# Making best use of permutations to compute sensitivity indices with replicated designs

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**Abstract**

In the field of sensitivity analysis, Sobol' indices are widely used to assess the importance of inputs of a model to its output. Among the methods that estimate these indices, the replication procedure is noteworthy for its efficient cost. However, gaining in efficiency and assessing the estimate precision still remains an issue, all the more important when one is dealing with limited computational budget. In this paper, we propose a new strategy to estimate the full set of first-order and second-order Sobol' indices with only two replicated designs based on orthogonal arrays of strength two. Such a procedure increases the precision of the estimation for a given computation budget. We also propose a bootstrap procedure for producing confidence intervals, that are compared to asymptotic ones in the case of first-order indices. Numerical simulations and applications to benchmarks assess the interest of our contributions.

*Keywords:* Bootstrap confidence intervals, Computer experiments, Replicated designs, Sensitivity Analysis, Sobol' indices

## 1. Introduction

Many mathematical models encountered in applied sciences involve a large number of poorly-known parameters as inputs. It is important for the practitioner to assess the impact of this uncertainty on the model output. This assessment can be performed via sensitivity analysis, which aims to identify the most sensitive parameters, that is, parameters having the largest influence on the output. In global stochastic sensitivity analysis (see for example [1] and references therein) the input variables are assumed to be independent random variables. Their probability distributions account for the practitioner's belief about the input uncertainty. This turns the model output into a random variable, whose total variance can be split down into different partial variances (this is the so-called Hoeffding decomposition, see [2, 3]). Each of these partial variances measures the uncertainty of the output induced by each input variable uncertainty. By considering the ratio of each partial variance to the total variance, we obtain a measure of importance for each input variable that is called the (first-order) *Sobol' index* or *sensitivity index* of the variable [3]; the most sensitive parameters can then be identified and ranked as the parameters with the largest Sobol' indices. Considering the uncertainty caused by the interaction in couples of input parameters (respectively, by an input parameter and its interaction with all other input parameters) similarly yields the so-called second-order (respectively, total) Sobol' indices.

Once the Sobol' indices have been defined, the question of their effective computation or estimation remains open. In practice, one has to estimate (in a statistical sense) those indices using a finite sample (of size typically in the order of hundreds of thousands) of evaluations of model outputs. Indeed, many Monte Carlo or quasi Monte Carlo approaches have been developed by the experimental sciences and engineering communities. This includes the Sobol' pick-freeze (SPF) scheme (see [3, 4]). In SPF a Sobol' index is viewed as the regression coefficient between the output of the model and its pick-freezed copy.

This copy is obtained by holding the value of the variable of interest (frozen variable) and by sampling the other variables (picked variables). Then, the regression coefficient can be empirically estimated. A basic SPF scheme has been studied in [5, 6], where the different input parameter values are sampled independently; this scheme can be used to estimate any (first-order, second-order, total) Sobol' index.

The main drawback of this basic scheme is that it requires a number of model evaluations which is proportional to the number of input parameters. In typical engineering applications, the number of input parameters can be very large, and, most importantly, the computation time required for a single model evaluation can also drastically restrict the total number of model outputs available.

This motivates the use of *replicated* designs, which can be used to estimate all first-order indices with a number of model evaluations which is *independent* of the number of input parameters. Replicated Latin Hypercube designs have first been introduced in [7]. The paper [8] uses such replicated Latin Hypercube designs to estimated first-order Sobol' indices, extending results in [9]. It also extends the replication procedure to the estimation of second-order Sobol' indices.

Apart from the required number of model evaluations, another problem arising in sensitivity indices estimation is the assessment of the precision of the reported numerical results, usually by giving confidence intervals. To do this, one can use empirical bootstrap confidence intervals [10], or use, when available, asymptotic confidence intervals derived from a theoretical analysis as done, for the first-order Sobol' indices with replicated Latin Hypercubes designs, in Proposition 3.2 of [8].

The goal of this paper is twofold: first, to improve the procedure in [8] so as to increase the accuracy of the estimation of first- and second-order Sobol' indices for a given computation budget, and, second, to propose a bootstrap procedure for producing confidence intervals.

The paper is organized as follows: in Section 2, definitions of the Sobol' indices and their pick-freeze estimators are recalled. Section 3 is devoted to the replication procedure. First, the classical version is presented, then a new version to estimate the full set of first-order and second-order Sobol' indices is proposed. This new approach makes use of only two replicated designs based on orthogonal arrays of strength two. Numerical illustrations of the new approach are provided in Section 4 along with a comparison to Saltelli's approach [11]; and a discussion on how to combine both of them in order to estimate the full set of first-, second-order and total Sobol' indices at a very competitive cost and with an improved accuracy. In addition, bootstrap confidence intervals resulting from the new approach are compared to the asymptotic intervals derived in [8] for the first-order Sobol' indices.

## 2. Background on Sobol' indices

### *2.1. Definition of Sobol' indices*

Denote by $\boldsymbol{x} = (x_1, \dots, x_d)$ the vector of inputs of a model $f$. We assume that $f$ is in some subset of $\mathbb{L}^2([0,1]^d)$ for which $f(\boldsymbol{x})$ is defined for all $\boldsymbol{x} \in [0,1]^d$, and $\mathcal{D} = \{1, \dots, d\}$ the set of dimension indices. Let $u$ be a subset of $\mathcal{D}$, $-u$ its complement and $|u|$ its cardinality. Then, $\boldsymbol{x}_u$ represents a point in $[0,1]^{|u|}$ with components $x_j, j \in u$. Given two points $\boldsymbol{x}$ and $\boldsymbol{x}'$, the hybrid point $\boldsymbol{w} = (\boldsymbol{x}_u : \boldsymbol{x}'_{-u})$ is defined as $w_j = x_j$ if $j \in u$ and $w_j = x'_j$ if $j \notin u$.

The uncertainty on $\boldsymbol{x}$ is modeled by a uniform random vector, namely $\boldsymbol{x} \sim \mathcal{U}([0,1]^d)$. The Hoeffding decomposition [2, 3, 12] of $f$ is:

$$f(\boldsymbol{x}) = f_{\varnothing} + \sum_{u \subseteq \mathcal{D}, u \neq \varnothing} f_u(\boldsymbol{x}), \tag{1}$$

where:

$$\begin{aligned} f_{\varnothing} &= \mathbb{E}[f(\boldsymbol{x})] = \mu, \\ f_u(\boldsymbol{x}) &= \int_{[0,1]^{|u|}} f(\boldsymbol{x}) d\boldsymbol{x}_{-u} - \sum_{v \subsetneq u} f_v(\boldsymbol{x}). \end{aligned}$$

Due to orthogonality, the variance of equation (1) leads to the variance decomposition of $f$:

$$\sigma^2 = \mathrm{Var}[f(\boldsymbol{x})] = \sum_{u \subseteq \mathcal{D}, u \neq \varnothing} \sigma_u^2,$$

$$\sigma_u^2 = \int_{[0,1]^{|u|}} f_u(\boldsymbol{x})^2 d\boldsymbol{x}_u.$$

From this decomposition, one can define the following two quantities:

$$\underline{\tau}_u^2 = \sum_{v \subseteq u} \sigma_v^2, \qquad \overline{\tau}_u^2 = \sum_{v \cap u \neq \varnothing} \sigma_v^2, \qquad u \subseteq \mathcal{D}.$$

These two quantities $\underline{\tau}_u^2$ and $\overline{\tau}_u^2$ measure the importance of variables $\boldsymbol{x}_u$: $\underline{\tau}_u^2$ quantifies the main effect of $\boldsymbol{x}_u$, that is the effect of all interactions between variables in $\boldsymbol{x}_u$, and $\overline{\tau}_u^2$ quantifies the main effect of $\boldsymbol{x}_u$ plus the effect of all interactions between variables in $\boldsymbol{x}_u$ and variables in $\boldsymbol{x}_{-u}$.

Both $\underline{\tau}_u^2$ and $\overline{\tau}_u^2$ satisfy the relation $0 \leqslant \underline{\tau}_u^2 \leqslant \overline{\tau}_u^2$. These two measures are commonly found in the literature in their normalized form: $\underline{S}_u = \underline{\tau}_u^2/\sigma^2$ is the closed $|u|$-order Sobol' index for inputs $u$, while $\overline{S}_u = \overline{\tau}_u^2/\sigma^2$ is the total effect Sobol' index of order $|u|$. In this paper, we focus on first-order and total effect Sobol' indices, corresponding to $|u| = 1$, $S_j = \underline{S}_{\{j\}}$ and $\overline{S}_{\{j\}}$, $j \in \mathcal{D}$, as well as on second-order Sobol' indices $S_{k,l} = \underline{S}_{\{k,l\}} - \underline{S}_{\{k\}} - \underline{S}_{\{l\}}$, $\{k,l\} \in \mathcal{D}^2; k \neq l$.

The computation of the normalized indices is performed based on the following integral formulas for their numerators:

$$\underline{\tau}_u^2 = \int_{[0,1]^{2d}} f(\boldsymbol{x}_u : \boldsymbol{x}'_{-u}) f(\boldsymbol{x}) d\boldsymbol{x} d\boldsymbol{x}' - \mu^2, \tag{2}$$

while variance and mean of $f$ are evaluated as:

$$\begin{aligned} \sigma^2 &= \int_{[0,1]^d} f(\boldsymbol{x})^2 d\boldsymbol{x} - \mu^2, \\ \mu &= \int_{[0,1]^d} f(\boldsymbol{x}) d\boldsymbol{x}. \end{aligned} \tag{3}$$

According to the law of total variance, the numerators of total effect Sobol' indices can be written as:

$$\overline{\tau}_{\{j\}}^2 = \sigma^2 - \underline{\tau}_{-\{j\}}^2. \tag{4}$$

Usually the complexity of $f$ causes the solution of integrals (2), (4) and (3) to be intractable. In such cases, one can instead estimate these quantities.

*2.2. Estimation of Sobol' indices*

In this section, starting from equation (2), we consider the following Monte Carlo procedure first introduced in [13] and then deeply studied in [5]. A design is a point set $\mathcal{P} = \{\boldsymbol{x}_i\}_{i=1}^n$ where each point is obtained by sampling each variable $x_j$ $n$ times. Each row of the design is a point $\boldsymbol{x}_i$ in $[0,1]^d$ and each column of the design refers to samples of a variable $x_j$. Consider $\mathcal{P} = \{\boldsymbol{x}_i\}_{i=1}^n$ and $\mathcal{P}' = \{\boldsymbol{x}'_i\}_{i=1}^n$ two designs where $(\boldsymbol{x}_i, \boldsymbol{x}'_i) \overset{\text{iid}}{\sim} \mathcal{U}([0,1]^{2d})$. One way to estimate the quantity in (2) and thus (4) is via:

$$\widehat{\underline{\tau}}_u^2 = \frac{1}{n}\sum_{i=1}^n f(\boldsymbol{x}_i) f(\boldsymbol{x}_{i,u} : \boldsymbol{x}'_{i,-u}) - \widehat{\mu}^2, \tag{5}$$

using for $\sigma^2$:

$$\widehat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^n \frac{f^2(\boldsymbol{x}_i) + f^2(\boldsymbol{x}_{i,u} : \boldsymbol{x}'_{i,-u})}{2} - \widehat{\mu}^2\,, \tag{6}$$

with $\widehat{\mu} = \dfrac{1}{n}\displaystyle\sum_{i=1}^n \frac{f(\boldsymbol{x}_i) + f(\boldsymbol{x}_{i,u} : \boldsymbol{x}'_{i,-u})}{2}$.

The Sobol' indices estimators are then:

$$\widehat{\underline{S}}_u = \widehat{\underline{\tau}}_u^2 / \widehat{\sigma}^2\,,\ u \subset \mathcal{D}\,,\ |u| = 1, 2\,, \tag{7}$$

and

$$\widehat{\overline{S}}_{\{j\}} = 1 - \frac{\frac{1}{n}\sum_{i=1}^n f(\boldsymbol{x}'_i) f(\boldsymbol{x}_{i,\{j\}} : \boldsymbol{x}'_{i,-\{j\}}) - \widehat{\mu}^2}{\widehat{\sigma}^2}\,. \tag{8}$$

Based on equations (5), (6), (7) and (8), we see easily that it is possible to compute the full set of first-order sensitivity indices as well as the full set of total-order sensitivity indices (a fairly common strategy in sensitivity analysis) with $d+2$ designs, namely with the designs $\{\boldsymbol{x}_{i,u} : \boldsymbol{x}'_{i,-u}\}_{i=1}^n$ constructed for $u \in \{\varnothing, \{1\}, \ldots, \{d\}, \mathcal{D}\}$. Tricky combinatorial arguments proposed in [11] lead to a cheaper strategy (called SAL02 variant B strategy in the following), which allows double estimates of the full set of first-order indices $S_j$, $j \in \mathcal{D}$ and total-order indices $\overline{S}_{\{j\}}$, $j \in \mathcal{D}$ as far as double estimates of the full set of closed second-order indices $\underline{S}_{\{k,l\}}$, $\{k,l\} \in \mathcal{D}^2$, $k \neq l$ with $2d+2$ designs (i.e. $n(2d+2)$

model evaluations). Later in Section 4.2, we introduce the cheaper strategy (called SAL02 variant A), which allows a simple estimate of all first-order and total Sobol' indices at a cost $n(d+2)$. Variant A does not provide second-order indices. In the following, we denote by SAL02 variant B of SAL02.

While ingenious, this last approach requires a number of model evaluations that grows linearly with respect to the input space dimension, which may be unaffordable for some real applications with limited budget. A reasonable solution to this issue lies in the use of the replication procedure, which allows the estimation of the full set of first- and second-order indices, at a cost independent from the input space dimension. The replication procedure is detailed in the next section.

## 3. Replication procedure

### 3.1. The usual strategy

The replication procedure has been introduced in [9] with the aim of evaluating all first-order indices at a reduced cost, namely $2n$ model evaluations. This procedure relies on the construction of two replicated designs. The notion of replicated designs was first introduced in [7] through the notion of replicated Latin Hypercubes. To extend this definition to other types of point sets, one may use the generalization from [14]:

**Definition 1.** *Let $\mathcal{P} = \{\boldsymbol{x}_i\}_{i=1}^n$ and $\mathcal{P}' = \{\boldsymbol{x}'_i\}_{i=1}^n$ be two point sets in $[0,1]^d$. Let $\mathcal{P}^u = \{\boldsymbol{x}_{i,u}\}_{i=1}^n$ (resp. $\mathcal{P}'^u$), $u \subsetneq \mathcal{D}$, denote the subset of dimensions of $\mathcal{P}$ (resp. $\mathcal{P}'$) indexed by $u$. $\mathcal{P}$ and $\mathcal{P}'$ are said to be two replicated designs of order $a \in \{1,\dots,d-1\}$ if for any $u \subsetneq \mathcal{D}$ such that $|u| = a$, $\mathcal{P}^u$ and $\mathcal{P}'^u$ are the same point set in $[0,1]^a$. We define by $\pi_u$ a permutation that rearranges the rows of $\mathcal{P}'^u$ into $\mathcal{P}^u$.*

The procedure introduced in [9] allows to estimate the full set of first-order Sobol' indices with only two replicated designs of order 1. This procedure has been deeply studied and generalized in Tissot and Prieur [8] to the estimation of the full set of closed second-order indices.

Let $\mathcal{P} = \{\boldsymbol{x}_i\}_{i=1}^n$ and $\mathcal{P}' = \{\boldsymbol{x}'_i\}_{i=1}^n$ be two replicated designs of order $|u|$. The key point of the procedure is to use the permutation $\pi_u$ resulting from Definition 1 to mimic the hybrid design $\{\boldsymbol{x}_{i,u} : \boldsymbol{x}'_{i,-u}\}_{i=1}^n$ used in equation (5). Denote by $\{y_i\}_{i=1}^n = \{f(\boldsymbol{x}_i)\}_{i=1}^n$ and $\{y'_i\}_{i=1}^n = \{f(\boldsymbol{x}'_i)\}_{i=1}^n$ the two sets of model evaluations obtained with $\mathcal{P}$ and $\mathcal{P}'$. From Definition 1, we know that $\boldsymbol{x}'_{\pi_u(i),u} = \boldsymbol{x}_{i,u}$. Then,

$$\begin{aligned} y'_{\pi_u(i)} &= f(\boldsymbol{x}'_{\pi_u(i),u} : \boldsymbol{x}'_{\pi_u(i),-u}) \\ &= f(\boldsymbol{x}_{i,u} : \boldsymbol{x}'_{\pi_u(i),-u}). \end{aligned}$$

Hence, each $\underline{\tau}_u^2$ can be estimated via formula (5) by using $y'_{\pi_u(i)}$ instead of $f(\boldsymbol{x}_{i,u} : \boldsymbol{x}'_{i,-u})$ without requiring further model evaluations for each $u$.

*Estimation of first-order indices.* Let us first consider the case when $|u| = 1$. As noted hereinbefore, the full set of first-order Sobol' indices can be estimated from two replicated designs of ordre 1, e.g. two replicated Latin hypercubes of size $n$.

*Estimation of second-order indices.* We now consider the case $|u| = 2$. The full set of closed second-order Sobol' indices can be estimated from two replicated designs of order 2, e.g. designs based on orthogonal arrays of strength 2 (see [8] for more details). The structure of orthogonal arrays has been introduced by Kishen [15] and further extended by Rao [16]. It is defined as follows:

**Definition 2.** *A $t-(q, d, \lambda)$ orthogonal array ($t \leqslant d$) is a $\lambda q^t \times d$ matrix whose entries are chosen from a $q$-set of $\mathbb{N}$ such that in every subset of $t$ columns of the array, every $t$-subset of points of this $q$-set appears in exactly $\lambda$ rows.*

From this definition by setting $t = 2$, we can construct a structure consisting of points in $\{1, \ldots, q\}^{\lambda q^2}$ where each 2-set of columns have the same 2-set of points $\lambda$ times.

In that paper, we use the so-called method of differences introduced by Bose and Bush [17] to construct $2-(d, q, 1)$ orthogonal arrays, with $q$ a prime number greater or equal to $d-1$. This last constraint is not that bad, as discussed in [8, 18], and can be relaxed when using other constructions (see e.g., [19]).

Thus, the replication procedure (called REP15 in the following) allows to estimate the full set of first- and closed second-order indices with a cost $2n+2q^2$, which depends on the input space dimension only through the constraint on $q$. REP15 is cheaper than SAL02 as far as $n > 2(d-1)$. For heavy applications with limited budget, one should prefer REP15, even if it does not allow the estimation of total-order Sobol' indices. We can also underline that in many applications, main effects and interactions of order 2 are leading the sensitivity of the model, higher-order interactions being less likely.

### *3.2. A more efficient strategy*

In this paper, we propose a more efficient strategy (called REP17 in the following), which allows the estimation of the full set of first- and second-order Sobol' indices from a single pair of replicated designs of order 2, as far as the derivation of associated bootstrap confidence intervals. We also propose in Section 4.2 to combine SAL02 with REP17 in case we can not assume that interactions of order higher or equal to three are negligible. This combined strategy (called REP17adapt in the following) allows the estimation of the full set of first-, second-order and total Sobol' indices at a cost of $n(d+2)$ model evaluations.

*Description of the new procedure.* Let us start with two replicated designs of order 2: $\mathcal{P} = \{\boldsymbol{x}_i\}_{i=1}^n$ and $\mathcal{P}' = \{\boldsymbol{x}'_i\}_{i=1}^n$. More precisely, replicated designs based on $2-(d,q,1)$ orthogonal arrays, each of size $n=q^2$ are chosen (see [8] for more details). Then, the procedure is based on the following results:

(a) for any subset $u$ of $\mathcal{D}$ such that $|u|=2$, these exists a unique permutation $\pi_u$ satisfying:

$$\boldsymbol{x'}_{\pi_u(i),u} = \boldsymbol{x}_{i,u}, \qquad \forall i \in \{1,\ldots,q^2\};$$

(b) for any $k \in \mathcal{D}$, there exists a set $\mathcal{H}_k = \{\pi_k^{(\ell)}, \ell \in \{1, \dots, q \times q!\}\}$ of $q \times q!$ mappings (or permutations) $\pi_k^{(\ell)}$, satisfying:

$$\boldsymbol{x'}_{\pi_k^{(\ell)}(i),k} = \boldsymbol{x}_{i,k}, \qquad \forall \ell \in \{1, \dots, q \times q!\}\,,\ \forall i \in \{1, \dots, q^2\}\,.$$

We then mimic the usual replication strategy described in Section 3.1 to estimate the full set of first- and second-order Sobol' indices from the single pair of replicated designs of order 2, $\mathcal{P} = \{\boldsymbol{x}_i\}_{i=1}^{n=q^2}$ and $\mathcal{P}' = \{\boldsymbol{x'}_i\}_{i=1}^{n=q^2}$. More precisely, for any $u$ subset of $\mathcal{D}$ with cardinal 2, for any $i \in \{1, \dots, q^2\}$, let

$$\begin{aligned}
y_i &= f(\boldsymbol{x}_i)\,, \\
y'_i &= f(\boldsymbol{x'}_i)\,, \\
y'_{\pi_u(i)} &= f(\boldsymbol{x'}_{\pi_u(i),u} : \boldsymbol{x'}_{\pi_u(i),-u}) \\
&= f(\boldsymbol{x}_{i,u} : \boldsymbol{x'}_{\pi_u(i),-u}).
\end{aligned}$$

For any $k \in \mathcal{D}$, for any $\ell \in \{1, \dots, q \times q!\}$, let

$$\begin{aligned}
y'_{\pi_k^{(\ell)}(i)} &= f(\boldsymbol{x'}_{\pi_k^{(\ell)}(i),k} : \boldsymbol{x'}_{\pi_k^{(\ell)}(i),-k}) \\
&= f(\boldsymbol{x}_{i,k} : \boldsymbol{x'}_{\pi_k^{(\ell)}(i),-k}).
\end{aligned}$$

Note that once we have computed $\{y_i\}_{i=1}^{q^2}$ and $\{y'_i\}_{i=1}^{q^2}$, we get $\{y'_{\pi_u(i)}\}_{i=1}^{q^2}$ for $u \subseteq \mathcal{D}, |u| = 2$ and $\{y'_{\pi_k^{(\ell)}(i)}\}_{i=1}^{q^2}$ with $k \in \mathcal{D}, \ell = 1, \dots, q \times q!$ without any additive evaluation of the model $f$, as the permutations $\pi_u$ and $\pi_k^{(\ell)}$ act as permutations of rows on the design $\mathcal{P}'$.

We then get Proposition 1 below.

**Proposition 1.** *Let $\mathcal{P} = \{\boldsymbol{x}_i\}_{i=1}^{n=q^2}$ and $\mathcal{P}' = \{\boldsymbol{x'}_i\}_{i=1}^{n=q^2}$ be two replicated designs based on $2-(d, q, 1)$ orthogonal arrays as in [8]. Evaluating the model on $\mathcal{P} = \{\boldsymbol{x}_i\}_{i=1}^{q^2}$ and $\mathcal{P}' = \{\boldsymbol{x'}_i\}_{i=1}^{q^2}$, it is possible to obtain:*

- *a single estimate for each $\underline{S}_u$, $|u| = 2$,*
- *$q \times q!$ estimates for each $S_k$, $k \in \mathcal{D}$.*

*Proof of Proposition 1.* Each $\underline{\tau}_u^2$, $|u| = 2$, can be estimated via formula (5) by using $y'_{\pi_u(i)}$ instead of $f(\boldsymbol{x}_{i,u} : \boldsymbol{x'}_{i,-u})$. Each $\underline{\tau}_k^2$, $k \in \mathcal{D}$, can be estimated via formula (5) by using $y'_{\pi_k^{(\ell)}(i)}$ instead of $f(\boldsymbol{x}_{i,k} : \boldsymbol{x'}_{i,-k})$. For each $k \in \mathcal{D}$, there exists $q \times q!$ choices for $\pi_k^{(\ell)}$. $\square$

*One example.* Let us illustrate the procedure of Proposition 1 on a simple example. Consider two replicated orthogonal arrays of strength two with $q = 3$ and $d = 4$:

$$\mathcal{P} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 2 & 1 & 3 & 2 \\ 3 & 1 & 2 & 3 \\ 2 & 2 & 2 & 1 \\ 3 & 2 & 1 & 2 \\ 1 & 2 & 3 & 3 \\ 3 & 3 & 3 & 1 \\ 1 & 3 & 2 & 2 \\ 2 & 3 & 1 & 3 \end{pmatrix} \qquad \mathcal{P}' = \begin{pmatrix} 2 & 1 & 2 & 1 \\ 3 & 3 & 2 & 2 \\ 2 & 3 & 3 & 3 \\ 3 & 2 & 3 & 1 \\ 1 & 1 & 3 & 2 \\ 3 & 1 & 1 & 3 \\ 1 & 3 & 1 & 1 \\ 2 & 2 & 1 & 2 \\ 1 & 2 & 2 & 3 \end{pmatrix}$$

Each column contains the three values 1, 2, 3 ; each of them being repeated three times. As an example, let us focus on the estimation of $\underline{S}_{\{1,2\}}$. Item (a) p.9 states that whatever the couple of columns one may pick in $\mathcal{P}$ and $\mathcal{P}'$, there exists a unique permutation that re-arranges the rows of the two first columns of $\mathcal{P}'$ in the order of the rows of the two first columns of $\mathcal{P}$, namely $\pi_{\{1,2\}} = (5, 1, 6, 8, 4, 9, 2, 7, 3)$. We now focus on the estimation of $S_1$. From Item (b), there exist $3 \times 3!$ permutations $\pi_1(\ell)$ that re-arrange the rows of the first column $C_1$ of $\mathcal{P}$ in the order of the rows of the first column $C'_1$ of $\mathcal{P}'$. On our example, we have:

$$C_1 = \begin{pmatrix} 1 \\ 2 \\ 3 \\ 2 \\ 3 \\ 1 \\ 3 \\ 1 \\ 2 \end{pmatrix}, \qquad C_1' = \begin{pmatrix} 2 \\ 3 \\ 2 \\ 3 \\ 1 \\ 3 \\ 1 \\ 2 \\ 1 \end{pmatrix}.$$

For each value $a_\ell \in \{1, 2, 3\}$, there exists 3! distinct permutations that re-arrange the three positions of $a_\ell$ in $C_1'$ in the three positions of $a_\ell$ in $C_1$. Let us take as an example $a_\ell = 1$, there exists 3! permutations to map positions $5, 7, 9$ of $C_1'$ in positions $1, 6, 8$ of $C_1$. The re-ordering of each value $a_\ell$ being independent, there exists a set $\mathcal{H}_1 = \{\pi_1^{(\ell)}, \ell \in \{1, \dots, 3 \times 3!\}\}$ of mappings between $C_1'$ and $C_1$ ensuring each:

$$\boldsymbol{x}'_{\pi_1^{(\ell)}(i),1} = \boldsymbol{x}_{i,1}, \qquad \forall i \in \{1, \dots, q^2\}.$$

The following permutation $\pi_1^{(1)}$ is one element of this set:

$$\pi_1^{(1)} = (5, 1, 2, 3, 4, 5, 6, 9, 8)\ .$$

Therefore, for each dimension $k \in \mathcal{D}$ one may pick one element of the corresponding set $\mathcal{H}_k$ to estimate the first-order index $S_k$.

To go further beyond, one may enhance the estimation of first-order indices by making use of the multiple mappings $\pi_k^{(\ell)}$ existing for each $k$. This is discussed in the next paragraph.

*One step beyond : augmenting the precision on first-order indices.* Let $k \in \mathcal{D}$. For each $S_k$, several estimations can be obtained, one for each permutation in $\mathcal{H}_k$. It is rather natural to consider the mean of these estimates, in order to outperform the accuracy of the procedure. In practice, we do not search for the existing $q \times q!$ permutations $\pi_k^{(\ell)}$ to estimate $S_k$. We choose $\kappa$ in $\{1, \dots, q \times q!\}$ and select randomly $\kappa$ permutations in $\mathcal{H}_k$. In Section 4, $\kappa$ has been chosen equal to 100. With that choice, the results are already very good. An optimal choice for $\kappa$, and an optimal selection procedure for the $\kappa$ permutations in $\mathcal{H}_k$ is out of the scope of that paper, but is an interesting perspective.

*Notation.* For any $u \subseteq \mathcal{D}$, $|u| = 2$, we estimate $\underline{S}_u$ by $\widehat{\underline{S}}_u$ associated with the permutation $\pi_u$ defined in (a) (p.9). Let $\kappa$ be a positive integer. For any $k \in \mathcal{D}$, we first choose randomly $\kappa$ permutations $\pi_k^{(\ell_1)}, \dots, \pi_k^{(\ell_\kappa)}$ in $\mathcal{H}_k$. We then estimate $S_k$ by

$$\widehat{S}_k^{(\ell_1,\dots,\ell_\kappa)} = \frac{1}{\kappa} \sum_{s=1}^{\kappa} \widehat{S}_k^{(\ell_s)} \tag{9}$$

where $\widehat{S}_k^{(\ell_s)}$ is the estimator associated with $\pi_k^{(\ell_s)}$ (see (b) p.9). We then deduce the estimate

$$\widehat{S}_{k,\ell}^{(\ell_1,\dots,\ell_\kappa)} = \widehat{\underline{S}}_{\{k,\ell\}} - \widehat{S}_k^{(\ell_1,\dots,\ell_\kappa)} - \widehat{S}_\ell^{(\ell_1,\dots,\ell_\kappa)} \tag{10}$$

for unclosed second-order Sobol' index associated to $u = \{k, \ell\}$. This new procedure is denoted by REP17 in the following.

### *3.3. Bootstrap intervals*

In this section, we propose bootstrap confidence intervals for the estimation of first- and second-order Sobol' indices with the procedure described in Section 3.2.

*Bias-corrected percentile method for bootstrap.* Sampling error in the estimation of Sobol' indices can be classically estimated for a moderate cost by using bootstrap resampling [20, 10]. More precisely, we use the bias-corrected (BC) percentile method presented in [21, 22]. The principle of this method can be summed up the following way: let $\widehat{\theta}(W_1, \dots, W_n)$ be an estimator for an unknown parameter $\theta$ in a reference population $\mathcal{Q}$. We generate a random i.i.d. $N$-sample $\{w_1, \dots, w_n\}$ from $\mathcal{Q}$, then we repeatedly, for $b = 1, \dots, B$, randomly draw $\{w_1[b], \ldots, w_n[b]\}$ with replacement from this sample and get a *replication* of $\widehat{\theta}$ by computing $\widehat{\theta}[b] = \widehat{\theta}(w_1[b], \ldots, w_n[b])$. This way we obtain a set $\mathcal{R} = \{\widehat{\theta}[1], \ldots, \widehat{\theta}[B]\}$ of replications of $\widehat{\theta}$.

We now show how this sample can be used to estimate a confidence interval for $\theta$. We denote by $\Phi$ the standard normal cdf:

$$\Phi(z) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{z} \exp\left(-\frac{t^2}{2}\right) \mathrm{d}t$$

and by $\Phi^{-1}$ its inverse.

Using $\mathcal{R}$ and the point estimate $\widehat{\theta} = \widehat{\theta}(w_1, \ldots, w_n)$, a "bias correction constant" $z_0$ can be estimated:

$$\widehat{z}_0 = \Phi^{-1}\left(\frac{\#\{\widehat{\theta}[b] \in \mathcal{R} \text{ s.t. } \widehat{\theta}[b] \leqslant \widehat{\theta}\}}{B}\right)$$

Then, for $\beta \in ]0;1[$, we define the "corrected quantile estimate" $\widehat{q}(\beta)$:

$$\widehat{q}(\beta) = \Phi(2\widehat{z}_0 + z_\beta)$$

where $z_\beta$ satisfies $\Phi(z_\beta) = \beta$.

The central BC bootstrap confidence interval of level $1-\alpha$ is then estimated by the interval whose endpoints are the $\widehat{q}(\alpha/2)$ and $\widehat{q}(1-\alpha/2)$ quantiles of $\mathcal{R}$.

*Application to the estimation of first- and second-order Sobol' indices.* Let $k \in \mathcal{D}$. The first-order Sobol' index is estimated by $\widehat{S}_k^{(\ell_1,\ldots,\ell_\kappa)}$ defined in equation (9). We apply the bootstrap procedure with $W = \left(Y, Y', Y'_{\pi_k^{(\ell_1)}}, \ldots, Y'_{\pi_k^{(\ell_\kappa)}}\right)$. Let $u \subseteq \mathcal{D}$, $|u| = 2$, $u = \{j_1, j_2\}$. The second-order Sobol' index $S_{j_1,j_2} = \underline{S}_{\{j_1,j_2\}} - S_{j_1} - S_{j_2}$ is estimated by $\widehat{S}_{j_1,j_2}^{(\ell_1,\ldots,\ell_\kappa)}$ defined in equation (10). We apply the bootstrap procedure with $W = \left(Y, Y', Y'_{\pi_{\{j_1,j_2\}}}, Y'_{\pi_{j_1}^{(\ell_1)}}, \ldots, Y'_{\pi_{j_1}^{(\ell_\kappa)}}, Y'_{\pi_{j_2}^{(\ell_1)}}, \ldots, Y'_{\pi_{j_2}^{(\ell_\kappa)}}\right)$.

## 4. Simulation study and application to benchmarks

The procedure REP17 is illustrated on two academic functions and two engineering examples. For the academic examples, results are assessed by computing bootstrap confidence intervals according to Section 3.3. Results are averaged over 100 repetitions and computed for three sizes of each of the two replicated designs: $n \in \{81, 529, 961\}$. The number of permutations $\kappa$ (see equations (9) and (10) in Section 3.2) and of bootstrap replications $B$ (see Section 3.3) are both fixed to 100.

True values of first-order and second-order Sobol' indices are estimated with a precision of 10 digits. For clarity purposes, in the following tables all results are rounded to 4 digits.

On the first academic example, we also provide a comparison between bootstrap confidence intervals and asymptotic ones in order to assess the estimation of first-order Sobol' indices (see Section 4.1.1 for more details). On the second academic example, we compare different approaches: REP17, SAL02, as well as a mix between both approaches REP17adapt.

### *4.1. Validation on test functions*

We consider in this section two academic examples: the Ishigami function introduced in [23] and the function introduced by Bratley *et al.* [24].

#### *4.1.1. Ishigami function*

The Ishigami function is defined as follows:

$$\begin{array}{rccc} f: & [-\pi,\pi]^3 & \to & \mathbb{R} \\ & x=(x_1,x_2,x_3) & \mapsto & \sin(x_1)+7\sin^2(x_2)+0.1\; x_3^4\sin(x_1) \end{array}$$

It is particularly interesting due to its strong nonlinearity and nonmonotonicity. Table 1 provides true values of first- and second-order Sobol' indices, means and bootstrap confidence intervals of the first- and second-order Sobol' estimates for the three sizes $n = 81$, $n = 529$ and $n = 961$. The means are represented as black dots in Figure 1 with their corresponding bootstrap confidence intervals (vertical bars).

For the first-order indices, one can observed that procedure REP17 yields already good results with $n = 529$. The precision of the bootstrap confidence intervals allows to distinguish the main effect of each of the three variables

Table 1: Means and bootstrap confidence intervals of the first- and second-order Sobol' estimates for the Ishigami function.

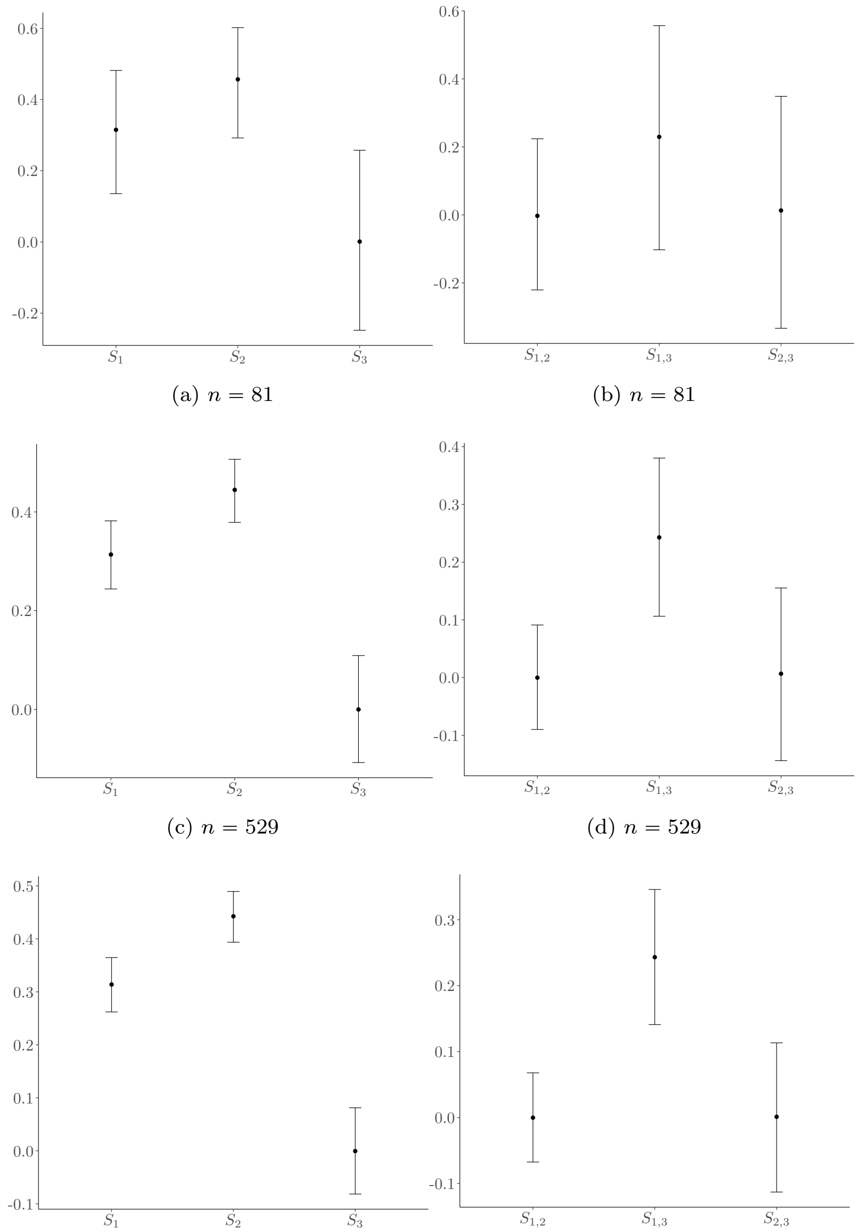
| | | Mean | | | bootstrap confidence interval | | |
|---|---|---|---|---|---|---|---|
| Index | Value | 81 | 529 | 961 | 81 | 529 | 961 |
| $S_1$ | 0.3139 | 0.3149 | 0.3137 | 0.3139 | $[0.1356, 0.4817]$ | $[0.2440, 0.3819]$ | $[0.2621, 0.3647]$ |
| $S_2$ | 0.4424 | 0.4567 | 0.4447 | 0.4425 | $[0.2920, 0.6018]$ | $[0.3788, 0.5067]$ | $[0.3937, 0.4895]$ |
| $S_3$ | 0 | 0.0009 | 0.0000 | 0.0029 | $[-0.2481, 0.2576]$ | $[-0.1076, 0.1091]$ | $[-0.0816, 0.0812]$ |
| $S_{1,2}$ | $< 10^{-9}$ | $-0.0027$ | $-0.0002$ | $-0.0001$ | $[-0.2206, 0.2239]$ | $[-0.0899, 0.0911]$ | $[-0.0674, 0.0679]$ |
| $S_{1,3}$ | 0.2436 | 0.2295 | 0.2429 | 0.2432 | $[-0.1026, 0.5565]$ | $[0.1063, 0.3802]$ | $[0.1411, 0.3460]$ |
| $S_{2,3}$ | 0 | 0.0130 | 0.0067 | 0.0013 | $[-0.3334, 0.3488]$ | $[-0.1440, 0.1552]$ | $[-0.1129, 0.1134]$ |

without any confusion. For indices $S_1$ and $S_2$ and $n = 961$, the radii of the bootstrap confidence intervals are lower than $5 \times 10^{-2}$.

Results for the second-order Sobol' indices are less accurate. This is expected due to the following reason: in procedure REP17, the estimation of the first-order Sobol' indices is obtained as an average over $\kappa$ different permutations (see equation (9)), but this is not the case for the estimation of closed second-order Sobol' indices. As such and given the formula (10), the accuracy of $\widehat{S}_{k,\ell}^{(\ell_1,\ldots,\ell_\kappa)}$ to estimate the unclosed second-order Sobol' index $S_{k,\ell}$ is mainly driven by the precision of $\widehat{\underline{S}}_{\{k,\ell\}}$, the corresponding closed second-order Sobol' estimate. Nonetheless, these results are still of good quality with respect to the values selected for $n$.

Table 2 provides a comparison between bootstrap and asymptotic confidence intervals for the estimation of first-order Sobol' indices with the replication procedure and estimates (5), (6) and (7) given in Section 2.2. Contrarily to bootstrap confidence intervals, asymptotic ones need new evaluations of the model. Moreover, the asymptotic theory for the estimation of second-order Sobol' indices via the replication method requires additional regularity assumptions on the model (see, e.g., [8]). We refer to the appendix for a detailed description on the way asymptotic confidence intervals are constructed for the estimation of first-order Sobol' indices with the replication procedure.

Figure 1: Means (black dots) and bootstrap confidence intervals (vertical bars) of the first- and second-order Sobol' estimates for the Ishigami function.




(a) $n = 81$ (b) $n = 81$

(c) $n = 529$ (d) $n = 529$

(e) $n = 961$ (f) $n = 961$

Table 2: Asymptotic and bootstrap confidence intervals (IC) of the first-order Sobol' indices for the Ishigami function. True values of the first-order indices are: $S_1 = 0.3139$, $S_2 = 0.4424$, $S_3 = 0$

| $n$ | IC | $S_1$ | $S_2$ | $S_3$ |
|---|---|---|---|---|
| 81 | bootstrap | $[0.1356, 0.4817]$ | $[0.2920, 0.6018]$ | $[-0.2481, 0.2576]$ |
| | asymptotic | $[0.1370, 0.4948]$ | $[0.2860, 0.5771]$ | $[-0.2848, 0.3093]$ |
| 529 | bootstrap | $[0.2440, 0.3819]$ | $[0.3788, 0.5067]$ | $[-0.1076, 0.1091]$ |
| | asymptotic | $[0.2467, 0.3859]$ | $[0.3770, 0.4926]$ | $[-0.1171, 0.1147]$ |
| 961 | bootstrap | $[0.2621, 0.3647]$ | $[0.3937, 0.4895]$ | $[-0.0816, 0.0812]$ |
| | asymptotic | $[0.2631, 0.3669]$ | $[0.4021, 0.4896]$ | $[-0.0891, 0.0854]$ |

#### *4.1.2. Bratley et al. function*

In this second example, we consider the Bratley *et al.* function defined by:

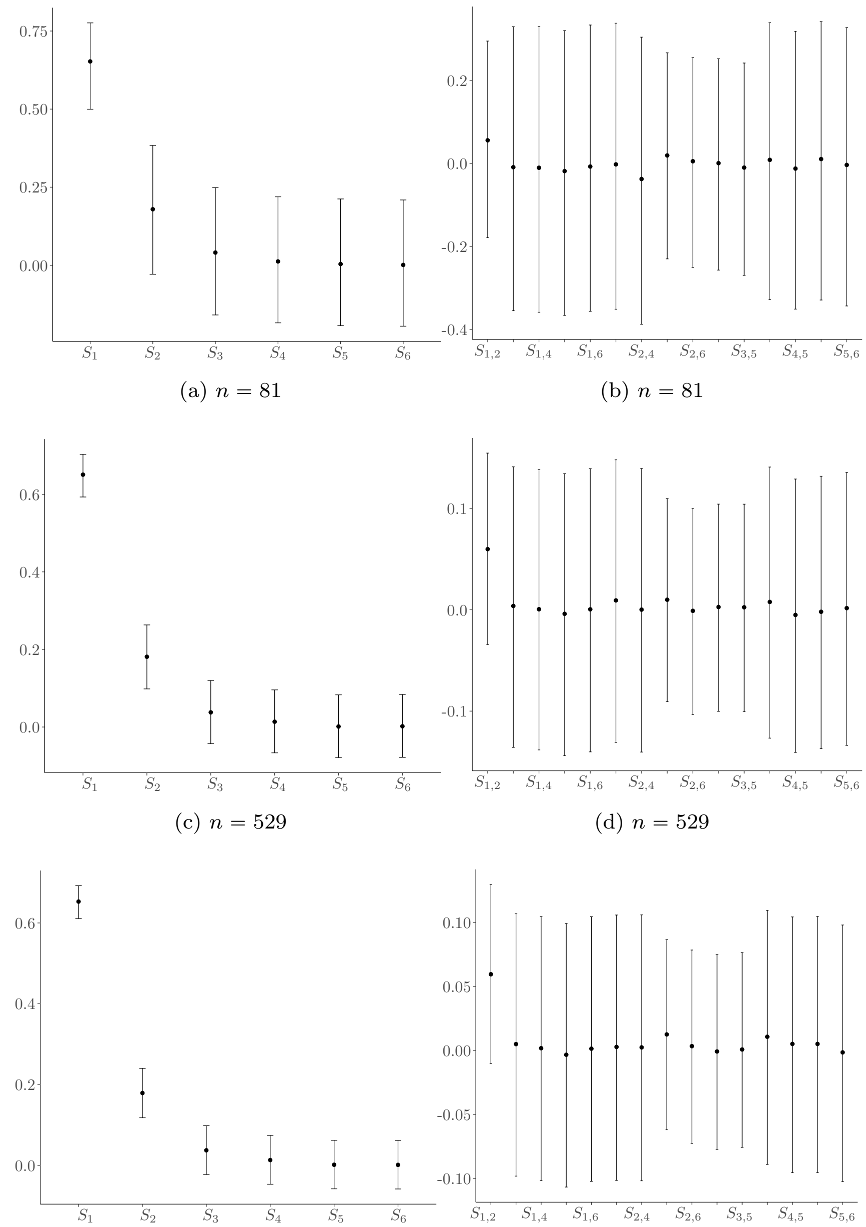
$$f(x_1, \ldots, x_6) = \sum_{i=1}^{6} (-1)^i \prod_{j=1}^{i} x_j \ .$$

The importance of each input $x_j$ depends on its own rank. More explicitly, $x_1$ is more influential than $x_2$ which is respectively more influential than $x_3$ and so on. The means of both first- and second-order estimates are represented as black dots in Figure 2 with their corresponding bootstrap confidence intervals (vertical bars).

Results for the first-order indices are similar to those obtained for the Ishigami function. For $n = 961$, the radii of the confidence intervals range from 0.04 to 0.06 and one can distinguish the influent inputs from the remaining ones.

For the second-order indices, results are slightly worse. For $n = 961$, the radii of the confidence intervals range from 0.07 to 0.10. The reason underlying these results is the same evoked for the Ishigami function. Note that most of the second-order Sobol' indices are close to zero for that example.

Figure 2: Means (black dots) and bootstrap confidence intervals (vertical bars) of the first- and second-order Sobol' estimates for the Bratley *et al.* function.



(a) $n = 81$ (b) $n = 81$

(c) $n = 529$ (d) $n = 529$

(e) $n = 961$ (f) $n = 961$

*4.2. Comparison with Saltelli procedure*

In this section, procedure REP17 is compared to procedure SAL02. Recall that SAL02 can be used to either:

*A*. simple estimate all first-order and total effect Sobol' indices at a cost of $n(d+2)$ evaluations of the model (Theorem 1 in [11]);

*B*. double estimates all first-order, second-order and total effect Sobol' indices at a cost of $n(2d+2)$ evaluations of the model (Theorem 2 in [11]).

Here, REP17 is compared to variant $B$ of SAL02 using the Ishigami test function. Results are compared by drawing boxplots of the estimation errors of first-order and second-order indices for each approach. These errors correspond to the absolute difference between the true values of the Sobol' indices and their estimates:

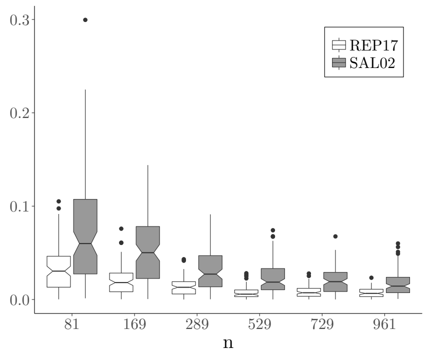
$$\delta_{S_u} = \left| S_u - \widehat{S}_u \right| , \qquad u \subset \mathcal{D} ,$$

where $S_u$ is the true value and $\widehat{S}_u$ the estimate.

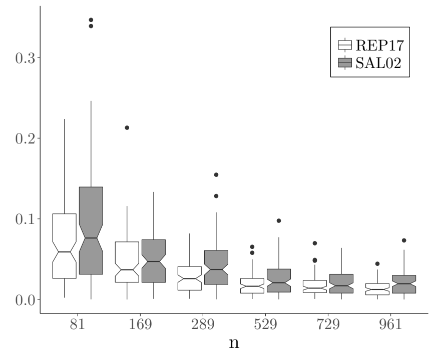
Results are averaged over 100 repetitions and computed for the following sizes of the designs: $n \in \{81, 169, 289, 529, 729, 961\}$. Figure 3 shows the results obtained with both approaches: REP17 and variant $B$ of SAL02. One can observe that REP17 performs the best for both the estimation of first-order and second-order indices. It is all the more noteworthy as the cost of SAL02 for that example is $n(2d+2) = 1134$ (*resp.* 2366, 4046, 7406, 10206 and 13454) for $n = 81$ (*resp.* 169, 289, 529, 729 and 961) instead of $2n = 162$ (*resp.* 338, 578, 1058, 1458 and 1922) for REP17.

Recall that REP17 as introduced in section 3.1 does not allow the estimation of total effect indices, which in some way offset the latter results. However, it is possible to go further and adapt REP17 (as REP17adapt) to estimate the same categories of Sobol' indices as variant $B$ of SAL02, with the computational cost of variant $A$. It proceeds as follows: first, all first-order and second-order indices are estimated with two replicated designs (*c.f.* Section 3.1). Then, all total effet Sobol' indices are estimated using the latter two replicated designs

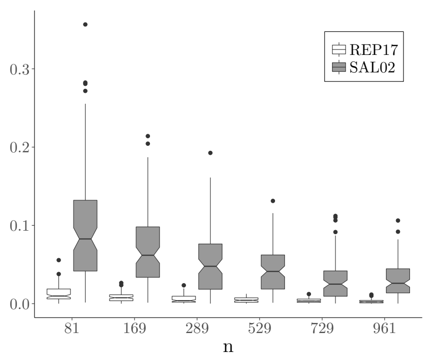
Figure 3: Boxplots of the estimation errors of the first- and second-order indices for the Ishigami function. The white boxplots refer to REP17, the grey boxplots refer to variant $B$ of SAL02. The x-axis indicates the size $n$ of the designs.



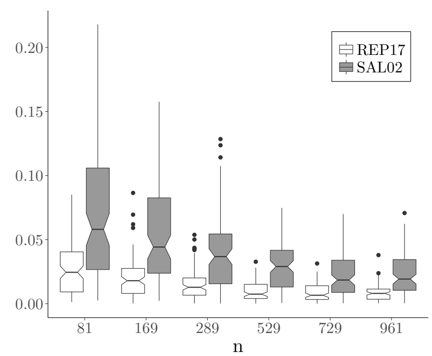

(a) Sobol' index $S_1$



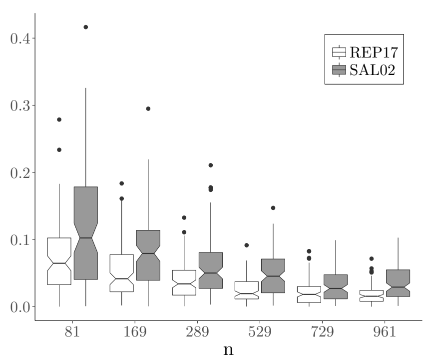

(b) Sobol' index $S_2$



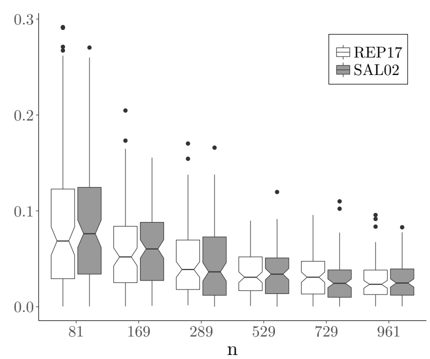

(c) Sobol' index $S_3$




(d) Sobol' index $S_{1,2}$




(e) Sobol' index $S_{1,3}$




(f) Sobol' index $S_{2,3}$

plus the $d$ designs constructed as in variant $A$. This extension can be viewed as a mix between REP17 and SAL02. The accuracy for the estimation of first-order Sobol' indices is increased with REP17adapt (with respect to SAL02 A) as first-order Sobol' indices are estimated as a mean over $\kappa$ different permutations (see equation (9)). Moreover, for the price of SAL02 A, we also get second-order Sobol' indices. The cost of REP17adapt is thus $n(d+2) = 648$ (*resp.* 1352, 2312, 4232, 5832 and 7688) for $n = 81$ (*resp.* 169, 289, 529, 729 and 961) for the full set of first-order, second-order and total Sobol' indices.

### *4.3. Application on Engineering examples*

#### *4.3.1. Wing weight function*

As a first application, consider the wing weight function introduced by Forrester *et al.* [25] and defined as follows:

$$f(\boldsymbol{x}) = 0.036 x_1^{0.758} x_2^{0.0035} \left( \frac{x_3}{\cos(x_4)^2} \right)^{0.6} x_5^{0.006} x_6^{0.04} \times \\ \times \left( \frac{100 x_7}{\cos(x_4)} \right)^{-0.3} (x_8 x_9)^{0.49} + x_1 x_{10}.$$

The parameters describing the behavior of the wing weight function are modeled by independent and uniformly distributed random variables that account for the uncertainty in the physical properties of the wing. Their range of variation and physical description are gathered in Table 3.

The motivation of this application is to test if procedure REP17 can capture the same set of influential inputs $(x_1, x_3, x_7, x_8, x_9)$ selected by the analysis of Forrester *et al.* which are those of value greater than 0.05. To do so, first-order and second-order Sobol' indices are estimated with two replicated designs of size $n = 71^2 = 5041$. Bootstrap confidence intervals are computed for each index.

First-order estimates are reported in Table 4. Figures 4 and 5 show first-order and second-order estimates (black dots) with their respective confidence interval (vertical bars). Overall, REP17 captures well the same set of influential inputs identified by Forrester *et al.*. Since the wing weight model is driven by main effects, all second-order indices are small. That explains the presence

Table 3: Parameters of the wing weight function and their ranges of variation. All inputs are uniformly distributed in their respective ranges.

| parameters | range | description |
|---|---|---|
| $x_1$ | $[150, 200]$ | wing area (ft$^2$) |
| $x_2$ | $[220, 300]$ | weight of fuel in the wing (lb) |
| $x_3$ | $[6, 10]$ | aspect ratio |
| $x_4$ | $[-10, 10]$ | quarter-chord sweep (degrees) |
| $x_5$ | $[16, 45]$ | dynamic pressure at cruise (lb/ft$^2$) |
| $x_6$ | $[0.5, 1]$ | taper ratio |
| $x_7$ | $[0.08, 0.18]$ | aerofoil thickness to chord ratio |
| $x_8$ | $[2.5, 6]$ | ultimate load factor |
| $x_9$ | $[1700, 2500]$ | flight design gross weight (lb) |
| $x_{10}$ | $[0.025, 0.08]$ | paint weight (lb/ft$^2$) |

Table 4: First-order Sobol' index estimates and bootstrap confidence intervals (CI) for the wing weight function.

| input | $\widehat{S}_u$ | bootstrap CI |
|---|---|---|
| $x_1$ | 0.1252 | $[0.0982, 0.1521]$ |
| $x_2$ | 0.0039 | $[-0.0238, 0.0315]$ |
| $x_3$ | 0.2187 | $[0.1930, 0.2445]$ |
| $x_4$ | 0.0037 | $[-0.0235, 0.0313]$ |
| $x_5$ | $-0.0002$ | $[-0.028, 0.0273]$ |
| $x_6$ | $-0.0014$ | $[-0.028, 0.0263]$ |
| $x_7$ | 0.1418 | $[0.1151, 0.1687]$ |
| $x_8$ | 0.4124 | $[0.3907, 0.4337]$ |
| $x_9$ | 0.0835 | $[0.0562, 0.1108]$ |
| $x_{10}$ | 0.0046 | $[-0.0225, 0.0324]$ |

of multiple negative estimates observed in Figure 5. Still, as all second-order estimates stand below the treshold 0.05, our procedure does not identify false influential parameters.

Figure 4: Plot of firt-order Sobol' index estimates for the wing weigth function. The vertical bars represent the bootstrap confidence intervals. The horizontal dotted line marks the threshold (0.05).

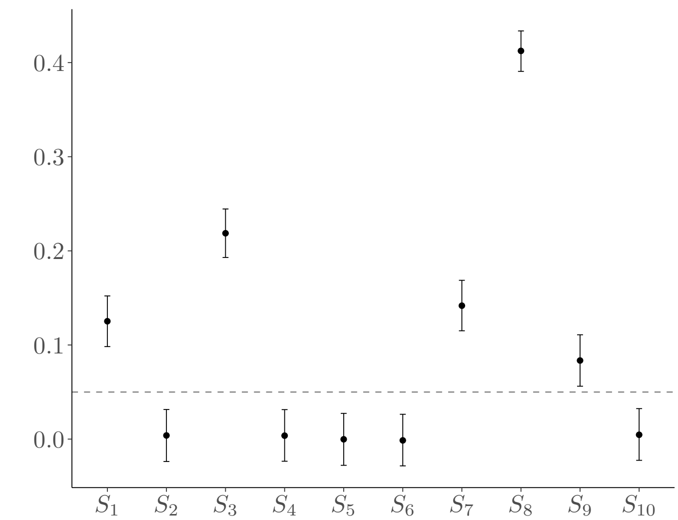



Figure 5: Plot of second-order Sobol' index estimates for the wing weigth function. The vertical bars represent the bootstrap confidence intervals. The horizontal dotted line marks the threshold (0.05).

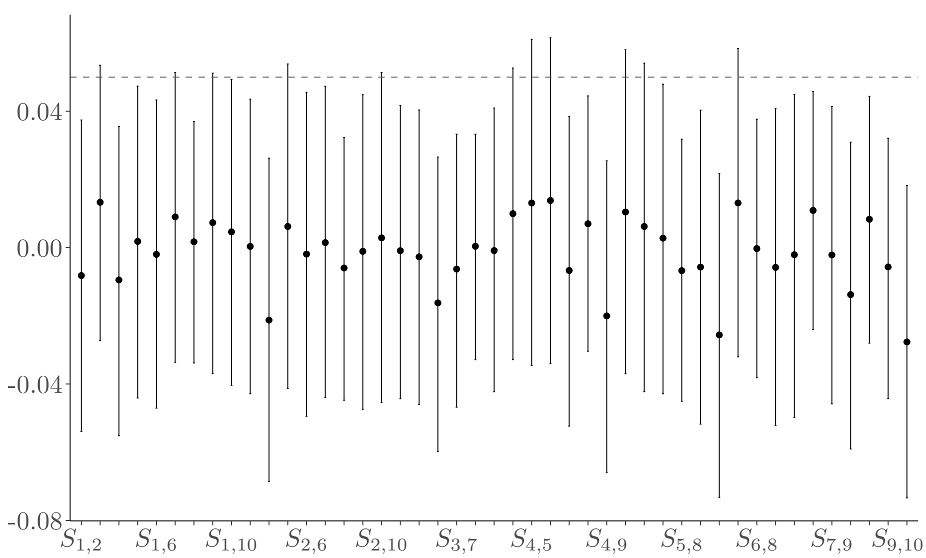


Table 5: Parameters of the Level E model and their distributions.

| parameters | distribution | range of variation | description |
|---|---|---|---|
| $x_1$ | uniform | $[100, 1000]$ | containment time (yr) |
| $x_2$ | log-uniform | $[10^{-3}, 10^{-2}]$ | leach rate for iodine (mols/yr) |
| $x_3$ | log-uniform | $[10^{-6}, 10^{-5}]$ | leach rate for Np chain (mols/yr) |
| $x_4$ | log-uniform | $[10^{-3}, 10^{-1}]$ | water velocity in the first geosphere layer (m/yr) |
| $x_5$ | uniform | $[100, 500]$ | length of the first geosphere layer (m) |
| $x_6$ | uniform | $[1, 5]$ | retention factor for iodine in the first layer |
| $x_7$ | uniform | $[3, 30]$ | retention factor for the chain elements in the first layer |
| $x_8$ | log-uniform | $[10^{-2}, 10^{-1}]$ | water velocity in the second geosphere layer (m/yr) |
| $x_9$ | uniforme | $[50, 200]$ | length of the second geosphere layer (m) |
| $x_{10}$ | uniform | $[1, 5]$ | retention factor for iodine in the first layer |
| $x_{11}$ | uniform | $[3, 30]$ | retention factor for the chain elements in the second layer |
| $x_{12}$ | log-uniform | $[10^5, 10^7]$ | stream flow rate ($m^3$/yr) |

*4.3.2. Level E model*

The Level E model has been used as a benchmark for sensitivity analysis by several authors (see [1] for a review). The model predicts the radiological dose to humans over geological time scales due to the underground migration of four radionuclides from a nuclear waste disposal site through two geosphere layers characterised by different hydro-geological properties.

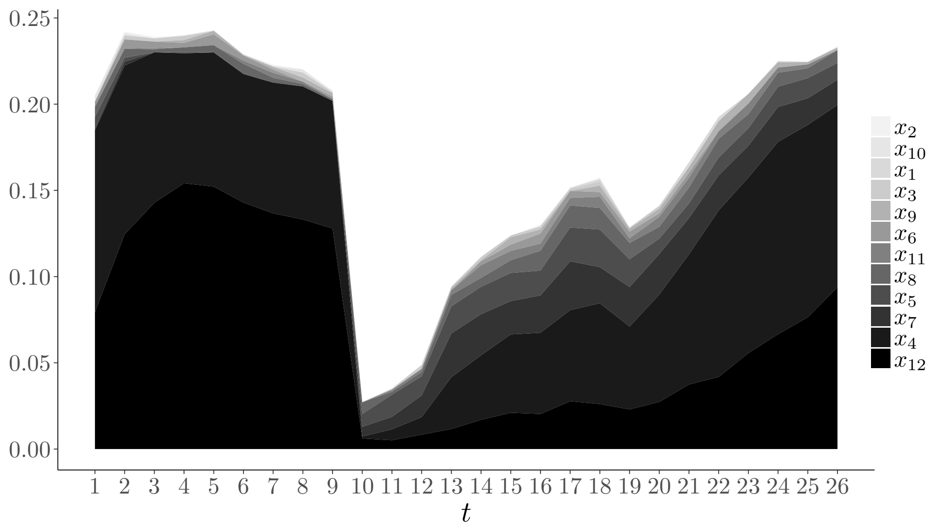
The model is mathematically represented by a set of partial differential equations modeling the different chemical processes that govern the underground migration of the nucleides (a detailed description of the equations can be found in [1][Section 3.4]). The quantity of interest $Y(t)$ corresponds to the annual radiological dose due to the four radionuclides. $Y(t)$ is evaluated at 26 time frames ranging from $2 \times 10^4$ to $9 \times 10^6$ years. Following the simplification proposed in [1], the twelve independent parameters listed in Table 5 are considered.

Procedure REP17 is applied to estimate first- and second-order indices associated to the twelve parameters. Two replicated designs of size $n = 5041$ are constructed to perform the estimation. The most influential parameters based on either main effects or second-order interactions are reported in Table 6. Since the quantity of interest $(Y(t_i), i = 1, \ldots, 26)$ is a vector, the results are displayed as cumulative area plots in Figures 6 and 7, on which we can

Table 6: Sets of most influential parameters for the levelE model at each time frame, based on either main effects or second-order interactions.

| time frame | set of most influential parameters | |
|---|---|---|
| | by main effect | by interaction |
| $t_1$ | $\{x_4, x_{12}\}$ | $\{x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_9, x_{11}, x_{12}\}$ |
| $t_2$ | $\{x_4, x_{12}\}$ | $\{x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_9, x_{10}, x_{11}, x_{12}\}$ |
| $t_3$ | $\{x_4, x_{12}\}$ | $\{x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_9, x_{10}, x_{11}, x_{12}\}$ |
| $t_4$ | $\{x_4, x_{12}\}$ | $\{x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_9, x_{10}, x_{11}, x_{12}\}$ |
| $t_5$ | $\{x_4, x_{12}\}$ | $\{x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_9, x_{10}, x_{11}, x_{12}\}$ |
| $t_6$ | $\{x_4, x_{12}\}$ | $\{x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_9, x_{10}, x_{11}, x_{12}\}$ |
| $t_7$ | $\{x_4, x_{12}\}$ | $\{x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_9, x_{10}, x_{11}, x_{12}\}$ |
| $t_8$ | $\{x_4, x_{12}\}$ | $\{x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_9, x_{10}, x_{11}, x_{12}\}$ |
| $t_9$ | $\{x_4, x_{12}\}$ | $\{x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_9, x_{10}, x_{11}, x_{12}\}$ |
| $t_{10}$ | $\varnothing$ | $\{x_2, x_5, x_6, x_7, x_8, x_9, x_{10}\}$ |
| $t_{11}$ | $\{x_5\}$ | $\{x_4, x_5, x_6, x_7, x_8, x_9, x_{10}, x_{11}, x_{12}\}$ |
| $t_{12}$ | $\{x_4, x_5, x_7\}$ | $\{x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_{10}, x_{11}, x_{12}\}$ |
| $t_{13}$ | $\{x_4, x_5, x_7, x_{12}\}$ | $\{x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_{10}, x_{11}, x_{12}\}$ |
| $t_{14}$ | $\{x_4, x_5, x_7, x_{12}\}$ | $\{x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_{10}, x_{11}, x_{12}\}$ |
| $t_{15}$ | $\{x_4, x_5, x_7, x_{12}\}$ | $\{x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_{10}, x_{11}, x_{12}\}$ |
| $t_{16}$ | $\{x_4, x_5, x_7, x_8, x_{12}\}$ | $\{x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_{10}, x_{11}, x_{12}\}$ |
| $t_{17}$ | $\{x_4, x_5, x_7, x_8, x_{12}\}$ | $\{x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_{10}, x_{11}, x_{12}\}$ |
| $t_{18}$ | $\{x_4, x_5, x_7, x_8, x_{12}\}$ | $\{x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_{10}, x_{11}, x_{12}\}$ |
| $t_{19}$ | $\{x_4, x_5, x_7, x_{12}\}$ | $\{x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_9, x_{10}, x_{11}, x_{12}\}$ |
| $t_{20}$ | $\{x_4, x_7, x_{12}\}$ | $\{x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_9, x_{10}, x_{11}, x_{12}\}$ |
| $t_{21}$ | $\{x_4, x_7, x_{12}\}$ | $\{x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_9, x_{10}, x_{11}, x_{12}\}$ |
| $t_{22}$ | $\{x_4, x_5, x_7, x_8, x_{12}\}$ | $\{x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_9, x_{10}, x_{12}\}$ |
| $t_{23}$ | $\{x_4, x_5, x_7, x_{12}\}$ | $\{x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_9, x_{10}, x_{11}, x_{12}\}$ |
| $t_{24}$ | $\{x_4, x_5, x_7, x_{12}\}$ | $\{x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_9, x_{10}, x_{12}\}$ |
| $t_{25}$ | $\{x_4, x_5, x_7, x_{12}\}$ | $\{x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_9, x_{10}, x_{11}, x_{12}\}$ |
| $t_{26}$ | $\{x_4, x_7, x_{12}\}$ | $\{x_1, x_2, x_3, x_4, x_6, x_7, x_8, x_9, x_{10}, x_{11}, x_{12}\}$ |

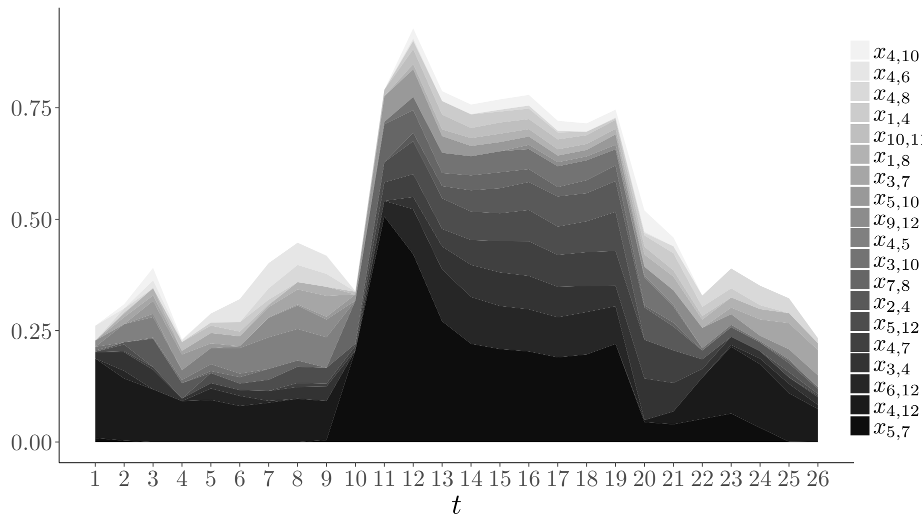
Figure 6: Cumulative area plot of first-order Sobol' index estimates for the levelE model. The y-axis indicates the sum of the estimates. The x-axis refers to the time frame $t$.




see the evolution in time. A parameter is judged influential if either its main effect or second-order interaction is higher than 0.01. The results obtained with REP17 match those obtained in [1] for the first-order indices. The observations are identical: only parameters $x_4$ and $x_{12}$ are influential for the first nine time frames, a drop is observed at time $t_{10}$, parameters $x_5, x_7, x_8$ become influential only after the drop. The sum of the first-order indices being always lower than 0.25, it is relevant to study the second-order indices.

Figure 7 shows that the model is driven by second-order interactions from time $t_{11}$ to $t_{19}$, where at least 75% of the model variance is explained. Based on Table 6, parameters $x_1, x_2, x_3, x_6, x_9, x_{11}, x_{12}$ are only influential through interactions. Since the sum of first-order and second-order indices is lower than 0.7 on the two time frames $[t_1, t_{10}]$ and $[t_{21}, t_{26}]$, a futur work would consist in testing the adaptation REP17adapt discussed in Section 4.2 to estimate total effect Sobol' indices on these two time frames.

Figure 7: Cumulative area plot of the 19 most influent second-order Sobol' index estimates for the levelE model. The y-axis indicates the sum of the estimates. The x-axis refers to the time frame $t$.




## 5. Conclusion

When estimating Sobol' indices, the question of how many model evaluations must be performed to reach a decent precision is often raised by practitioners. This question is all the more critical as the number of available evaluations is often bounded (wheter by time or budget constraints). The new procedure proposed in this article offers a practical solution with the estimation of the full set of first-order and second-order Sobol' indices. Aside from halving the cost of the original replication procedure [8], this new approach was shown to drastically enhance the precision of the estimates. The assessment of this precision was made by computing bootstrap confidence intervals. The comparison against asymptotic intervals suggests that the produced bootstrap intervals are a reliable tool to gauge the quality of the estimation.

Additionally, if one is interested by total effect Sobol' indices, it was discussed that the procedure can be mixed with Saltelli approach to estimate the latter indices together with all first-order and second-order indices at a competitive cost.

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## 6. Appendix

In this appendix, we describe the construction of asymptotic confidence intervals for first-order Sobol' indices estimated with the replication procedure.

Let $u = \{\ell\} \subseteq \{1, \ldots, d\}$. We estimate $\underline{S}_u = S_\ell$ with the replication procedure and formulas (5), (6) and (7) given in Section 2.2. Let $\mathbf{x} = (x_\ell, \mathbf{x}_{-\ell}) =$

$(X, Z) \in \mathbb{R} \times \mathbb{R}^{d-1}$. We denote by $X', Z', Z'', Z'''$ independent copies of $X$ (resp. $Z$). Asymptotic confidence intervals are constructed as follows: let $g_T : \mathbb{R}^{2d-1} \to \mathbb{R}^3$ defined by

$$g_T(x, z, z') = \begin{pmatrix} (f(x,z) - \mu)(f(x,z') - \mu) \\ f(x,z) + f(x,z') - 2\mu \\ (f(x,z) - \mu)^2 + (f(x,z') - \mu)^2 \end{pmatrix}$$

where $x \in \mathbb{R}$, $z, z' \in \mathbb{R}^{d-1}$ and $\mu = \mathbb{E}(f(\mathbf{x}))$.

We denote by $g_{T\,add}$ the best additive (in $X, Z, Z'$) approximation as defined in [26], and set $g_{T\,rem} = g_T - g_{T\,add}$.

Then, we let:

$$\Phi_T(x, y, z) = \frac{x - (\frac{y}{2})^2}{\frac{z}{2} - (\frac{y}{2})^2},$$

and, finally,

$$\mathbf{a}_T = \big(\mathrm{Cov}(Y, Y'), 0, 2\mathrm{Var}(Y)\big)^T$$

for $Y' = f(X, Z')$.

Then, the asymptotic variance in the central limit theorem for $\widehat{S}_\ell$ (*c.f* equation (7)) is defined as

$$\sigma_T^2 = (\nabla \Phi_T(\mathbf{a_T}))^T \; \Sigma_T \; \nabla \Phi_T(\mathbf{a_T})$$

where $\Sigma_T$ is the $(3 \times 3)$ covariance matrix of $g_{T\,rem}$. A proof of these expressions is given in (ii) of Proposition 3.2. of [8].

It remains to explain how the $\Sigma_T$ matrix can be estimated.

We decompose $g_T$ as:

$$g_T(X, Z, Z') = m + g_{T\,add}(X, Z, Z') + g_{T\,rem}(X, Z, Z')$$

where $m = \mathbb{E}(g_T(X, Z, Z'))$ and

$$g_{T\,add}(X, Z, Z') = g_{T\,a1}(X) + g_{T\,a2}(Z) + g_{T\,a3}(Z')$$

is the best additive approximation of $g_T$.

We want to estimate the covariance matrix of the $\mathbb{R}^m$-valued random variable $g_{Trem}(X, Z, Z')$. For $i, j \in \{1, \ldots, m\}$, we denote by $C_{i,j}$ the $(i, j)$-coefficient of this matrix.

Let $(X, Z, Z', Z'', Z''')_k$, $k = 1, \ldots, n$ be a $n$-sample of $(X, Z, Z', Z'', Z''')$. Let us define $Y_i, Y_j, Y_j'$ and $Y_j''$ as:

$$Y_i = g_T((X, Z, Z')_i) = m_i + g_{Ta1}(X)_i + g_{Ta2}(Z)_i + g_{Ta3}(Z')_i + g_{Trem}(X, Z, Z')_i$$

$$Y_j = g_T((X, Z, Z')_j) = m_j + g_{Ta1}(X)_j + g_{Ta2}(Z)_j + g_{Ta3}(Z')_j + g_{Trem}(X, Z, Z')_j$$

$$Y_j' = g_T((X, Z'', Z''')_j) = m_j + g_{Ta1}(X)_j + g_{Ta2}(Z'')_j + g_{Ta3}(Z''')_j + g_{Trem}(X, Z'', Z''')_j$$

$$Y_j'' = g_T((X', Z, Z''')_j) = m_j + g_{Ta1}(X')_j + g_{Ta2}(Z)_j + g_{Ta3}(Z'')_j + g_{Trem}(X', Z, Z'')_j$$

$$Y_j''' = g_T((X', Z'', Z')_j) = m_j + g_{Ta1}(X')_j + g_{Ta2}(Z'')_j + g_{Ta3}(Z')_j + g_{Trem}(X', Z'', Z')_j$$

We also define:

$$A_{i,j} = \mathrm{Cov}(g_{Ta1}(X)_i, g_{Ta1}(X)_j)$$

$$B_{i,j} = \mathrm{Cov}(g_{Ta2}(Z)_i, g_{Ta2}(Z)_j)$$

$$D_{i,j} = \mathrm{Cov}(g_{Ta3}(Z')_i, g_{Ta3}(Z')_j)$$

Thanks to independance, and $L^2-$orthogonality between $g_{Trem}(X, Z, Z')$ and functions of $X$ (resp. $Z$, $Z'$) alone, we have:

$$\mathrm{Cov}(Y_i, Y_j) = A_{i,j} + B_{i,j} + D_{i,j} + C_{i,j}$$

$$\mathrm{Cov}(Y_i, Y_j') = A_{i,j}$$

$$\mathrm{Cov}(Y_i, Y_j'') = B_{i,j}$$

$$\mathrm{Cov}(Y_i, Y_j''') = D_{i,j}$$

Hence:

$$C_{i,j} = \mathrm{Cov}(Y_i, Y_j) - \mathrm{Cov}(Y_i, Y_j') - \mathrm{Cov}(Y_i, Y_j'') - \mathrm{Cov}(Y_i, Y_j''')$$

which gives rise to a natural empirical estimator $\widehat{C}_{i,j}$ of $C_{i,j}$ using a sample of $Y_i, Y_j, Y_j'$ and $Y_j''$.

In practice, one can re-use the samples of input variables used during sensitivity indices estimation (both first-order and second-order), so as to avoid new model evaluations for estimating the asymptotic variances. However, our numerical experiments below are made using new Monte-Carlo samples.

It is also worth noting that $g_{\mathrm{add}}$ could be estimated using, for instance, the semi-parametric methods in the `R` package GAM [27], but we have noticed in our experiments that this choice induces some significative bias in the estimation of $\Sigma_T$, leading to a bias in the estimation of the asymptotic variance of $\hat{T}$.