{\mathbf{X}^0 \rightarrow \mathbf{X}^1}] \quad (26)$$

and

$$D_g^{\text{Int}} = \frac{\sum_{i=1}^d \mathbb{E}[g(\mathbf{X}^0) \cdot \Lambda_i^{\mathbf{X}^0 \rightarrow \mathbf{X}^1}]}{\sigma_Y^2}. \quad (27)$$

Proposition 7 implies that the global interaction indices Λ_i^2 can be obtained as averages of local indices $\Lambda_i^{\mathbf{X}^0 \rightarrow \mathbf{X}^1}$, weighted by the initial point $g(\mathbf{X}^0)$. Note that, without this weights, we would have $\mathbb{E}[\Lambda_i^{\mathbf{X}^0 \rightarrow \mathbf{X}^1}] = \mathbb{E}[\tau_i^{\mathbf{X}^0 \rightarrow \mathbf{X}^1}] - \mathbb{E}[\phi_i^{\mathbf{X}^0 \rightarrow \mathbf{X}^1}] = -\mathbb{E}[\phi_i^{\mathbf{X}^1 \rightarrow \mathbf{X}^0}] - \mathbb{E}[\phi_i^{\mathbf{X}^0 \rightarrow \mathbf{X}^1}] = 0$. Eq. (26) shows that to recover global (Λ_i^2) from local ($\Lambda_i^{\mathbf{X}^0 \rightarrow \mathbf{X}^1}$) interaction indices we need to adopt a forward-backward-pass strategy. We discuss this aspect further in next section.

4. Full-forward or forward-and-backward?

The possibility of exchanging the forward and backward passes highlighted in the previous section leads to a potential tradeoff between exploration of the input space and insights about interactions. Suppose computational budget allows for a fixed number of model runs C . This cap leads to an overall maximum number of locations to be explored equal to $N^* = C/(d+2)$. The analyst may consider using a forward trajectory, computing for each input the sequence $(\phi_i^{0 \rightarrow 1})_{(k)}$, or using half of the points for a forward trajectory and half of the points for the corresponding backward trajectory.

An analyst can allocate all $N^*(d+2)$ runs to forward-passes, obtaining N^* first order effects $(\phi_i^{0 \rightarrow 1})_{(k)}$ for each input, from which she can estimate the elements of $\mathbb{C}(\Phi)$ in (18). Thus, information on global interactions can be obtained from the variance-covariance matrix and from taking the differences between global total effects in (21) and the first-order effects in (23). All these quantities can be estimated with forward passes. Alternatively, the analyst can opt for allocating $\frac{N^*(d+2)}{2}$ runs to forward-passes and $\frac{N^*(d+2)}{2}$ runs to the corresponding backward-passes. By Proposition 1, the analyst still obtains N^* local main effects from which to estimate the variance-covariance matrix, and, in addition, obtains $\frac{N^*}{2}$ local interaction effects $(\Lambda_i^{0 \rightarrow 1})_{(k)}$ at randomized locations. The selection depends on the goal of the analysis. If focus is on exploration of the input space, a forward strategy allows a more thorough exploration of the input space, because the model is evaluated at $N^*(d+2)$ different points. Conversely, if the goal is to obtain also local insights on interactions, then a forward-backward design is to be chosen, because the analyst obtains triplets of individual, total and overall local interaction effects at $N^*/2$ randomized locations that communicate insights regarding the relevance of interactions at the finite scale. We stress this aspect since having information about interactions on the global scale does not imply information on the local scale, as next example shows.

Example 8. In this example we consider the wing-weight simulator of Forrester, Söbester, & Keane (2008). This simulator describes the weight of the wings of a small aircraft as a function of 10 engineering and physical inputs subject to uncertainty. From a sample of local interaction effects $(\Lambda_i^{0 \rightarrow 1})_{(k)}$, with $k = 1, 2, \dots, 10,000$ for

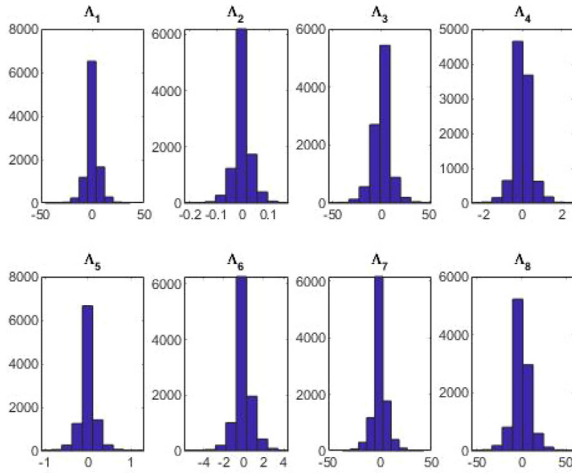


Fig. 2. Histograms of the local interaction indices Δ_i for the first inputs $i = 1, 2, \dots, 8$. These plots show that some values can be significantly different from zero.

each input, we find that $D_g^{Int} = 0.0463$ using (27), and consequently $D_g^{Add} = 0.9537$. Thus, this simulator response is additive on a global scale, a result in accordance with the findings in Jiménez Rugama & Gilquin (2018). However, an examination of the magnitudes of local interaction effects shows that they might be non-negligible. Fig. 2 displays the histograms of the 10,000 local interaction effects $(\Delta_i^{0 \rightarrow 1})_{(k)}$ for the first eight inputs $i = 1, 2, \dots, 8$.

As expected, the mean of the empirical distributions is null. Nonetheless, the histograms show that particularly inputs 1, 3, 7, 8 are involved in non-negligible local interaction effects. Indeed, considering that this simulator response has mean 278.16 and standard deviation 52.36, we note that several local interaction effects are of the same or higher magnitude of the model output standard deviation.

5. The exact relationship between Morris and Sobol' total indices

The method of Morris (1991) is one of the most popular screening techniques in the simulation literature. It is based on a sample of forward-passes in which inputs are shifted one-at-a-time with fixed step Δ . Given a randomly sampled trajectory $\mathbf{x}^1, \mathbf{x}^2, \dots, \mathbf{x}^N$, Morris (1991) introduces the elementary effects

$$EE_i^k = \frac{g(x_1^k, x_2^k, \dots, x_i^k + \Delta, \dots, x_d^k) - g(\mathbf{x}^k)}{\Delta}, \quad (28)$$

where $\mathbf{x}^k$ is a point in the trajectory and $(x_1^k, x_2^k, \dots, x_i^k + \Delta, \dots, x_d^k)$ is the point obtained by shifting X_i by Δ . With this definition EE_i^k , an elementary effect in (28) is the random quantity

$$EE_i = \frac{\Delta \Phi_i}{\Delta}, \quad (29)$$

where

$$\Delta \Phi_i = g(X_i + \Delta : \mathbf{X}_{-i}) - g(\mathbf{X}), \quad (30)$$

We note that the Morris main effect $\Delta \Phi_i$ differs from the local main effect Φ_i in (16) because the inputs are shifted by a fixed step Δ . Differently from Φ_i , $\Delta \Phi_i$ do not have null expectation, because

$$\mathbb{E}[\Delta \Phi_i] = \mu_i \Delta, \quad (31)$$

where $\mu_i = \mathbb{E}[EE_i]$ is the mean of the Morris effects for the i th input. The variance of the Morris effects is denoted by $\sigma_{EE_i}^2$.

Morris (1991) considers two sensitivity measures: The empirical mean of the elementary effects²

$$\hat{\mu}_i = \frac{\sum_{k=1}^N EE_i^k}{N} = \frac{\Delta \Phi_i}{\Delta}, \quad i = 1, 2, \dots, d, \quad (32)$$

and their empirical variance

$$\hat{\sigma}_{EE_i}^2 = \frac{\sum_{k=1}^N (EE_i^k - \hat{\mu}_i)^2}{N-1} = \frac{\sum_{k=1}^N (\Delta \phi_i^k - \hat{\mu}_i \Delta)^2}{(N-1)\Delta^2}, \quad (33)$$

as a measure of non-linearity and interaction, where we have denoted a realization of $\Delta \Phi_i$ by $\Delta \phi_i^k$, that is, for $k = 1, 2, \dots, N$,

$$\Delta \phi_i^k = g(x_i^k + \Delta : \mathbf{x}_{-i}^k) - g(\mathbf{x}^k). \quad (34)$$

One also has

$$\mathbb{V}[\hat{\mu}_i] = \frac{\hat{\sigma}_{EE_i}^2}{N} \quad i = 1, \dots, d. \quad (35)$$

Because the elementary effects EE_i are Newton quotients, we are effectively sampling approximations of partial derivatives at randomized locations in $\mathcal{X}$. This way of proceeding resembles the estimation of sensitivity measures in the Distributed Evaluation of Local Sensitivity Analysis (DELSA), in derivative-based methods and in radial design sampling (Campolongo et al., 2011; Rakovec et al., 2014; Sobol' & Kucherenko, 2009).

Since $\Delta \Phi_i$ are random variables, we consider the quantity

$$\Delta \bar{\tau}_i^2 = \frac{1}{2} \mathbb{E}[(\Delta \Phi_i)^2]. \quad (36)$$

This index is similar to the Jansen estimator of the total Sobol' index $\bar{\tau}_i^2$ in (20). However, the difference is that $\Delta \bar{\tau}_i^2$ is constructed from Morris main effects in (30) rather than local main effects. It is then possible to rewrite the variance of the Morris effects as

$$\sigma_{EE_i}^2 = 2 \frac{\Delta \bar{\tau}_i^2}{\Delta^2} - \mu_i^2. \quad (37)$$

Eq. (36) is associated with the empirical second order moment of $\Delta \phi_i^k$,

$$\Delta \hat{\tau}_i^2 = \frac{\sum_{k=1}^N (\Delta \phi_i^k)^2}{2N}. \quad (38)$$

The index $\Delta \hat{\tau}_i^2$ in (38) is still an average of main effects, but these main effects are computed across points whose coordinates differ by the fixed step Δ . In particular, the sample variance can be written as

$$\hat{\sigma}_{EE_i}^2 = \frac{N}{N-1} \frac{2\Delta \hat{\tau}_i^2}{\Delta^2} - \frac{N}{N-1} \hat{\mu}_i^2. \quad (39)$$

Notice that (39) coincides with the statistic proposed by Shi, Shang, & Zhigang (2016) for hypothesis testing in the controlled Morris method. However, the quantity $\Delta \hat{\tau}_i^2$ is not an estimate of the total Sobol' index $\bar{\tau}_i^2$, as the next result shows.

Proposition 9. Under the assumptions of Theorem 3, one finds

$$\sigma_{EE_i}^2 = \frac{2}{\Delta^2} (\bar{\tau}_i^2 - \text{Bias}(\bar{\tau}_i^2 - \Delta \bar{\tau}_i^2)) - \mu_i^2, \quad (40)$$

where

$$\begin{aligned} \text{Bias}(\bar{\tau}_i^2 - \Delta \bar{\tau}_i^2) &= \frac{1}{2} \mathbb{E}[(g(X_i^1 : \mathbf{X}_{-i}^0) - g(X_i^0 + \Delta : \mathbf{X}_{-i}^0)) \\ &\quad \cdot (g(X_i^1 : \mathbf{X}_{-i}^0) + g(X_i^0 + \Delta : \mathbf{X}_{-i}^0) - 2g(\mathbf{X}^0))]. \end{aligned} \quad (41)$$

² Campolongo et al. (2011) propose the absolute value of Morris elementary effects before averaging, to take into account potential annihilating effects in (29) when g is not monotonic (see also Becker & Saltelli, 2015). Because (32) is prevalent in the simulation arena (see Shi & Chen, 2019; Shi, Chen, & Shang, 2018), we will focus on this equation in the reminder.

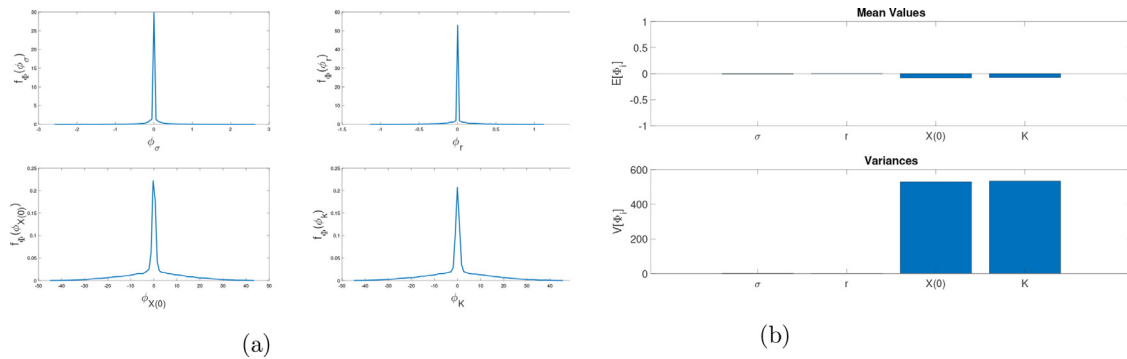


Fig. 3. Asian Option: Empirical densities of Φ obtained via the Matlab ksdensity.m subroutine (a) and corresponding empirical mean and variances (b).

Proposition 9 establishes the exact relationship between Sobol' total indices and Morris $\sigma_{EE_i}^2$. It formalizes the intuition of previous literature that considers Morris $\sigma_{EE_i}^2$ as a measure that captures interactions and nonlinear effects. In particular, it shows that Morris $\sigma_{EE_i}^2$ is a biased estimator of $\bar{\tau}_i^2$. However, Eq. (41) allows one to correct for such bias. Note that the quantity $\Delta \bar{\tau}_i^2$ plays a role both in the total Sobol' index (when debiased) and the Morris measure $\sigma_{EE_i}^2$.

Example 10 (Example 5 continued). Suppose that an analyst carried out a Morris method analysis for the same mapping and input distributions as in Example 5. Analytically, it is $\mu_i = 1$, $\sigma_{EE_i}^2 = 3$ and $\Delta \bar{\tau}_i^2 = 2 \cdot \Delta^2$. From (41), we find $\text{Bias}(\bar{\tau}_i^2 - \Delta \bar{\tau}_i^2) = 4 - 2 \cdot \Delta^2$ for all $i = 1, 2, 3$. Resolving (40) for $\bar{\tau}_i^2$, we get $\bar{\tau}_i^2 = (4 - \mu_i^2 + \mu_i^2) \frac{\Delta^2}{2} + 4 - 2 \cdot \Delta^2$, whence $\bar{\tau}_i^2 = 4$.

6. Asymptotic analysis and a conservative screening criterion

In estimation it is of practical interest to obtain measures of the error at finite sample sizes. Towards this end, in this section we present asymptotic results the quantities introduced in the previous sections.

In Theorem 3, we have seen that the random variables Φ_i have null mean and variance $2\bar{\tau}_i^2$. By the Central Limit Theorem and the

$$\Gamma_{S_i} = \frac{\mathbb{V}[g(\mathbf{X}^1) \cdot \Phi_i^{\mathbf{X}^0 \rightarrow \mathbf{X}^1}] + S_i^2(\mu_{(4)} - \sigma_Y^4) - 2S_i \mathbb{C}[g(\mathbf{X}^1) \cdot \Phi_i^{\mathbf{X}^0 \rightarrow \mathbf{X}^1}, (g(\mathbf{X}^0) - \mu)^2]}{\sigma_Y^4}, \quad (50)$$

$$\Gamma_{T_i} = \frac{\mu_{(4)} - 4\bar{\tau}_i^4 + 4T_i^2(\mu_{(4)} - \sigma_Y^4) - 4T_i \mathbb{C}[(\Phi_i^{\mathbf{X}^0 \rightarrow \mathbf{X}^1})^2, (g(\mathbf{X}^0) - \mu)^2]}{4\sigma_Y^4} \quad (51)$$

and

$$\Gamma_{D_g} = \frac{d\mu_{(4)} - 4 \sum_{i=1}^d \bar{\tau}_i^4 + 4D_g^2(\mu_{(4)} - \sigma_Y^4) - 4D_g \mathbb{C}[\sum_{i=1}^d (\Phi_i^{\mathbf{X}^0 \rightarrow \mathbf{X}^1})^2, (g(\mathbf{X}^0) - \mu)^2]}{4\sigma_Y^4}. \quad (52)$$

Law of Large Numbers, the average $\bar{\Phi}_i$ of N local main effects is asymptotically distributed with null mean and variance $2\bar{\tau}_i^2/N$. This result allows us to investigate the asymptotic behaviour of the estimators of the variance-based indices and of the mean dimension. We let

$$S_i = \frac{\bar{\tau}_i^2}{\sigma_Y^2}, \quad T_i = \frac{\bar{\tau}_i^2}{\sigma_Y^2} \quad \text{and} \quad I_i = \frac{\Lambda_i^2}{\sigma_Y^2} \quad (42)$$

denote the normalized individual, total and interaction indices respectively. Note that, by (25), $D_g = \sum_{i=1}^d (S_i + I_i)$.

Theorem 11. Assume that $\mathbb{E}[g(\mathbf{X})^4] = \mu_{(4)} < \infty$ and all inputs are independent. Then, for $N \rightarrow \infty$ we have

$$\sqrt{N}(\hat{\tau}_{i,N}^2 - \bar{\tau}_i^2) \rightarrow \mathcal{N}(0, \mathbb{V}[g(\mathbf{X}^0) \cdot \Phi_i^{\mathbf{X}^1 \rightarrow \mathbf{X}^0}]), \quad (43)$$

$$\sqrt{N}(\hat{\tau}_{i,N}^2 - \bar{\tau}_i^2) \rightarrow \mathcal{N}\left(0, \frac{\mu_{(4)} - 4\bar{\tau}_i^4}{4}\right) \quad (44)$$

and

$$\sqrt{N}\left(\sum_{i=1}^d \hat{\tau}_{i,N}^2 - \sum_u |u| \sigma_u^2\right) \rightarrow \mathcal{N}\left(0, \frac{d\mu_{(4)} - 4 \sum_{i=1}^d \bar{\tau}_i^4}{4}\right). \quad (45)$$

For the normalized indices we have:

$$\sqrt{N}(\hat{S}_{i,N} - S_i) \rightarrow \mathcal{N}(0, \Gamma_{S_i}), \quad (46)$$

$$\sqrt{N}(\hat{T}_{i,N} - T_i) \rightarrow \mathcal{N}(0, \Gamma_{T_i}) \quad (47)$$

and

$$\sqrt{N}(\hat{D}_N - D_g) \rightarrow \mathcal{N}(0, \Gamma_{D_g}), \quad (48)$$

where the estimates are given by

$$\hat{S}_{i,N} = \frac{\hat{\tau}_{i,N}^2}{\hat{\sigma}_Y^2}, \quad \hat{T}_{i,N} = \frac{\hat{\tau}_{i,N}^2}{\hat{\sigma}_Y^2} \quad \text{and} \quad \hat{D}_N = \frac{\sum_{i=1}^d \hat{\tau}_{i,N}^2}{\hat{\sigma}_Y^2} \quad (49)$$

and the asymptotic variances are

Theorem 11 suggests that main effect-based estimators of sensitivity indices are asymptotically normal, unbiased and their variance tends to zero as the sample size increases. The assumption of a finite fourth moment implies that the variance of estimators is well defined. In particular, Eqs. (43) and (44) yield confidence intervals for variance-based sensitivity indices.

Eqs. (46) and (47) illustrate the asymptotic distribution of the estimators of the normalized Sobol' indices in (49).

Before us, Janon, Klein, Lagnoux, Nodet, & Prieur (2014) and Gamboa, Janon, Klein, Lagnoux, & Prieur (2016) investigate the

asymptotic distribution of the variance-based indices S_u computed via the pick-and-freeze design. We employ a similar technique in our proof. The difference lies in the estimator, that allows us to extend the asymptotic analysis to the total indices and the mean dimension as well.

It can be also shown that for the population of EE_i 's we have:

$$\sqrt{N}(\hat{\mu}_i - \mu_i) \rightarrow \mathcal{N}\left(0, \frac{2}{\Delta^2} \cdot \Delta \bar{\tau}_i^2 - \mu_i^2\right) \quad (53)$$

for $N \rightarrow \infty$, where μ_i is the mean value of the elementary effect EE_i . This result suggests that, fixed Δ , Newton quotients are asymptotically normal with mean μ_i and variance $\frac{2}{\Delta^2} \cdot \Delta \bar{\tau}_i^2 - \mu_i^2$. This fact connects with earlier findings. [Zazanis & Suri \(1993\)](#) investigate the asymptotic convergence rate of Newton quotients; in particular, they show that, if Δ^* is chosen to be the optimal increment (i.e. the increment that minimizes the mean square error of the finite-difference estimator), then the corresponding estimator $\hat{\mu}_i^*$ converges at a rate of order $N^{-1/4}$, which is smaller than the Monte Carlo rate $O(N^{-1/2})$.

A special case in which we can find the exact analytical values of all EE_i and μ_i is that of a deterministic linear model (In Section 2 in the Supplementary Appendix, we provide further results connecting these findings to the case of linear models plus noise often used in metamodeling).

In practical applications, analysts resort to screening thresholds: a simulator input is judged irrelevant if the associated importance measure falls below a certain threshold (see [Sarrazin, Pianosi, & Wagener, 2016](#) among others). For instance, one can state that X_i is screened if $\bar{\tau}_i^2 < \mathcal{K} \cdot \sigma_Y^2$, where $\mathcal{K}$ is a given percentage of the total simulator output variance (e.g., $\mathcal{K} = 0.01$ or 0.05). The results of the asymptotic analysis can be employed to introduce a slight modification that takes into account uncertainty in the estimates. Let $0 \leq \alpha \leq 1$ and let $z_{(1-\alpha)/2}$ denote the α -quantile of the standard normal distribution. From [Eq. \(44\)](#), we can write

$$\bar{\tau}_i^2 \leq \hat{\tau}_{i,N}^2 + z_{(1-\alpha)/2} \sqrt{\frac{\hat{\mu}_{(4)} - 4\hat{\tau}_{i,N}^4}{4N}}. \quad (54)$$

This equation suggests that $\bar{\tau}_i^2$ is smaller than the current estimate plus a positive quantity that decreases as N increases. Therefore, at $N > N_0$, if we register that the quantity $\hat{\tau}_{i,N}^2 +$

$z_{(1-\alpha)/2} \sqrt{\frac{\hat{\mu}_{(4)} - 4\hat{\tau}_{i,N}^4}{4N}}$ is smaller than $\mathcal{K} \cdot \sigma_Y^2$, we are reassured that also $\bar{\tau}_i^2 < \mathcal{K} \cdot \sigma_Y^2$. That is, we are reassured that X_i is not relevant with $\alpha\%$ confidence (see [Section 7.2](#) for an application).

7. Case studies

In this section, we report results on numerical experiments performed on the Asian simulator [Nelson \(2013\)](#) and on the NASA probabilistic risk assessment [Borgonovo & Smith \(2011\)](#) case studies.

7.1. Asian option value

Asian options are among the most popular and studied path-dependent financial options ([Wang & Sloan, 2011](#)). The payoff of an Asian option depends on the average price of the underlying asset over a time period. [Nelson \(2013\)](#) considers the simulation of the value of an Asian option

$$v = \mathbb{E}[e^{-rT}(\bar{X}(T) - K)^+], \quad (55)$$

where $T = 1$ is the maturity, r is the risk-free interest rate and K is the strike price. The underlying asset has initial value $X(0)$ and volatility σ^2 . The quantity $\bar{X}(T) = \int_0^T X(t)dt$ is the time-average of

the Brownian motion. We regard σ , r , $X(0)$, and K as simulation inputs. Notice that these inputs have different characteristics and their values can be assigned with alternative methods: K is user-defined, $X(0)$ is known at the moment the contract starts, but uncertain before, σ and r are statistically estimated or calibrated to market data. As in [Nelson \(2013\)](#), we set the base-case scenario of the simulation at $(\sigma, r, X(0), K) = (0.3, 0.05, 50, 55)$. In order to demonstrate the design, we consider a variation range for each input with low and high extremes equal, respectively, to 5% and 195% of the base-case value. For every input combination, we use 10,000 replicates of the option pricing model and average to find the estimated expected value $\hat{v}$.

As a screening design, we opt for the mirror scheme, with 10,000 forward and 10,000 backward replications, for a total of about 80,000 evaluations of $\hat{v}$. The analysis requires 2 hours and 45 minutes on a personal computer with 64 GB RAM, and processor Intel(R) Core(TM) i7-7700HQ, 2.80 GHz. The subroutines are developed in MATLAB. [Fig. 3a](#) reports the empirical distributions of the local main effects of the four simulator inputs. The realizations of $\Phi_{X(0)}$ and Φ_K display greater variability around the mean value (zero) than the realizations of Φ_σ and Φ_r . This is confirmed by the barplots in [Fig. 3b](#), that report the corresponding local main effects mean values and variances. The variance of $\Phi_{X(0)}$ and Φ_K are much larger than the corresponding variances of Φ_σ and Φ_r , that are close to zero.

Regarding global sensitivity measures, [Fig. 4a](#) reports the point estimates and corresponding confidence intervals of the total indices T_i as N increases, following [Eqs. \(47\)–\(49\)](#). Across all N , the point estimates $\hat{T}_K$ and $\hat{T}_{X(0)}$ are greater than the point estimates of $\hat{T}_\sigma$ and $\hat{T}_r$. However, the confidence intervals allow one to clearly separate their importance after $N > 400$. As N increases, the confidence intervals shrink towards the point estimates. At $N = 10,000$, we find $\hat{T}_{X(0)} = 0.6025$ with 95% confidence interval given by $[0.5646, 0.6404]$. At this sample size, the empirical normalized variance-covariance matrix of the local main effects in [\(18\)](#):

$$\frac{\widehat{\mathbb{C}}(\Phi)}{\hat{\sigma}_Y^2} = \begin{pmatrix} 0.0043 & 0.0002 & 0.0014 & 0.0020 \\ 0.0002 & 0.0008 & 0.0005 & 0.0000 \\ 0.0014 & 0.0005 & 1.2048 & 0.2043 \\ 0.0020 & 0.0000 & 0.2043 & 1.2122 \end{pmatrix}.$$

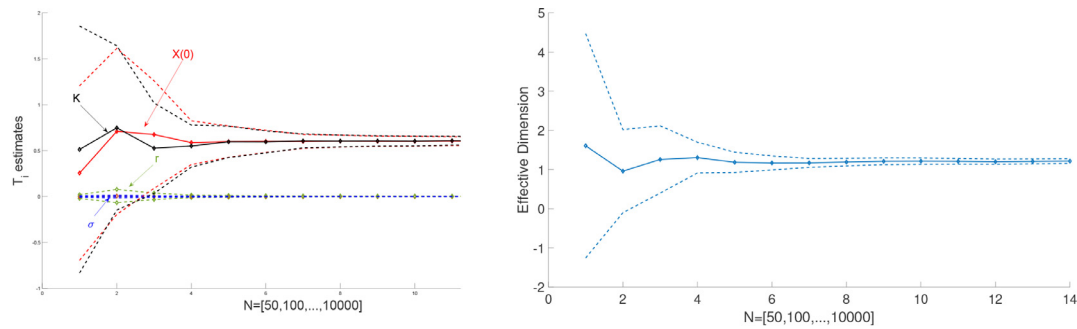
The matrix shows that $X(0)$ and K owe their influence not only to their individual contribution but also to their strong interaction, as can be seen from the off-diagonal entries.

We then perform experiments considering the elementary effects for the Asian Option simulator ([Fig. 5](#)).

[Fig. 5](#) a reports the estimates based on the variance-covariance matrix and the debiased finite-changes estimator with constant step $\Delta = 0.1$ as N increases up to $N = 100$. Panel a) shows that the two estimators are very close even at small sample sizes. Conversely, taking into account the Morris $\sigma_{EE_i}^2$ measure might lead to very different insights. To illustrate, consider the barchart in [Fig. 5b](#), that compares the Morris $\hat{\sigma}_{EE_i}$ measures at $N = 100$ to the estimates of the Sobol' total indices. An analyst would attribute to input r a relevance greater than what, in fact, it has.

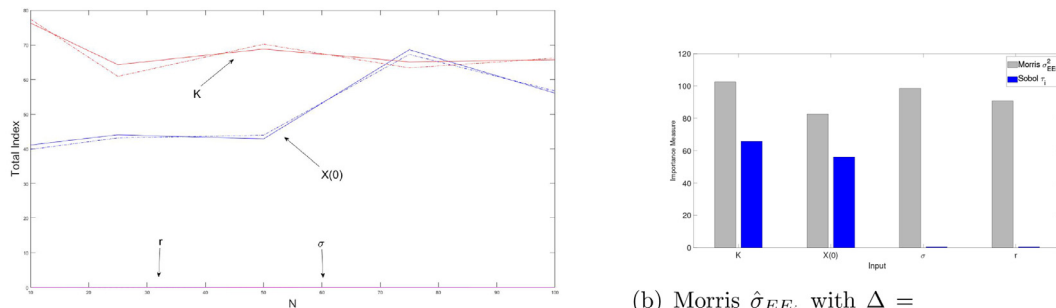
Regarding interactions, the design also allows one to estimate the mean dimension of the simulator. [Fig. 4b](#) shows $\hat{D}_g$ in [\(49\)](#) as N increases. Starting at about $N \simeq 2000$ the mean dimension is at about $\hat{D}_g = 1.25$, with 95% confidence interval $[1.06, 1.44]$. At $N = 10,000$, we obtain $\hat{D}_g = 1.22$, with 95% confidence interval $[1.16, 1.28]$. This result is consistent with the results in $\widehat{\mathbb{C}}(\Phi)$, and indicates that, on average, interactions of order greater than 2 are not expected to play a major role.

Taking a local viewpoint, [Fig. 6a](#) displays the Generalized Tornado Diagram for this case study. This plot shows the local main



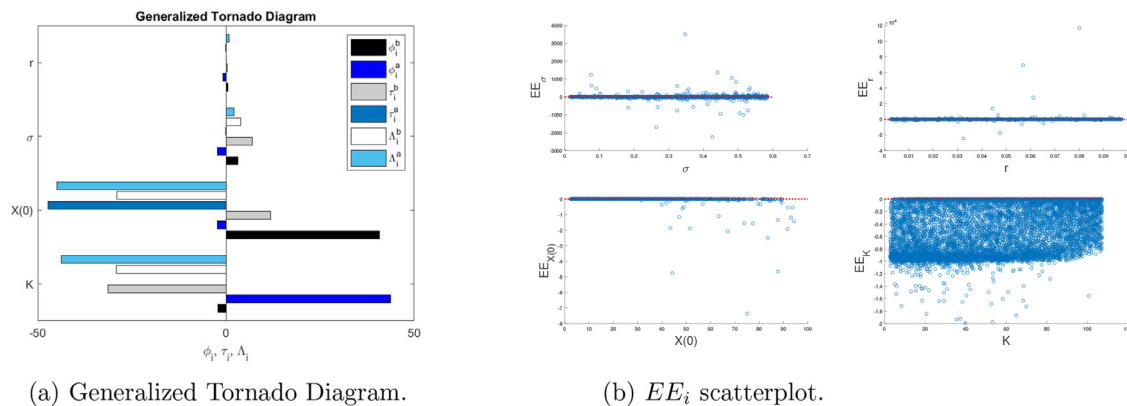
(a) $\hat{T}_i$ (continuous lines) and corresponding 95% (b) $\hat{D}_g$ and corresponding 95% confidence interval.

Fig. 4. Asian Option: Estimates of Sobol' indices and D_g with corresponding 95% confidence intervals as N increases.



(a) Comparison between the variance-covariance estimators of the total effects τ_i^2 (dotted lines) and the Morris-debiased ones $\Delta \tau_i^2 + \text{Bias}(\tau_i^2 - \Delta \tau_i^2)$ (continue lines), for $i = 1, \dots, 4$.

Fig. 5. Sobol' total indices and comparison with Morris $\hat{\sigma}_{EE_i}$ for the Asian Option simulator.



(a) Generalized Tornado Diagram.

(b) EE_i scatterplot.

Fig. 6. Asian Option: Generalized Tornado Diagram (a) and scatterplot of individual effects providing indications on sign of direction of change (b). In the Generalized Tornado Diagram the points we consider are the base-case scenario (0.3, 0.05, 50, 55), a stressed scenario $a = (0.015, 0.0025, 2.5, 2.75)$ at the 5% of the base-case value and a stressed scenario $b = (0.585, 0.0975, 97.5, 107.25)$ at the 195% of the base-case value.

ϕ_i , interaction Λ_i and total effects τ_i when shifting the inputs from the base-case values to their 5% and 195% lower and upper values respectively. The inputs r and σ are associated with very low importance indices, while the model variations are mostly driven by $X(0)$ and K , in agreement with results on a global scale. Consider the finite change from the base-case to the 5% input values: we register an almost null total effect for K , because $\phi_K + \Lambda_K \approx 0$. This null local importance of K is not in contrast with the results of the global analysis, because the global total indices are based on the squared averages of local main effects. Similarly, for $X(0)$ we register a relevant local total effect $\tau_{X(0)}$ but a very small local main effect. This input is also important globally: in Remark 4 we have

seen that the estimator of the global total index can be obtained also by averaging squared local total effects. Concerning the local interaction analysis, K and $X(0)$, the inputs with strongest local effects, show negligible interactions with the other two inputs.

Finally, regarding direction of change, the scatterplots of Morris elementary effects (i.e., Newton quotients) in Fig. 6b show that their sign is consistently negative for $X(0)$ and K , while they are both positive and negative for σ and r . Note that the most appropriate setting for the use of Newton quotients (elementary effects EE_i) is direction of change rather than prioritization. In fact, if one were to calculate Morris $\hat{\sigma}_{EE_i}^2$ directly from the realizations of the Newton quotients in Fig. 6b, one would rank σ and r higher than

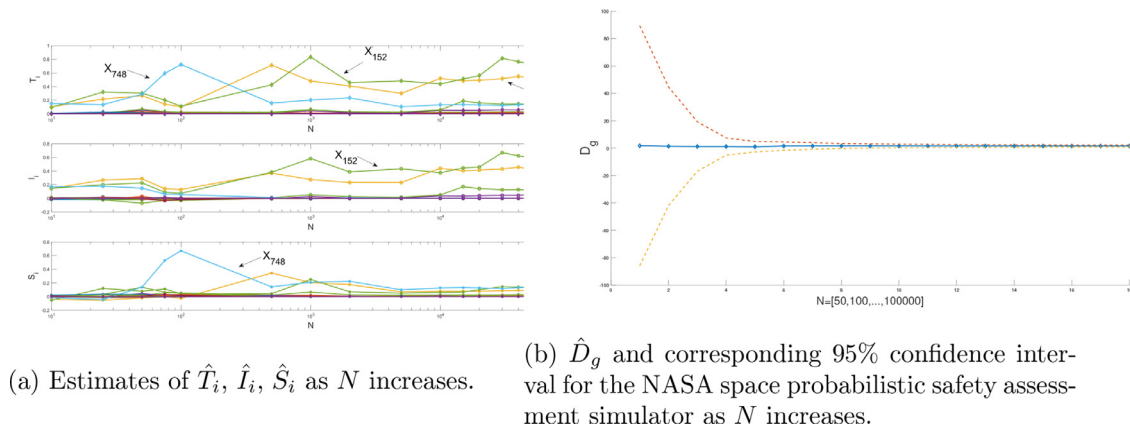


Fig. 7. NASA space probabilistic safety assessment simulator: Estimates of variance-based sensitivity indices and dimension distribution as N increases.

Table 2

Relevant inputs identified at a level $\kappa = 0.005$, for $N = 10, 25, 100$. Note that already at $N = 10$ one screens 855 inputs. At $N = 100,000$ the relevant inputs reduce to seven.

N	Index of identified inputs
10	66, 143, 145, 152, 174, 176, 177, 179, 180, 205, 361, 362, 748, 785, 786, 791, 794
25	66, 143, 145, 152, 174, 177, 179, 180, 205, 361, 362, 748, 785, 786, 791
100	143, 145, 152, 177, 179, 180, 361, 362, 748, 786
100,000	143, 145, 152, 177, 179, 362, 748

$X(0)$ and K . However, the Newton quotients of r and K have different units and, consequently, $\hat{\sigma}_{EE_K}^2$ and $\hat{\sigma}_{EE_r}^2$ cannot be compared. In order to compare them, one would have to recompute Morris $\hat{\sigma}_{EE_i}^2$ after standardizing all the inputs on the $[0,1]$ a-dimensional scale. This step is not necessary if one uses the empirical variance of local main effects.

7.2. Probabilistic safety assessment simulator for NASA space missions

In this section, we discuss the application of our framework to the probabilistic safety assessment simulator used in [Borgonovo & Smith \(2011\)](#). The simulator, developed to support the design and planning of a NASA lunar space mission, is aimed at providing insights to risk managers towards ensuring the highest levels of performance and safety. The model simulates eight phases from launch to final Earth landing. The output is the probability of loss of mission, modeled as a function of 872 inputs, which for privacy reasons are labeled by $X_1, X_2, \dots, X_{872}$. In previous literature, the simulator is analyzed with a generalized Tornado approach. The inputs are assigned ranges taking as extremes the fifth and ninety-fifth quantiles of the assigned lognormal distributions. The simulator is run with the inputs varying one-at-a-time at the two extremes of the input hypercube using Cotter's the fold-over design. In the notation of the present work, one obtains one local main effect $\phi_i^{0 \rightarrow 1}$, one local total order interaction effect $\Lambda_i^{0 \rightarrow 1}$ and one local total effect $\tau_i^{0 \rightarrow 1}$ for each input. Based on the theory developed in the previous sections, we perform a randomized evaluation of the sensitivities under the fold-over design (We thank C.L. Smith for making the code available). This allows us to have a comparison of results obtained with a sensitivity carried out at the extremes of the input space vs an approach that evaluates the simulator across the entire space.

We use increasing sample sizes up to $N = 100,000$ randomized pairs. The points are sampled using crude Monte Carlo from the same distributions assigned in [Borgonovo & Smith \(2011\)](#). At the end of the simulations, a sample of 200,000 local main effects ϕ_i is available for each input. The computation takes 2.5 hours on the

above-mentioned calculator, with a parallel calculus provision and 4 cores.

[Fig. 7](#) reports the estimates of the total (T_i), interaction (I_i) and individual (S_i) indices defined in (42) as the sample size increases from $N = 100$ to $N = 100,000$. For T_i and I_i we record stable estimates at $N \geq 4 \times 10^4$ (we do not display confidence intervals for the sake of space).

The most important inputs are X_{152} and X_{143} , whose total order index is five times greater than the total order index of X_{748} the third most important input. These inputs are also the three most important inputs according to S_i . From the second and third graphs in [Fig. 7a](#), one observes that X_{152} and X_{143} are involved in significant interactions, while X_{748} is not. We note that [Borgonovo & Smith \(2011\)](#), where the analysis is limited to the exploration of the two extreme scenarios, inputs X_{152} , X_{143} and X_{374} are identified as the most important. Thus, input X_{374} is important for the finite change across the two extreme scenarios, but not when the input space is explored more thoroughly.

[Fig. 7b](#) displays the point estimates and confidence interval of the mean dimension as the sample size increases; the estimated mean dimension converges towards the value $\hat{D}_g = 1.63$, with a 95% confidence interval $D_g \in [0.971, 2.295]$. This result shows that, on average interactions are dominated by low order groups, with interactions of higher orders expected to have a negligible role. For a simulator with 872 inputs, this result indicates a low impact of interactions.

Regarding trend, all realizations of Morris elementary effects are non-negative. This result confirms the monotonically increasing dependence of the probability of loss of mission on the simulator inputs due to the fact that the underlying system is coherent (for further details on the system, see [Borgonovo & Smith \(2011\)](#)). Regarding the sign of interactions, results show (we do not display the graphs for space reasons) that the indices $\Lambda_i^{0 \rightarrow 1}$ are both be positive and negative. Thus, overall interactions can be antagonistic or synergistic.

The discussion carried out thus far has concerned asymptotic results and we have allowed the number of replicates to grow up to tens of thousands of runs. We now consider the same case study

but we suppose that there is a budget limitation up to $N = 100$. We then employ the conservative screening criterion of Section 6, deeming a simulator input irrelevant if the upper bound of the corresponding total index is smaller than 5 per thousand of the overall simulator output variance (In the notation of Section 6, $\frac{\bar{\tau}_i^2}{\sigma_Y^2} < \mathcal{K}$, with $\mathcal{K} = 0.005$.) Table 2 reports the simulator inputs deemed as relevant for $N = 10, 25, 100$. At $N = 10$ randomized evaluations, a total of 855 inputs are screened out, because their 95% – $\hat{\tau}_i$ -upper bound is below the threshold, while at $N = 100$ we are left with ten relevant simulator inputs; (this is a consequence of the fact that the confidence intervals become less wide). The groups always include the inputs deemed most important at $N = 100, 000$.

8. Discussion and conclusions

A rich body of literature has proposed the randomized evaluation of one-at-a-time sensitivities as a bridge between local and global methods. Previous works on derivative-based sensitivity measures and on the Morris method have hinted at possible links between screening sensitivity measures and Sobol' total indices. This work has derived the exact relationship between Sobol' total indices and Morris $\hat{\sigma}_{EE}^2$. The specific form of the link evidences that the way in which one-at-a-time sensitivities are randomized matters. If, as in the original Morris design, one randomly samples points in the input space and then considers radial and equally spaced (constant Δ) input variations, then one estimates Morris sensitivity measures. Conversely, the local main effects in Jansen's estimators involve one-at-a-time sensitivities in which the extremes are randomly sampled. Moreover, the covariance of these main effects yields Liu and Owen's $\Upsilon_{i,j}^2$ interaction indices. We have a connection between the local and global scales, in which global total indices are the average of local total indices, so that what is important at a local scale is also important at a global scale.

Moreover, we have exploited the randomization of main effects in a forward and backward trajectory (a fold-over design). We have seen that this strategy, while leading to the same number of local main effects, also yields local interaction effects, which are invariant with respect to the direction of the pass (forward or backward). This new measure of interaction is also directly connected to global measures of interaction previously defined in Design of Experiments. We have then defined the global analog of this local interaction measure and compared it to Liu and Owen's superset importance measure. The numerical experiments show that application of this design allows the analyst to infer insights regarding direction of change, and the overall relevance of interactions, as well as input importance.

The proposed approach is also open to refinements that we have not had the possibility to address here due to space constraints, such as the optimal selection of locations or the application of a sequential sampling with optimal stopping.

At the same time, several of our results rely on the independence assumption. The approach is valid within a screening exercise, in an exploratory modelling phase. However, the independence assumption would interfere with a subsequent uncertainty quantification, if further data collection would reveal input dependencies. The extend to which the conclusions of preliminary experiments are impacted by input dependencies needs to be investigated with further numerical experiments. Preliminarily, we can say that local results are formally not impacted, but the links from local to global results are. In fact, the definition itself of the mean dimension as well as the interpretation of total indices as providing information about the relevance of interactions rely on the independence assumption. Their interpretation/calculation for dependent

inputs is a topical research subject, and part of future research by the authors as well.

Supplementary material

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.ejor.2022.05.002

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