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Reliable error estimation for Sobol' indices

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Dear associate editor and reviewers,
we would like to thank you for the positive and constructive feedback. Below we have compiled a detailed list of answers (blue text) to the issues raised in the review reports. The corresponding modifications in the manuscript are colored in purple.
Further aknowledgments have been added ahead of time to thank both the associate editor and the two reviewers work.
Best regards,
Laurent Gilquin and Lluís Antoni Jiménez Rugama

Report on "Reliable error estimation for Sobol' indices"

Reviewer 1

Minor comments:

1. page 2, column 1, line 1: replace "convergence rates are of" by "convergence rates can be", as these convergence rates only hold under some conditions, and the "are of" without any mention of conditions makes it sound as if these rates always held
2. page 4, column 1, line 9, italicize d in "dimension d"
3. page 4, column 2, lines 42-43: replace "and" by "an" before "automatic"
4. page 6, column 2, lines 22-23: replace "incur" by "result"
5. page 7, line 9 of column 2: regarding item f of the minor comments in my previous review, although it is now more clear how the points are constructed, the "iid" mention is still slightly confusing. I think you mean that the 3d coordinates are independent but not that the points themselves are independent (since even after scrambling the points of the scrambled sequence are dependent). I would remove the iid mention, assuming it is meant to describe the property of the 3d coordinates, as it is implicit when saying that each point follow a $\mathcal{U}([0,1)^{3d})$.
6. page 8, column 1, lines 32-33: "academic example": what does this mean? Why not just say "application" as indicated in the title of your Section 5.2 on page 10?
7. page 11, column 1, lines 51-52: should read "expensive"

* Points 1, 2, 3, 4 and 7 have all been addressed accordingly.
* Concerning point 5, we intended to mention Owen's estimator in its original form, designed with uniform iid points. Since it uses iid uniform points, the integral (or expected value to be estimated) is defined over the uniform measure. Hence, because the integral is defined over the uniform measure, we can apply quasi-Monte Carlo points instead of uniform iid

points. This does not imply that the quasi-Monte Carlo points need to be independent. As the reviewer mentions, since this is confusing, we have followed the suggested correction and removed the *iid* mention.

* Concerning point 6, we simply missed this correction during the first review. We thank the reviewer for catching it.

Reviewer 2

Minor comments:

1. p2 line 33 Left: there is an extra $\in$
2. p3 eq (7): you can get a better estimate of σ^2 using all 2n observations, not just the first n.
3. p3 line 37 Left: 'we generalized' is not quite precise, since ref [4] had 4 other authors
4. Rereading my original comment about definition 1, I see it was a bit ambiguous. Sorry about that. Something extra needed to be said to rule out bad point sets. That could either be in the definition itself, or put in a comment right at the place where points satisfying the definition get used. The revision puts it into the definition. This is ok, but it leaves you with a longer definition than you might have wanted.
5. p3 line 14 Right: ref 21 has only two authors, so why not just say Tissot and Prieur instead of Tissot et al?
6. p3 line 26 Right: asymptotical → asymptotic
7. p5 eq (15) replace period by comma
8. sec 5.1.1 for readers who don't know a lot about QMC, it would help to explain why the new g function is not as qmc friendly as the previous one.
9. p5 line 51 Right: propose to draw boxplots → draw boxplots
10. p9 and elsewhere: influent → influential. Influential means important. Influent refers to water flowing in:
    http://www.dictionary.com/browse/influent?s=t
11. p10 55 Left shwon → shown
12. p11 52 Left expansive → expensive

* Points 1, 5, 6, 7, 9, 10, 11 and 12 have all been addressed accordingly.

* Concerning point 2, although this is a great idea, this is not as convenient if we use the error estimation from Section 3. We could proceed by estimating μ (the same method for σ^2) with $f(\mathbf{x}_i)$ and computing the error bound, estimating μ with $f(\mathbf{x}'_i)$ and computing the error bound. Then, if $\mu \in [a, b]$ and $\mu' \in [a', b']$, the new estimator would be the mid point in

$[a, b] \cap [a', b']$. This would require including the computation of the fast Fourier transform for the $f(\mathbf{x}'_i)$ evaluations which could be too costly for the benefits it provides (given that the hard integral is in the numerator). As the reviewer suggests, it is important to consider that we have the $f(\mathbf{x}'_i)$ evaluations and this could always be used. We added a comment after equation (7) explaining this point.

* Concerning point 3, 'we generalized' has been replaced by 'we use the generalization from' to answer the issue.

* Concerning point 4, we decided to keep the modification in the definition to stress that bad point sets are ruled out.

* Concerning point 8, further explainations were added on the new g-function (inspired from the reviewer's comments on the first review).

Noname manuscript No.
(will be inserted by the editor)

Reliable error estimation for Sobol' indices

Lluís Antoni Jiménez Rugama · **Laurent Gilquin**

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Abstract In the field of sensitivity analysis, Sobol' indices are sensitivity measures widely used to assess the importance of inputs of a model to its output. The estimation of these indices is often performed through Monte Carlo or quasi-Monte Carlo methods. A notable method is the replication procedure that estimates first-order indices at a reduced cost in terms of number of model evaluations.

An inherent practical problem of this estimation is how to quantify the number of model evaluations needed to ensure that estimates satisfy a desired error tolerance. This article addresses this challenge by proposing a reliable error bound for first-order and total effect Sobol' indices. Starting from the integral formula of the indices, the error bound is defined in terms of the discrete Walsh coefficients of the different integrands.

We propose a sequential estimation procedure of Sobol' indices using the error bound as a stopping criterion. The sequential procedure combines Sobol' sequences with either Saltelli's strategy to estimate both first-order and total effect indices, or the replication procedure to estimate only first-order indices.

Keywords Sobol' index · error bound · sequential method · quasi-Monte Carlo

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1 Introduction

Let f represent a deterministic numerical model in $[0,1]^d$, $d \geqslant 1$. Sensitivity measures, also known as Sobol' indices, are used to assess which inputs of f are influential for the output. The normalized indices are scalars between 0 and 1 whose values are interpreted as follows: the closer to 1 the more influential the index. Alternatively, they can be interpreted as the percentage of the variance explained by the inputs. Among all Sobol' indices one can distinguish first-order and total effect indices. The first measure the effect of a single input, while the second measure the effect of a single input plus all its interactions with other inputs.

When dealing with complex numerical models, analytical expressions of Sobol' indices are often inaccessible. In such cases, one must rely on an estimation of these indices. The original estimation procedure is due to Sobol' [20]. However, this procedure requires several model evaluations which are usually expensive. Later on, Saltelli [18] proposed strategies to estimate sets of Sobol' indices at once through the use of a combinatorial formalisms. While elegant, these strategies still require a large number of model evaluations. A cost efficient alternative to estimate first-order indices was introduced in [13]. This alternative, called the replication procedure, has recently been further studied in [21] and generalized to the estimation of closed second-order indices.

A practical problem concerning the use of these methods is how to quantify the number of model evaluations required to ensure that Sobol' estimates are accurate enough. This article addresses this challenge by proposing a reliable error bound for Sobol' indices based on digital sequences. One reason to use digital sequences is that the numerical integra-

tion convergence rates can be $\mathcal{O}(n^{-1+\delta})$ (n being the number of function values) instead of the usual $\mathcal{O}(n^{-1/2})$ for iid Monte Carlo methods. In addition, the error bound in this article is defined in terms of the discrete Walsh coefficients of the integrands involved in the Sobol' indices definition. We propose a sequential estimation procedure of Sobol' indices using the error bound as our stopping criterion. The procedure operates under the assumption that all integrands lie inside a particular cone of functions (see [5]).

Firstly, Section 2 introduces Sobol' indices and reviews both Saltelli's strategy to estimate first-order and total effect Sobol' indices, and the replication procedure. Our main contribution is detailed in Section 3. There, we review the construction of the error bound proposed in [5] for the estimation of integrals based on digital sequences, and then we generalize it for Sobol' indices. Section 4 is devoted to analyze the cost in terms of model evaluations of our sequential estimation algorithm. It combines the error bound in Section 3 and either one of the two estimation procedures of Section 2. We also discuss a potential improvement to estimate small first-order indices according to [17]. Finally, examples and illustrations of our procedure are presented in Section 5.

2 Background on Sobol' indices

2.1 Definition of Sobol' indices

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

The uncertainty on $\mathbf{x}$ is modeled by a uniform random vector, namely $\mathbf{x} \sim \mathscr{U}([0,1]^d)$. The Hoeffding decomposition [8,20] of f is:

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

where:

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

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

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

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

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

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

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

Both $\underline{\tau}_u^2$ and $\overline{\tau}_u^2$ satisfy the following relations: $0 \leqslant \underline{\tau}_u^2 \leqslant \overline{\tau}_u^2$ and $\underline{\tau}_u^2 = \sigma^2 - \overline{\tau}_{-u}^2$. 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 our framework, we are only interested in single input indices, namely $|u| = 1$. The computation of the normalized indices is performed based on the following integral formulas for their numerators:

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

$$\overline{\tau}_u^2 = \frac{1}{2} \int_{[0,1]^{d+1}} (f(\mathbf{x}') - f(\mathbf{x}_u : \mathbf{x}'_{-u}))^2 d\mathbf{x}_u d\mathbf{x}', \; u \in \mathscr{D}, \tag{3}$$

while variance and mean of f are evaluated as:

$$\sigma^2 = \int_{[0,1]^d} f(\mathbf{x})^2 d\mathbf{x} - \mu^2,$$
$$\mu = \int_{[0,1]^d} f(\mathbf{x}) d\mathbf{x}, \tag{4}$$

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

2.2 Estimation of Sobol' indices

In this section we review two Monte Carlo procedures for the estimation of Sobol' indices. A design is a point set $\mathscr{P} = \{\mathbf{x}_i\}_{i=0}^{n-1}$ where each point is obtained by sampling each variable x_j n times. Each row of the design is a point $\mathbf{x}_i$ in $[0,1]^d$ and each column of the design refers to samples of a variable x_j. Consider $\mathscr{P} = \{\mathbf{x}_i\}_{i=0}^{n-1}$ and $\mathscr{P}' = \{\mathbf{x}'_i\}_{i=0}^{n-1}$ two designs where $(\mathbf{x}_i, \mathbf{x}'_i) \overset{\text{iid}}{\sim} \mathscr{U}([0,1]^{2d})$. One way to estimate the two quantities (2) and (3) is via:

$$\widehat{\underline{\tau}}_u^2 = \frac{1}{n} \sum_{i=0}^{n-1} \left(f(\mathbf{x}_{i,u} : \mathbf{x}'_{i,-u}) - f(\mathbf{x}'_i)\right) f(\mathbf{x}_i), \tag{5}$$

$$\widehat{\overline{\tau}}_u^2 = \frac{1}{2n} \sum_{i=0}^{n-1} (f(\mathbf{x}'_i) - f(\mathbf{x}_{i,u} : \mathbf{x}'_{i,-u}))^2, \qquad u \in \mathscr{D}, \tag{6}$$

using for σ^2:

$$\widehat{\sigma}^2 = \frac{1}{n-1}\sum_{i=0}^{n-1}(f(\mathbf{x}_i)-\widehat{\mu})^2, \text{ with } \widehat{\mu} = \frac{1}{n}\sum_{i=0}^{n-1} f(\mathbf{x}_i). \quad (7)$$

Equation (7) can be improved if we use the $2n$ evaluations $f(\mathbf{x}_i)$ and $f(\mathbf{x}'_i)$. While this would be an important improvement to estimate the indices' denominator, the error construction described in Section 3 would require additional computations. Because of these new computations in the algorithm, the additional benefit of using $2n$ evaluations could become more costly than beneficial.

The Sobol' indices estimators are:

$$\widehat{\underline{S}}_u = \widehat{\underline{\tau}}^2_u/\widehat{\sigma}^2, \qquad \widehat{\overline{S}}_u = \widehat{\overline{\tau}}^2_u/\widehat{\sigma}^2. \quad (8)$$

Based on equation (8), the estimation of a single pair $(\widehat{\underline{S}}_u, \widehat{\overline{S}}_u)$ requires $3n$ evaluations of the model f. Thus, for all first order and total effect indices, one would need $3nd$ model evaluations. Using a combinatorial formalism, in [18] Saltelli proposes the following estimation strategy:

Theorem 1 *The $d+2$ designs $\{\mathbf{x}_{i,u} : \mathbf{x}'_{i,-u}\}_{i=0}^{n-1}$ constructed for $u \in \{\varnothing, \{1\}, \ldots, \{d\}, \mathscr{D}\}$ allow to estimate all first-order and total effect Sobol' indices at a cost of $n(d+2)$ evaluations of the model.*

The main idea of the theorem is that there is no need to reevaluate $f(\mathbf{x}_i)$ and $f(\mathbf{x}'_i)$ for each u. Hence, we can simply evaluate $f(\mathbf{x}_i)$ n times, $f(\mathbf{x}'_i)$ n times, and $f(\mathbf{x}_{i,u} : \mathbf{x}'_{i,-u})$ nd times, which accounts for the $n(d+2)$ evaluations.

The $d+2$ designs of Theorem 1 are obtained by substituting columns of $\mathscr{P}$ for columns of $\mathscr{P}'$ according to u. While elegant, this approach requires a number of model evaluations that grows linearly with respect to the input space dimension.

A more efficient alternative to evaluate all first-order indices was proposed in [13] and only requires $2n$ model evaluations. This alternative relies on the construction of two replicated designs. The notion of replicated designs was first introduced by McKay through his replicated Latin Hypercubes in [14]. In order to apply this definition to other types of points, we use the generalization from [4].

Definition 1 Let $\mathscr{P} = \{\mathbf{x}_i\}_{i=0}^{n-1}$ and $\mathscr{P}' = \{\mathbf{x}'_i\}_{i=0}^{n-1}$ be two point sets in $[0,1]^d$. In these sets, all points $\mathbf{x}_i$ (resp. $\mathbf{x}'_i$) are coordinate-wise different, i.e. for all $(i_1, i_2) \in \{0, \ldots, n-1\}^2$ such that $i_1 \neq i_2$:

$$x_{i_1,j} \neq x_{i_2,j}, \qquad \text{for any } j = 1, \ldots, d.$$

Let $\mathscr{P}^u = \{\mathbf{x}_{i,u}\}_{i=0}^{n-1}$ (resp. $\mathscr{P}'^u$), $u \subsetneq \mathscr{D}$, denote the subset of dimensions of $\mathscr{P}$ (resp. $\mathscr{P}'$) indexed by u. We say that $\mathscr{P}$ and $\mathscr{P}'$ are two replicated designs of order $a \in \{1, \ldots, d-1\}$ if for any $u \subsetneq \mathscr{D}$ such that $|u| = a$, $\mathscr{P}^u$ and $\mathscr{P}'^u$ are the same point set in $[0,1]^a$. We define by π_u the permutation that rearranges the rows of $\mathscr{P}'^u$ into $\mathscr{P}^u$ and exclude the trivial case $\mathbf{x}_i = \mathbf{x}'_i$ for all $i \in \{0, \ldots, n-1\}$.

The method introduced in [13] allows to estimate all first-order Sobol' indices with only two replicated designs of order 1. The key point of this method is to use the permutations resulting from the structure of the two replicated designs to mimic the hybrid points in equation (5).

More precisely, let $\mathscr{P} = \{\mathbf{x}_i\}_{i=0}^{n-1}$ and $\mathscr{P}' = \{\mathbf{x}'_i\}_{i=0}^{n-1}$ be two replicated designs of order 1. Denote by $\{y_i\}_{i=0}^{n-1} = \{f(\mathbf{x}_i)\}_{i=0}^{n-1}$ and $\{y'_i\}_{i=0}^{n-1} = \{f(\mathbf{x}'_i)\}_{i=0}^{n-1}$ the two sets of model evaluations obtained with $\mathscr{P}$ and $\mathscr{P}'$. From Definition 1, we know that $\mathbf{x}'_{\pi_u(i),u} = \mathbf{x}_{i,u}$. Then,

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

Hence, each $\underline{\tau}^2_u$ can be estimated via formula (5) by using $y'_{\pi_u(i)}$ instead of $f(\mathbf{x}_{i,u} : \mathbf{x}'_{i,-u})$ without requiring further model evaluations for each u. This estimation method has been studied deeply and generalized in Tissot and Prieur [21] to the case of closed second-order indices. In the following we will refer to this method as the replication procedure.

2.3 Towards a reliable estimation

The aim of this article is to propose a sequential procedure to estimate first-order and total effect Sobol' indices. A practical problem concerning the estimation of these indices is how large to choose the number of evaluations to ensure that Sobol' estimates are accurate enough. Asymptotic results show that Sobol' estimates are normally distributed ([9, Proposition 2.2], [21, Proposition 3.5]). As a consequence, errors can be estimated through confidence intervals. However, these error estimates are only guaranteed asymptotically as the number of model evaluations goes to infinity.

Additional sequential procedures are the replicated procedure and McKay's procedure respectively proposed in [3] and [22]. Nevertheless, in those two cases, the stopping criterion is a purely empirical quantity of interest, built directly upon the estimates. Such stopping criteria often involve hyper-parameters that are difficult to tweak but more importantly, fail to guarantee any error bound on the estimates.

Our sequential procedure stands apart from others since it proposes a robust stopping criterion, not costly to compute. This criterion is an error bound based on the Walsh series decomposition of the integrands in (2), (3) and (4), and exploits the group properties of digital nets. As such, our procedure relies on an iterative construction of Sobol' sequences. This construction is performed accordingly to the multiplicative approach presented in [4].

The description of the error bound is introduced in the following section and our sequential procedure is detailed in Section 4.

3 Reliable error bound for Sobol' indices

We start by reviewing the construction of the error bound proposed in [5] for the estimation of d-dimensional integrals. Then, we present an extension of this error bound for normalized Sobol' indices. This extension is built upon the integral formula of a Sobol' index.

3.1 Reliable integral estimation using digital sequences

We will assume that we have an embedded sequence of digital nets in $[0,1]^d$, base b and dimension d as described in [5, Sec. 2-3],

$$\mathscr{P}_0 = \{\mathbf{0}\} \subset \cdots \subset \mathscr{P}_m = \{\mathbf{x}_i\}_{i=0}^{b^m-1} \subset \cdots \subset \mathscr{P}_\infty = \{\mathbf{x}_i\}_{i=0}^{\infty}. \quad (9)$$

The Sobol' sequence is an example of a digital net in base two satisfying (9), which in dimension one corresponds to: $\mathscr{P}_0 = \{0\}$, $\mathscr{P}_1 = \{0, 0.5\}$, $\mathscr{P}_2 = \{0, 0.5, 0.25, 0.75\}$, $\mathscr{P}_3 = \{0, 0.5, 0.25, 0.75, 0.125, 0.625, 0.375, 0.875\}$,...

For this sequence of digital nets, each $\mathscr{P}_m$ has a group structure under the digitwise addition:

$$\mathbf{x} \oplus \mathbf{t} = \left(\sum_{\ell=1}^{\infty} [(x_{j\ell} + t_{j\ell}) \bmod b] b^{-\ell} \pmod 1 \right)_{j=1}^{d},$$

where $x_{j\ell}$ and $t_{j\ell}$ are the b-adic decompositions of the j^{th} component of points $\mathbf{x}$ and $\mathbf{t}$, i.e.

$$x_j = \sum_{\ell=1}^{\infty} x_{j\ell} b^{-\ell}, \qquad t_j = \sum_{\ell=1}^{\infty} t_{j\ell} b^{-\ell}.$$

For $b = 2$, the digitwise addition is equivalent to the XOR operation.

In addition, we consider the *wavenumber* space of non-negative integers $\mathbb{N}_0^d$. These non-negative integers will index the frequencies in which we decompose our integrand as a Walsh series. The space $\mathbb{N}_0^d$ is also a group under the digitwise addition:

$$\mathbf{k} \oplus \mathbf{l} = \left(\sum_{\ell=0}^{\infty} [(k_{j\ell} + l_{j\ell}) \bmod b] b^{\ell} \right)_{j=1}^{d},$$

where $k_{j\ell}$ and $l_{j\ell}$ are the b-adic decompositions of the j^{th} components,

$$k_j = \sum_{\ell=0}^{\infty} k_{j\ell} b^{\ell}, \qquad l_j = \sum_{\ell=0}^{\infty} l_{j\ell} b^{\ell}.$$

To relate the group structure of $\mathscr{P}_m$ with the integration error, we introduce the *dual net* which establishes the link between any digital net and the *wavenumber* space. A dual net $\mathscr{P}_m^\perp$ is

$$\mathscr{P}_m^\perp = \{\mathbf{k} \in \mathbb{N}_0^d : \langle \mathbf{k}, \mathbf{x} \rangle = 0, \text{ for all } \mathbf{x} \in \mathscr{P}_m\},$$

$$\langle \mathbf{k}, \mathbf{x} \rangle = \left(\sum_{j=1}^{d} \sum_{\ell=0}^{\infty} k_{j\ell} x_{j,\ell+1} \pmod b \right) / b,$$

and inherits the inverted embedded structure (9),

$$\mathscr{P}_0^\perp = \mathbb{N}_0^d \supset \cdots \supset \mathscr{P}_\infty^\perp = \{\mathbf{0}\}. \quad (10)$$

As shown in [5, Sec. 3], the group structure of digital nets guarantees the property below affecting any Walsh basis function $\varphi_{\mathbf{k}}(\mathbf{x}) = \mathrm{e}^{2\pi\sqrt{-1}\langle \mathbf{k}, \mathbf{x} \rangle}$,

$$\frac{1}{b^m} \sum_{\mathbf{x} \in \mathscr{P}_m} \varphi_{\mathbf{k}}(\mathbf{x}) = \begin{cases} 1, & \mathbf{k} \in \mathscr{P}_m^\perp, \\ 0, & \mathbf{k} \notin \mathscr{P}_m^\perp. \end{cases} \quad (11)$$

Therefore, using the Walsh decomposition of $f \in \mathbb{L}^2([0,1]^d)$:

$$f(\mathbf{x}) = \sum_{\mathbf{k} \in \mathbb{N}_0^d} \hat{f}_{\mathbf{k}} \varphi_{\mathbf{k}}(\mathbf{x}),$$

and defining the value of the integral,

$$I = \int_{[0,1]^d} f(\mathbf{x}) \, d\mathbf{x},$$

property (11) leads to

$$\begin{aligned} \left| I - \frac{1}{b^m} \sum_{\mathbf{x} \in \mathscr{P}_m} f(\mathbf{x}) \right| &= \left| \hat{f}_{\mathbf{0}} - \frac{1}{b^m} \sum_{\mathbf{x} \in \mathscr{P}_m} \sum_{\mathbf{k} \in \mathbb{N}_0^d} \hat{f}_{\mathbf{k}} \varphi_{\mathbf{k}}(\mathbf{x}) \right|, \\ &= \left| \sum_{\mathbf{k} \in \mathscr{P}_m^\perp \setminus \{\mathbf{0}\}} \hat{f}_{\mathbf{k}} \right| \\ &\leqslant \sum_{\mathbf{k} \in \mathscr{P}_m^\perp \setminus \{\mathbf{0}\}} \left| \hat{f}_{\mathbf{k}} \right|. \end{aligned} \quad (12)$$

Based on the size of $\left|\hat{f}_{\mathbf{k}}\right|$ and the structure of dual nets (10), in [5, Sec. 4.1] we proposed an ordering of the *wavenumbers* $\tilde{\mathbf{k}}(\cdot) : \mathbb{N}_0 \to \mathbb{N}_0^d$. This ordering $\tilde{\mathbf{k}}$ is a one-to-one and onto mapping between $\mathbb{N}_0$ and $\mathbb{N}_0^d$. Thus, we can identify each $\mathbf{k} \in \mathbb{N}_0^d$ with one $\kappa \in \mathbb{N}_0$ such that $\tilde{\mathbf{k}}(\kappa) = \mathbf{k}$. The ordering is not unique and one should choose it such that large values of κ are mapped to smaller values of $\left|\hat{f}_{\tilde{\mathbf{k}}(\kappa)}\right|$. It also ensures that $\mathscr{P}_m^\perp \setminus \{\mathbf{0}\} = \{\tilde{\mathbf{k}}(\lambda b^m)\}_{\lambda=1}^{\infty}$. If we identify $\hat{f}_\kappa = \hat{f}_{\tilde{\mathbf{k}}(\kappa)}$, the error bound (12) becomes,

$$\left| I - \frac{1}{b^m} \sum_{\mathbf{x} \in \mathscr{P}_m} f(\mathbf{x}) \right| \leqslant \sum_{\lambda=1}^{\infty} \left| \hat{f}_{\lambda b^m} \right|. \quad (13)$$

The use of the error bound (13) to design an automatic algorithm requires the knowledge of the Walsh coefficients. To avoid this assumption, we will estimate them via the fast transform obtained using the precomputed function values already used to estimate the mean. We will refer to the discrete coefficients as $\widetilde{f}_{m,\kappa}$,

$$\widetilde{f}_{m,\kappa} = \widetilde{f}_{m,\tilde{\mathbf{k}}(\kappa)} = \frac{1}{b^m} \sum_{\mathbf{x} \in \mathscr{P}_m} f(\mathbf{x}) \overline{\varphi_{\tilde{\mathbf{k}}(\kappa)}(\mathbf{x})}.$$

As shown in [5, Sec. 3], the error of estimating the true coefficients using the discrete coefficients can be measured,

$$\widetilde{f}_{m,\kappa} = \hat{f}_\kappa + \sum_{\lambda=1}^{\infty} \hat{f}_{\kappa+\lambda b^m}, \qquad \text{for all } \kappa \in \mathbb{N}_0. \quad (14)$$

However, since there are at most b^m distinct values of $\widetilde{f}_{m,\kappa}$, we require some assumptions on the decay rate of $\hat{f}_\kappa$ to transform (13) into a new error bound in terms of the discrete coefficients.

For $\ell, m \in \mathbb{N}_0$ and $\ell \leqslant m$ we introduce the following notation,

$$S_m(f) = \sum_{\kappa=\lfloor b^{m-1} \rfloor}^{b^m-1} \left|\hat{f}_\kappa\right|, \ \widehat{S}_{\ell,m}(f) = \sum_{\kappa=\lfloor b^{\ell-1} \rfloor}^{b^\ell-1} \sum_{\lambda=1}^{\infty} \left|\hat{f}_{\kappa+\lambda b^m}\right|,$$

$$\breve{S}_m(f) = \widehat{S}_{0,m}(f) + \cdots + \widehat{S}_{m,m}(f) = \sum_{\kappa=b^m}^{\infty} \left|\hat{f}_\kappa\right|,$$

$$\widetilde{S}_{\ell,m}(f) = \sum_{\kappa=\lfloor b^{\ell-1} \rfloor}^{b^\ell-1} \left|\widetilde{f}_{m,\kappa}\right|.$$

The sums $S_m(f)$, $\widehat{S}_{\ell,m}(f)$, $\breve{S}_m(f)$, and $\widetilde{S}_{\ell,m}(f)$ are different from the normalized Sobol' indices $\underline{S}_u$ and $\overline{S}_u$. Unfortunately, the notation in articles [5,6,10] coincides and should not be confused with the normalized Sobol' indices notation.

Among these sums, one should notice that $\widehat{S}_{0,m}(f)$ corresponds to the error bound appearing in (13). Thus, $\breve{S}_m(f)$ is an infinite sum of Walsh coefficients that contain the error bound coefficients. To have a control on the decay rate of the coefficients, we also define the finite sum of true coefficients $S_m(f)$. Note that from these sums, we can only observe $\widetilde{S}_{\ell,m}(f)$.

Finally, we define the set of functions $\mathscr{C}$,

$$\mathscr{C} := \{f \in \mathbb{L}^2([0,1]^d) : \widehat{S}_{\ell,m}(f) \leqslant \widehat{\omega}(m-\ell)\breve{S}_m(f), \ \ell \leqslant m, \\ \breve{S}_m(f) \leqslant \mathring{\omega}(m-\ell)S_\ell(f), \ \ell_* \leqslant \ell \leqslant m\}. \quad (15)$$

for a fixed $\ell_* \in \mathbb{N}$, and $\widehat{\omega}$ and $\mathring{\omega}$ two non-negative valued functions with $\lim_{m\to\infty} \mathring{\omega}(m) = 0$. The decay rate assumptions on the Walsh coefficients are encoded in $\mathscr{C}$ and controlled by $\widehat{\omega}$ and $\mathring{\omega}$. First, we assume that $\breve{S}_m(f)$ bounds $\widehat{S}_{\ell,m}(f)$ through $\widehat{\omega}$, in particular it bounds $\widehat{S}_{0,m}(f)$. This means that we can use $\breve{S}_m(f)$ as an indicator of the error bound. Then, we also need $S_\ell(f)$ to bound $\breve{S}_m(f)$ which helps transforming the infinite sum into a finite sum. In this step, we are assuming that if $S_\ell(f)$ is small enough, we expect the high frequency coefficients, i.e. $\breve{S}_m(f)$, to also be small. By defining $r = m - \ell$ with $\widehat{\omega}(r)\mathring{\omega}(r) < 1$ and $r \in \mathbb{N}$, one may intuitively see r as the distance between $S_\ell(f)$ and $\breve{S}_m(f)$. One only needs to choose the appropriate r: larger values of r will imply a smaller error bound but more dependence on smaller Walsh coefficients. Finally, we can write the error bound in terms of $\widetilde{S}_{\ell,m}(f)$ instead of $\breve{S}_m(f)$ by using (14). With this reasoning, in [5, Sec. 4.2] we showed that for any $f \in \mathscr{C}$,

$$\left| I - \frac{1}{b^m} \sum_{\mathbf{x}\in\mathscr{P}_m} f(\mathbf{x}) \right| \leqslant \widetilde{S}_{m-r,m}(f) \underbrace{\frac{\widehat{\omega}(m)\mathring{\omega}(r)}{1-\widehat{\omega}(r)\mathring{\omega}(r)}}_{\mathfrak{C}(m)} = \varepsilon_{\widehat{I}}, \quad (16)$$

where one may increase m until the error bound $\varepsilon_{\widehat{I}}$ is small enough.

Details concerning the algorithm, the mapping of the *wavenumber* space, or the meaning and properties of $\mathscr{C}$, are provided in [5].

For our problem, only Sobol' sequences [19] have been considered. Their major interest comes from their fast and easy implementation. Further details concerning Sobol' sequences can be found in [12,15].

3.2 Extension to Sobol' indices

In this section we will extend the definition of the error bound (16) to Sobol' indices. To achieve this goal, we consider the two integral formulas of the first-order and total effect Sobol' indices with $|u| = 1$:

$$\underline{S}_u(\mathbf{I}) = \frac{\int_{[0,1]^{2d}} (f(\mathbf{x}_u : \mathbf{x}'_{-u}) - f(\mathbf{x}')) f(\mathbf{x}) d\mathbf{x} d\mathbf{x}'}{\int_{[0,1]^d} f(\mathbf{x})^2 d\mathbf{x} - \left(\int_{[0,1]^d} f(\mathbf{x}) d\mathbf{x}\right)^2},$$

$$\underline{S}_u(\mathbf{I}) = \frac{I_1}{I_3 - (I_4)^2},$$

$$\overline{S}_u(\mathbf{I}) = \frac{\frac{1}{2}\int_{[0,1]^{d+1}} (f(\mathbf{x}') - f(\mathbf{x}_u : \mathbf{x}'_{-u}))^2 d\mathbf{x}_u d\mathbf{x}'}{\int_{[0,1]^d} f(\mathbf{x})^2 d\mathbf{x} - \left(\int_{[0,1]^d} f(\mathbf{x}) d\mathbf{x}\right)^2},$$

$$\overline{S}_u(\mathbf{I}) = \frac{I_2}{I_3 - (I_4)^2},$$

where $\mathbf{I} = (I_1, I_2, I_3, I_4)$ is a vector of integral values. Indices $\underline{S}_u(\mathbf{I})$ and $\overline{S}_u(\mathbf{I})$ are defined as functions over the vector $\mathbf{I}$. If we estimate $\mathbf{I}$ by $\widehat{\mathbf{I}}$ with known error bounds $\varepsilon_{\widehat{\mathbf{I}}} = (\varepsilon_{\widehat{I}_1}, \varepsilon_{\widehat{I}_2}, \varepsilon_{\widehat{I}_3}, \varepsilon_{\widehat{I}_4})$ according to (16), we know that $\mathbf{I} \in B_{\varepsilon_{\widehat{\mathbf{I}}}}(\widehat{\mathbf{I}}) = [\widehat{\mathbf{I}} - \varepsilon_{\widehat{\mathbf{I}}}, \widehat{\mathbf{I}} + \varepsilon_{\widehat{\mathbf{I}}}]$.

Then, as an alternative to the common Sobol' indices estimators (8), we can define the following two estimators with their respective error bounds:

$$\widehat{\underline{S}}_u = \frac{1}{2}\left(\min\left(\max_{\mathbf{I}\in B_{\varepsilon_{\widehat{\mathbf{I}}}}(\widehat{\mathbf{I}})} \underline{S}_u(\mathbf{I}), 1\right) + \max\left(\min_{\mathbf{I}\in B_{\varepsilon_{\widehat{\mathbf{I}}}}(\widehat{\mathbf{I}})} \underline{S}_u(\mathbf{I}), 0\right)\right)$$

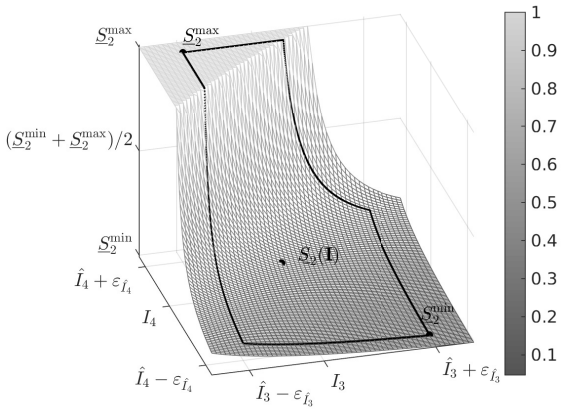
$$\varepsilon_{\widehat{\underline{S}}_u} = \frac{1}{2}\left(\min\left(\max_{\mathbf{I}\in B_{\varepsilon_{\widehat{\mathbf{I}}}}(\widehat{\mathbf{I}})} \underline{S}_u(\mathbf{I}), 1\right) - \max\left(\min_{\mathbf{I}\in B_{\varepsilon_{\widehat{\mathbf{I}}}}(\widehat{\mathbf{I}})} \underline{S}_u(\mathbf{I}), 0\right)\right) \quad (17)$$

and,

$$\widehat{\overline{S}}_u = \frac{1}{2}\left(\min\left(\max_{\mathbf{I}\in B_{\varepsilon_{\widehat{\mathbf{I}}}}(\widehat{\mathbf{I}})} \overline{S}_u(\mathbf{I}), 1\right) + \max\left(\min_{\mathbf{I}\in B_{\varepsilon_{\widehat{\mathbf{I}}}}(\widehat{\mathbf{I}})} \overline{S}_u(\mathbf{I}), 0\right)\right)$$

$$\varepsilon_{\widehat{\overline{S}}_u} = \frac{1}{2}\left(\min\left(\max_{\mathbf{I}\in B_{\varepsilon_{\widehat{\mathbf{I}}}}(\widehat{\mathbf{I}})} \overline{S}_u(\mathbf{I}), 1\right) - \max\left(\min_{\mathbf{I}\in B_{\varepsilon_{\widehat{\mathbf{I}}}}(\widehat{\mathbf{I}})} \overline{S}_u(\mathbf{I}), 0\right)\right) \quad (18)$$

Fig. 1 The delimited region in the figure represents the possible values of $\underline{S}_2$ for $\mathbf{I} \in B_{(0,0,0.05,0.1)}(\hat{\mathbf{I}})$ (Bratley *et al.* function). There, $\underline{S}_2^{\min} = \max\left(\min_{\mathbf{I}\in B_{\mathfrak{E}_\mathbf{I}}(\hat{\mathbf{I}})} \underline{S}_2(\mathbf{I}), 0\right)$, $\underline{S}_2^{\max} = \min\left(\max_{\mathbf{I}\in B_{\mathfrak{E}_\mathbf{I}}(\hat{\mathbf{I}})} \underline{S}_2(\mathbf{I}), 1\right)$, and $\hat{\underline{S}}_2 = (\underline{S}_2^{\min} + \underline{S}_2^{\max})/2$.



Because numerator and denominator are both known to be positive, maximizing $\underline{S}_u(\mathbf{I})$ (resp. $\overline{S}_u(\mathbf{I})$) is done through maximizing the numerator I_1 (resp. I_2) and minimizing the denominator $I_3 - I_4^2$. Analogously, to minimize $\underline{S}_u(\mathbf{I})$ (resp. $\overline{S}_u(\mathbf{I})$) one minimizes the numerator I_1 (resp. I_2) and maximizes the denominator $I_3 - I_4^2$. As an example, Figure 1 illustrates the region of possible values of $\underline{S}_2(\mathbf{I})$ given the true value of I_1 for the test function of Bratley *et al.* [1]. This function is further described in Section 5.

By construction, under the assumption that each integrand in $\underline{S}_u$ and $\overline{S}_u$ lies inside $\mathscr{C}$, these new estimators satisfy:

$$\underline{S}_u \in \left[\hat{\underline{S}}_u - \varepsilon_{\hat{\underline{S}}_u}, \hat{\underline{S}}_u + \varepsilon_{\hat{\underline{S}}_u}\right], \qquad \overline{S}_u \in \left[\hat{\overline{S}}_u - \varepsilon_{\hat{\overline{S}}_u}, \hat{\overline{S}}_u + \varepsilon_{\hat{\overline{S}}_u}\right].$$

Because we do not assume the knowledge of the Walsh coefficients, it is hard to verify whether all the integrands lie in $\mathscr{C}$. Nevertheless, some data-based necessary conditions are provided in [6]. These conditions can be used to automatically enlarge the cone according to each integrand. For the rest of the article, we will consider $\hat{\underline{S}}_u$ and $\hat{\overline{S}}_u$ as defined in formulas (17) and (18).

4 Sequential estimation procedure

The sequential estimation procedure we propose combines error bounds $\varepsilon_{\hat{\underline{S}}_u}$ and $\varepsilon_{\hat{\overline{S}}_u}$ presented in the previous section with either one of the two estimation strategies of Section 2.2: Saltelli's strategy and the replication procedure.

We start by detailing our procedure under the form of an algorithm. Then, we discuss a possible improvement by considering a new estimator introduced in [17] for the estimation of first-order indices.

It is important to note that the function evaluations performed to estimate the Sobol' indices are also used to compute the discrete Walsh coefficients. As a result, no additional function evaluations are required to compute the error bound. The only computation cost that could be expensive is the fast Walsh transform. However, the fast transform cost becomes inexpensive when dealing with time consuming models.

4.1 Sequential algorithm and cost

Algorithm 1 summarizes the main steps of our sequential procedure. First, one must fix the tolerance $\varepsilon > 0$ at which Sobol' indices must be estimated, and set $m = \ell_* + r$, where ℓ_* and r are the two hyper-parameters defined in (15). The choice of ℓ_* must be large enough to ensure that each integrand of $\underline{S}_u$ and $\overline{S}_u$ (Section 3.2) is in $\mathscr{C}$ (see (15)). Parameter r should also be chosen carefully: larger values of r will imply a smaller error bound and more dependence on smaller Walsh coefficients, while smaller of values of r might result in aliasing errors.

Then, one must construct the two designs $\mathscr{P}_m = \{\mathbf{x}_i\}_{i=0}^{2^m-1}$ and $\mathscr{P}'_m = \{\mathbf{x}'_i\}_{i=0}^{2^m-1}$ at Step 5 according to the multiplicative approach detailed in [4]. This approach iteratively constructs a $2d$-dimensional Sobol' sequence. Then, it assigns its first d coordinates to $\mathscr{P}_m$ and its last d coordinates to $\mathscr{P}'_m$. The $2d$-dimensional Sobol' sequence is generated based on the direction numbers found in [11]. These direction numbers optimize the two-dimensional projections of the Sobol' sequence. Although this is the authors choice, one may choose any other Sobol' construction for $\mathscr{P}_m$ and $\mathscr{P}'_m$ as long as the $2d$ dimensions are each generated with different primitive polynomials. In addition, $\mathscr{P}_m$ and $\mathscr{P}'_m$ are also independently scrambled using Owen's scrambling [7, 16].

The sets $\mathscr{P}_m$ and $\mathscr{P}'_m$ can be used with Saltelli's strategy to estimate all first-order indices and total effect Sobol' indices. This option is referred as Variant *A* in Algorithm 1.

Alternatively, $\mathscr{P}_m$ and $\mathscr{P}'_m$ can be used with the replication procedure to estimate all first-order Sobol' indices. This option is referred as Variant *B* in Algorithm 1. In this case, the scrambling applied to both designs must be identical to ensure that $\mathscr{P}_m$ and $\mathscr{P}'_m$ are replicated designs of order one.

In both cases we always check if the respective error bounds $\varepsilon_{\hat{\underline{S}}_u}$ and $\varepsilon_{\hat{\overline{S}}_u}$ are lower than the tolerance ε. For Variant *A* the stopping criterion is $\varepsilon_{\hat{\underline{S}}_u} \leqslant \varepsilon$ and $\varepsilon_{\hat{\overline{S}}_u} \leqslant \varepsilon$ for all $u \in \mathscr{D}$. For Variant *B* it is $\varepsilon_{\hat{\underline{S}}_u} \leqslant \varepsilon$ for all $u \in \mathscr{D}$.

If the stopping criterion is satisfied, the algorithm stops and Sobol' estimates are returned. Otherwise, m is incremented by one to perform a new estimation.

The cost of our algorithm, in terms of model evaluations, varies whether Variant *A* or Variant *B* is selected. To discuss

Algorithm 1 Sequential estimation of Sobol' indices

choose $\varepsilon > 0$
set: $m \leftarrow \ell_* + r$
$bool \leftarrow false$
while $!bool$ **do**
  $\mathscr{P}_m \leftarrow \mathscr{P}_{m-1} \cup B_m$
  $\mathscr{P}'_m \leftarrow \mathscr{P}'_{m-1} \cup B'_m$
  for $u = 1, \dots, d$ **do**
    if Variant A **then**
      if $!bool_u$ **then**
        compute $\widehat{\underline{S}}_u$ and $\widehat{\overline{S}}_u$ with formulas (17) and (18), and Saltelli's strategy
        $bool_u \leftarrow \varepsilon_{\widehat{\underline{S}}_u} \leqslant \varepsilon \;\&\; \varepsilon_{\widehat{\overline{S}}_u} \leqslant \varepsilon$
        $m_u \leftarrow m$
      end if
    end if
    if Variant B **then**
      if $!bool_u$ **then**
        estimate $\widehat{\underline{S}}_u$ with formula (17) and the replication procedure
        $bool_u \leftarrow \varepsilon_{\widehat{\underline{S}}_u} \leqslant \varepsilon$
        $m_u \leftarrow m$
      end if
    end if
  end for
  $bool \leftarrow \forall u : \; bool_u$
  $m \leftarrow m + 1$
end while
return the Sobol' estimates.

this cost we note by $m^\star$ the ending iteration. If Variant A is selected, the cost of our algorithm is:

$$\sum_{u \in \mathscr{D}} 2^{m_u} + 2 \times 2^{m^\star}, \qquad m^\star = \max_{u \in \mathscr{D}} m_u,$$

where:

- 2^{m_u} is the number of evaluations $f(\mathbf{x}_{i,u} : \mathbf{x}'_{i,-u})$ used to estimate both the first-order index $\underline{S}_u$ and the total effect index $\overline{S}_u$,
- $2 \times 2^{m^\star}$ is the number of evaluations $f(\mathbf{x}_i)$ and $f(\mathbf{x}'_i)$ used in the estimation of each first-order and total effect indices.

If all m_u are equal, the cost of Variant A becomes $2^{m^\star}(d+2)$ and we recover the cost specified in Theorem 1 with $n = 2^{m^\star}$. If Variant B is selected, the cost of our algorithm equals $2 \times 2^{m^\star}$. This cost corresponds to the one of the replication procedure introduced in Section 2.2, where $2n = 2 \times 2^{m^\star}$ independent of d.

4.2 Improvement

When $\underline{S}_u$ is small, it usually becomes harder to estimate. For this reason, we consider the use of a new estimator to evaluate small first-order Sobol' indices in Variant A. This estimator called "Correlation 2" has been introduced by Owen in [17]. In this article, he discussed and highlighted the efficiency of "Correlation 2" when estimating small first-order indices. Our aim is to show that the use of "Correlation 2" in Variant A improves the estimation of small first-order indices while potentially reducing the total number of model evaluations required. This new estimator is,

$$\widehat{\underline{\tau}}^2_u = \frac{1}{n} \sum_{i=0}^{n-1} (f(\mathbf{x}_i) - f(\mathbf{z}_{i,u} : \mathbf{x}_{i,-u}))(f(\mathbf{x}_{i,u} : \mathbf{x}'_{i,-u}) - f(\mathbf{x}'_i)).$$

As proposed by Owen in [17], the sample points are $(\mathbf{x}_i, \mathbf{x}'_i, \mathbf{z}_i) \sim \mathscr{U}([0,1])^{3d}$. For our algorithm, we extend Owen's estimator by replacing the uniform points with a scrambled Sobol' sequence in dimension $3d$. In either case, this estimator requires an additional set of n model evaluations to estimate $\underline{\tau}^2_u$.

We discuss below the potential improvement brought by using "Correlation 2" in Variant A. The idea is to replace the current estimator (5) by "Correlation 2" for each small first-order index.

Assume that the number of small first-order indices is known and equals γ. We denote by $u_1, \dots, u_\gamma$ the indices of the corresponding inputs and $\Gamma = \{1, \dots, \gamma\}$. The cost of Variant A including "Correlation 2" becomes,

$$\sum_{j \in \Gamma} 2^{m''_{u_j}} + \sum_{j \in \Gamma} 2^{m'_{u_j}} + \sum_{j \in \mathscr{D} \setminus \Gamma} 2^{m_{u_j}} + 2 \times 2^{m^\star}, \tag{19}$$

where:

- for $j \in \Gamma$, $2^{m''_{u_j}}$ is the number of evaluations $f\left(\mathbf{z}_{i,u_j} : \mathbf{x}_{i,-u_j}\right)$ to estimate $\underline{S}_{u_j}$,
- for $j \in \Gamma$, $2^{m'_{u_j}}$ is the number of evaluations $f\left(\mathbf{x}_{i,u_j} : \mathbf{x}'_{i,-u_j}\right)$ to estimate both $\underline{S}_{u_j}$ and $\overline{S}_{u_j}$,
- likewise, for $j \in \mathscr{D} \setminus \Gamma$, $2^{m_{u_j}}$ is the number of evaluations $f\left(\mathbf{x}_{i,u_j} : \mathbf{x}'_{i,-u_j}\right)$ to estimate both $\underline{S}_{u_j}$ and $\overline{S}_{u_j}$,
- $2 \times 2^{m^\star}$ is the number of evaluations $f(\mathbf{x}_i)$ and $f(\mathbf{x}'_i)$ used in the estimation of each first-order and total effect index.

We recall the cost of Variant A without "Correlation 2",

$$\sum_{j \in \Gamma} 2^{m_{u_j}} + \sum_{j \in \mathscr{D} \setminus \Gamma} 2^{m_{u_j}} + 2 \times 2^{m^\star}. \tag{20}$$

The difference (19) $-$ (20) equals:

$$\sum_{j \in \Gamma} 2^{m_{u_j}} \left(2^{m''_{u_j} - m_{u_j}} + 2^{m'_{u_j} - m_{u_j}} - 1\right) = \sum_{j \in \Gamma} c_j. \tag{21}$$

The sign of (21) indicates whether or not using "Correlation 2" brings an improvement to Variant A. A negative sign would mean an improvement. We distinguish two cases :

1) for $j \in \Gamma$, if the total effect index $\overline{S}_{u_j}$ requires as much or more evaluations than the first-order index $\underline{S}_{u_j}$. Since the total effect estimator is the same, as a consequence we have $m'_{u_j} = m_{u_j}$ and $c_j > 0$.

2) for $j \in \Gamma$, if the total effect index $\overline{S}_{u_j}$ requires less evaluations than the first-order index $\underline{S}_{u_j}$. In this case, if both $m''_{u_j} < m_{u_j}$ and $m'_{u_j} < m_{u_j}$ then $c_j \leqslant 0$.

We assume that the numerator in $\underline{S}_u$ is harder to estimate than the numerator in $\overline{S}_u$. This assumption is tested in the numerical examples presented in Section 5.1 by comparing the number of evaluations required by $\underline{S}_u$ and $\overline{S}_u$.

If this assumption holds, we expect to observe case 2) more often than case 1). Furthermore, in case 2), we expect the two conditions $m''_{u_j} < m_{u_j}$ and $m'_{u_j} < m_{u_j}$ to usually hold as "Correlation 2" is shown to perform better for small first-order indices (*c*.f. [17]).

In practice, one does not know which are the small Sobol' indices $(u_1, \dots, u_\gamma)$. To overcome this issue, we propose the following alternative for Variant *A*. If at the end of the first iteration $\widehat{\underline{S}}_u$ is smaller than a threshold (in our case 0.1, as suggested by Owen), then the estimator (5) is switched to "Correlation 2" for this particular u. In this case, a third Sobol' sequence $\mathscr{P}''_m = \{\mathbf{z}_i\}_{i=0}^{2^m-1}$ is constructed to obtain the corresponding evaluations $f(\mathbf{z}_{i,u} : \mathbf{x}_{i,-u})$. $\mathscr{P}''$ can be generated assigning and scrambling the last d coordinates of a $3d$-dimensional Sobol' sequence.

5 Applications

We illustrate our sequential estimation procedure with two classical test functions and one application. In each case, Sobol' indices are estimated with the following three variants:

- Variant *A*.*a* as Variant *A* without using "Correlation 2".
- Variant *A*.*b* as Variant *A* using "Correlation 2".
- Variant *B*.

The threshold to decide whether or not a first-order index is small is set to 0.1.

For the two test functions, the results of the three variants are compared based on the true estimation errors. These errors correspond to the absolute difference between the true values and their estimates:

$$\delta_{\underline{S}_u} = \left| \underline{S}_u - \widehat{\underline{S}}_u \right|, \qquad \delta_{\overline{S}_u} = \left| \overline{S}_u - \widehat{\overline{S}}_u \right|.$$

The true values of Sobol' indices are estimated with a precision of 10 digits. For clarity purposes, in the following tables all results are rounded to 4 digits.

We also compare the total number of evaluations of each variant to verify the assumption in Section 4.2. Results are averaged over 100 repetitions, each computed with different random scramblings. For all repetitions, we fix the tolerance $\varepsilon = 5 \cdot 10^{-3}$, set $\ell_* = 5$, and $r = 4$ (the algorithm starts with 512 Sobol' points). The error bound factor described in (16) is set to $\mathfrak{C}(m) = 10 \times 2^{-m}$.

For these examples we do not know the true Walsh coefficients of the integrands. Indeed, since the mapping $\tilde{\mathbf{k}}$ is chosen heuristically, the cone conditions will also depend on each scrambling. Therefore, we cannot say whether the integrands lie inside the cone. For this reason, we define the failure rates $r_{\delta_{\underline{S}_u}}$ and $r_{\delta_{\overline{S}_u}}$ over the 100 repetitions. These rates are the proportion of the repetitions in which the true errors failed to satisfy $\delta_{\underline{S}_u} \leqslant \varepsilon$ and $\delta_{\overline{S}_u} \leqslant \varepsilon$. When $\delta_{\underline{S}_u} > \varepsilon$ or $\delta_{\overline{S}_u} > \varepsilon$, we can infer that our algorithm parameters that define the cone are not conservative enough and at least one integrand (I_1, I_2, I_3, or I_4) falls outside the cone (15).

5.1 Classical test functions

The two classical test functions considered in this article are a non qMC (quasi-Monte Carlo) friendly version of the g-function introduced by Sobol' [20], and the function introduced by Bratley *et al.* [1]. The idea is to test our method over two categories of functions: additive (Bratley *et al.*) and multiplicative (g-function).

5.1.1 Sobol' g-function

The non qMC friendly version of the g-function is defined as follows:

$$f(\mathbf{x}) = \prod_{j=1}^{d} g_j(x_j), \qquad g_j(x_j) = \frac{|3x_j - 2| + a_j}{1 + a_j}, \; a_j \geqslant 0.$$

In many cases, qMC points are generated in base two. In addition, the derivative $\partial f(\mathbf{x})/\partial x_j$ is discontinuous at $x_j = 2/3$. Since $2/3$ does not have a finite binary representation, $f(\mathbf{x})$ does not benefit from the stratification properties of qMC points as well as the original Sobol' g-function. Each value a_j determines the relative importance of the x_j. When the value of a_j gets closer to zero the variable x_j becomes more influential. For this example, we chose $d = 6$ and $a_1 = 0, a_2 = 0.5, a_3 = 3, a_4 = 9, a_5 = 99$, and $a_6 = 99$.

Table 1 shows the averaged estimation errors obtained with Variant *A*.*a* as well as the averaged total number of evaluations performed. Table 2 shows the same results obtained with Variant *A*.*b*.

The main observation is that both approaches give similar results both in terms of estimation errors, failure rates and averaged total number of evaluations. The use of "Correlation 2" in Variant *A*.*b* to estimate the four small first-order Sobol' indices $\underline{S}_3, \underline{S}_4, \underline{S}_5, \underline{S}_6$ does seem to bring an improvement. In particular, the failure rate for input x_3 is reduced to 0. We draw boxplots of the estimation errors to further investigate the results.

Figure 2 shows boxplots of the 100 estimation errors $\delta_{\underline{S}_u}$ obtained with both Variant *A*.*a* and Variant *A*.*b* for the four

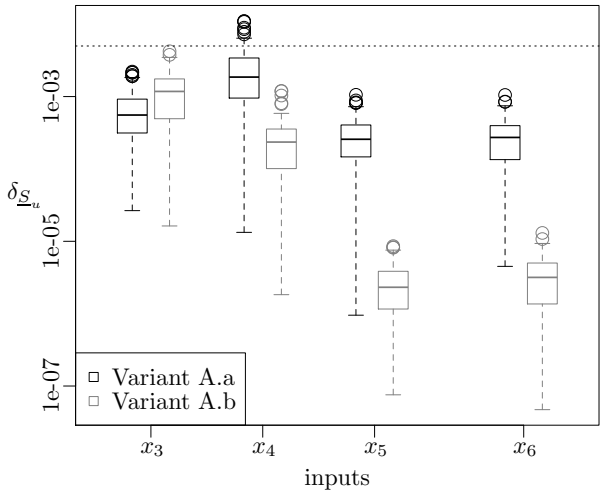
Table 1 Averaged estimation errors $\delta_{\underline{S}_u}$ and $\delta_{\overline{S}_u}$, failure rates $r_{\delta_{\underline{S}_u}}$ and $r_{\delta_{\overline{S}_u}}$, and averaged total number of evaluations for Variant *A.a*.

input	$\underline{S}_u$	$\delta_{\underline{S}_u}$	$r_{\delta_{\underline{S}_u}}$	$\overline{S}_u$	$\delta_{\overline{S}_u}$	$r_{\delta_{\overline{S}_u}}$
x_1	0.6043	0.0005	0	0.7252	0.0001	0
x_2	0.2360	0.0006	0	0.3481	0.0007	0
x_3	0.0286	0.0007	0	0.0483	0.0005	0
x_4	0.0043	0.0025	0.11	0.0075	0.0004	0
x_5	$4\cdot10^{-5}$	0.0003	0	$7\cdot10^{-5}$	$<10^{-4}$	0
x_6	$4\cdot10^{-5}$	0.0003	0	$7\cdot10^{-5}$	$<10^{-4}$	0
Total number of evaluations: 120 638						

Table 2 Averaged estimation errors $\delta_{\underline{S}_u}$ and $\delta_{\overline{S}_u}$, failure rates $r_{\delta_{\underline{S}_u}}$ and $r_{\delta_{\overline{S}_u}}$, and average total number of evaluations for Variant *A.b*.

input	$\underline{S}_u$	$\delta_{\underline{S}_u}$	$r_{\delta_{\underline{S}_u}}$	$\overline{S}_u$	$\delta_{\overline{S}_u}$	$r_{\delta_{\overline{S}_u}}$
x_1	0.6043	0.0005	0	0.7252	0.0001	0
x_2	0.2360	0.0006	0	0.3481	0.0007	0
x_3	0.0286	0.0013	0	0.0483	0.0005	0
x_4	0.0043	0.0003	0	0.0075	0.0004	0
x_5	$4\cdot10^{-5}$	$<10^{-4}$	0	$7\cdot10^{-5}$	$<10^{-4}$	0
x_6	$4\cdot10^{-5}$	$<10^{-4}$	0	$7\cdot10^{-5}$	$<10^{-4}$	0
Total number of evaluations: 120 832						

Fig. 2 Boxplots of estimation errors $\delta_{\underline{S}_u}$ for the four inputs x_3, x_4, x_5, x_6 obtained with both Variant *A.a* and Variant *A.b*. The dashed horizontal line marks the tolerance $\varepsilon = 5\cdot10^{-3}$.



inputs x_3, x_4, x_5, x_6. The dashed horizontal line marks the tolerance $\varepsilon = 5\cdot10^{-3}$.As expected, we observe that the use of "Correlation 2" in Variant *A.b* results in lower estimation errors for these four inputs. The discrepancy observed does not stand out in Table 2 due to its low magnitude (10^{-4} to 10^{-6}).

Table 3 shows the average number of evaluations performed in Variant *A.a* to estimate $\underline{S}_u$ and $\overline{S}_u$. The column *N* indicates the number of times where $\overline{S}_u$ required more evaluations than $\underline{S}_u$. We observe that $\overline{S}_u$ never requires more evaluations than $\underline{S}_u$.

Table 3 Average number of evaluations performed to estimate $\underline{S}_u$ and $\overline{S}_u$ in Variant *A.a*. Column *N* shows the number of times among the 100 repeats where $\overline{S}_u$ required more evaluations than $\underline{S}_u$.

input	$\underline{S}_u$	$\overline{S}_u$	*N*
x_1	32768	32768	0
x_2	16384	16384	0
x_3	4096	2048	0
x_4	830	512	0
x_5	512	512	0
x_6	512	512	0

Table 4 Averaged estimation errors $\delta_{\underline{S}_u}$, failure rates $r_{\delta_{\underline{S}_u}}$, and averaged total number of evaluations for Variant *B*.

input	$\underline{S}_u$	$\delta_{\underline{S}_u}$	$r_{\delta_{\underline{S}_u}}$
x_1	0.6043	0.0005	0
x_2	0.2360	0.0010	0
x_3	0.0286	0.0018	0.02
x_4	0.0043	0.0016	0
x_5	$4\cdot10^{-5}$	0.0034	0
x_6	$4\cdot10^{-5}$	0.0035	0
Total number of evaluations: 65 536			

Table 4 shows the averaged estimation errors $\delta_{\underline{S}_u}$, failure rates $r_{\delta_{\underline{S}_u}}$, and averaged total number of evaluations for Variant *B*. Variant *B* leads to slightly higher estimation errors than those obtained with Variant *A.a* or Variant *A.b*. However, the averaged total number of evaluations is half as large. As such, this approach remains interesting when one wants to estimate only first-order indices.

5.1.2 Bratley et al. function

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

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

The importance of each variable x_j depends on their own rank. More explicitly, x_1 is more influential than x_2 which is respectively more influential than x_3 and so on.

As for the g-function, Tables 5 and 6 show averaged estimation errors, failure rates, and averaged total number of evaluations for Variant *A.a* and Variant *A.b*.

Variant *A.b* gives lower estimation errors and fewer failure rates than Variant *A.a* on all four small first-indices $\underline{S}_3$, $\underline{S}_4, \underline{S}_5$, $\underline{S}_6$ which highlights the good performance of "Correlation 2". The discrepancy is particularly notable for input x_3 where Variant *A.a* reaches a failure rate of 78% against

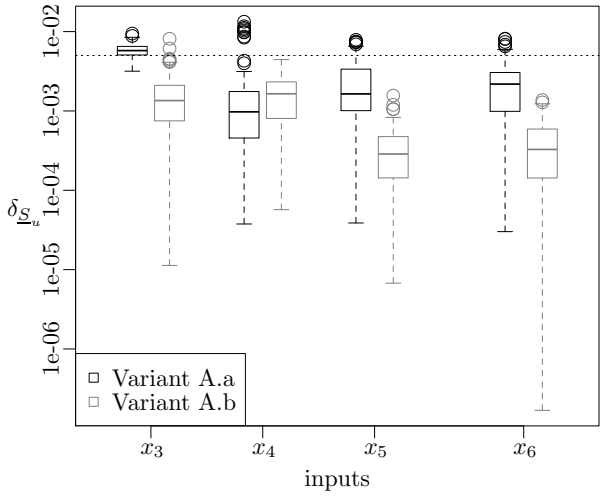
Table 5 Averaged estimation errors $\delta_{\underline{S}_u}$ and $\delta_{\overline{S}_u}$, failure rates $r_{\delta_{\underline{S}_u}}$ and $r_{\delta_{\overline{S}_u}}$, and averaged total number of evaluations for Variant *A.a*.

input	$\underline{S}_u$	$\delta_{\underline{S}_u}$	$r_{\delta_{\underline{S}_u}}$	$\overline{S}_u$	$\delta_{\overline{S}_u}$	$r_{\delta_{\overline{S}_u}}$
x_1	0.6529	0.0005	0	0.7396	0.0002	0.
x_2	0.1791	0.0006	0	0.2659	0.0005	0
x_3	0.0370	0.0058	0.78	0.0764	0.0015	0.01
x_4	0.0133	0.0019	0.09	0.0343	0.0018	0.02
x_5	0.0015	0.0024	0.13	0.0062	0.0016	0.05
x_6	0.0015	0.0023	0.09	0.0062	0.0011	0
Total number of evaluations: 68 404						

Table 6 Averaged estimation errors $\delta_{\underline{S}_u}$ and $\delta_{\overline{S}_u}$, failure rates $r_{\delta_{\underline{S}_u}}$ and $r_{\delta_{\overline{S}_u}}$, and averaged total number of evaluations for Variant *A.b*.

input	$\underline{S}_u$	$\delta_{\underline{S}_u}$	$r_{\delta_{\underline{S}_u}}$	$\overline{S}_u$	$\delta_{\overline{S}_u}$	$r_{\delta_{\overline{S}_u}}$
x_1	0.6529	0.0005	0	0.7396	0.0002	0
x_2	0.1791	0.0006	0	0.2659	0.0005	0
x_3	0.0370	0.0017	0.02	0.0764	0.0015	0.01
x_4	0.0133	0.0017	0	0.0343	0.0018	0.02
x_5	0.0015	0.0003	0	0.0062	0.0016	0.05
x_6	0.0015	0.0004	0	0.0062	0.0011	0
Total number of evaluations: 66 821						

Fig. 3 Boxplots of estimation errors $\delta_{\underline{S}_u}$ for the four inputs x_3, x_4, x_5, x_6 obtained with both Variant *A.a* and Variant *A.b*. The dashed horizontal line marks the tolerance $\varepsilon = 5 \cdot 10^{-3}$.



only 2% for Variant *A.b*. Furthermore, Variant *A.b* requires less evaluations than Variant *A.a*. The boxplots presented in Figure 3 emphasize the latter observations.

Table 7 shows the average number of evaluations performed in Variant *A.a* to estimate $\underline{S}_u$ and $\overline{S}_u$. The column *N* indicates the number of times where $\overline{S}_u$ required more evaluations than $\underline{S}_u$. In this case, we observe that $\overline{S}_u$ requires more evaluations than $\underline{S}_u$ in only 4 of the 100 estimations.

Table 7 Average number of evaluations performed to estimate $\underline{S}_u$ and $\overline{S}_u$ in Variant *A.a*. Column *N* shows the number of times among the 100 repeats where $\overline{S}_u$ required more evaluations than $\underline{S}_u$.

input	$\underline{S}_u$	$\overline{S}_u$	*N*
x_1	16876	16384	0
x_2	8520	8192	0
x_3	4096	2786	0
x_4	3794	1096	4
x_5	635	512	0
x_6	712	512	0

Table 8 Averaged estimation errors $\delta_{\underline{S}_u}$, failure rates $r_{\delta_{\underline{S}_u}}$, and averaged total number of evaluations for Variant *B*.

input	$\underline{S}_u$	$\delta_{\underline{S}_u}$	$r_{\delta_{\underline{S}_u}}$
x_1	0.6529	0.0004	0
x_2	0.1791	0.0006	0
x_3	0.0370	0.0007	0
x_4	0.0133	0.0037	0.25
x_5	0.0015	0.0023	0
x_6	0.0015	0.0025	0
Total number of evaluations: 65 536			

Averaged estimation errors $\delta_{\underline{S}_u}$, failure rates $r_{\delta_{\underline{S}_u}}$, and averaged total number of evaluations for Variant *B* are shown in Table 8. The estimation errors are lower than those of Variant *A.a* but higher than those of Variant *A.b*. Failure rates are similar but slightly higher than those of Variant *A.b*. Since the averaged total number of evaluations is close to the one of Variant *A.b*, Variant *B* does not bring much improvement for this example.

From the results of these two test functions, the main conclusion is that Variant *A.b* performs best. This highlights the efficiency of "Correlation 2" to estimate small first-order indices with quasi-Monte Carlo methods. Even if "Correlation 2" originally requires more model evaluations, this drawback is overridden when this estimator is included into a sequential procedure such as ours. For the case where we are only interested in estimating first-order indices, Variant *B* could be the best choice as the number of function evaluations is less than for Variants *A.a* and *A.b*.

5.2 Application

As an application, we will study the wing weight function introduced by Forrester *et al.* [2] and defined as follows:

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

Table 9 Inputs and their ranges of variation. All inputs are uniformly distributed in their respective ranges.

inputs	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)
$x_{11}, \ldots, x_{15}$	$[0, 1]$	"noise"

All inputs are described in Table 9 including their distribution and their physical representation. To illustrate the performance of our procedure, five additional inert inputs x_{11}, $\ldots$, x_{15} are added to serve only as "noise" to the sensitivity analysis.

The motivation of this application is to test if our procedure captures 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.

A second motivation is to compare the performance of each variant (*A.a*, *A.b* and *B*) on a function where the true values of Sobol' indices are unknown. The comparison is based on averaged Sobol' indices estimates and averaged total number of evaluations over 100 repetitions.

Tables 10 and 11 show the results obtained with Variant *A.a* and Variant *A.b*. Both variants capture well the presence of inert inputs. Variant *A.b* is more expensive but validates the property that first-order indices are lower or equal to total-effect indices. Conversely, Variant A.a fails to guarantee this property for inputs with small main effects: x_2, x_4, x_5, x_6. Once again, this highlights the efficiency of "Correlation 2". The boxplots presented in Figure 4 emphasize the latter observation where Variant *A.b* shows less variance in the estimates.

Table 12 shows the results obtained with Variant *B*. Variant *B* does not identify the inputs x_{11}, $\ldots$, x_{15} as inert inputs. However, all the estimated values for these inputs are smaller than the threshold $5 \cdot 10^{-3}$. The overestimation of the first-order indices for the inert inputs is balanced by the improvement in terms of total number of evaluations.

Overall, each variant captures well the same set of influential inputs identified by Forrester *et al.*

Table 10 Averaged values of $\widehat{\underline{S}}_u$, $\widehat{\overline{S}}_u$, and averaged total number of evaluations of Variant *A.a*.

input	$\widehat{\underline{S}}_u$	$\widehat{\overline{S}}_u$
x_1	0.1245	0.1279
x_2	0.0001	$< 10^{-4}$
x_3	0.2203	0.2261
x_4	0.0022	0.0006
x_5	0.0011	0.0001
x_6	0.0037	0.0024
x_7	0.1410	0.1452
x_8	0.4116	0.4196
x_9	0.0851	0.0877
x_{10}	0.0038	0.0043
$x_{11}, \ldots, x_{15}$	0	0
Total number of evaluations: 87 844		

Table 11 Averaged values of $\widehat{\underline{S}}_u$, $\widehat{\overline{S}}_u$ and averaged total number of evaluations of Variant *A.b*.

input	$\widehat{\underline{S}}_u$	$\widehat{\overline{S}}_u$
x_1	0.1245	0.1279
x_2	$< 10^{-4}$	$< 10^{-4}$
x_3	0.2203	0.2261
x_4	0.0006	0.0006
x_5	0.0001	0.0001
x_6	0.0023	0.0024
x_7	0.1410	0.1452
x_8	0.4116	0.4196
x_9	0.0851	0.0877
x_{10}	0.0043	0.0043
$x_{11}, \ldots, x_{15}$	0	0
Total number of evaluations: 93 881		

5.3 Comparison with the iid Monte Carlo method

In this section, our procedure is compared to a simpler method based on iid sampling and straightforward confidence intervals. This method corresponds to Saltelli's procedure described in Section 2.2 using iid uniform points instead of Sobol' sequences. The Bratley *et al.* function is used to compare the iid sampling approach with Variant *A.b*. The iid sampling method proceeds as follows: each Sobol' index is evaluated with the same number of evaluations used in Variant *A.b*. Then, we compute bootstrap confidence intervals to compare the error bounds. The confidence levels of the bootstrap intervals are set to 95%. The bounds are respectively the 2.5% and 97.5% quantile of the bootstrap sample.

The results are averaged over 100 repetitions and compared in Table 13. The comparison is made based on the estimation errors and failures rates. The column *precision*

Fig. 4 Boxplots of first-order indices $\underline{S}_u$ for inputs $x_2, x_4, x_5, x_6, x_{10}$ obtained with both Variant *A.a* and Variant *A.b*.

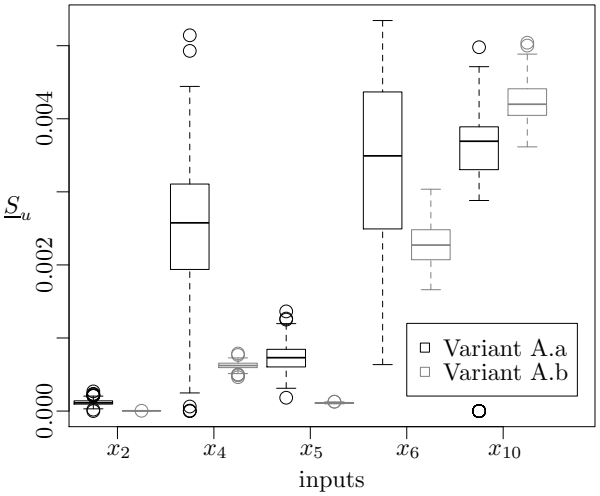


Table 12 Averaged values of $\widehat{\underline{S}}_u$ and averaged total number of evaluations of Variant *B*.

input	$\widehat{\underline{S}}_u$
x_1	0.1243
x_2	0.0035
x_3	0.2202
x_4	0.0033
x_5	0.0021
x_6	0.0037
x_7	0.1410
x_8	0.4117
x_9	0.0673
x_{10}	0.0043
$x_{11}, \ldots, x_{15}$	$\in [0,\ 0.005)$
Total number of evaluations: 65 536	

corresponds to the width of the bootstrap confidence interval for the iid sampling method.

The main observation is that our procedure performs the best. The random sampling method has high failure rates for inputs x_1, x_2 and slightly worse failure rates than Variant *A.b* for inputs x_3, x_4. The average *precision* values only fall below the tolerance $\varepsilon = 5 \cdot 10^{-3}$ for inputs x_5 and x_6. Figures 5 and 6 emphasize the latter observations.

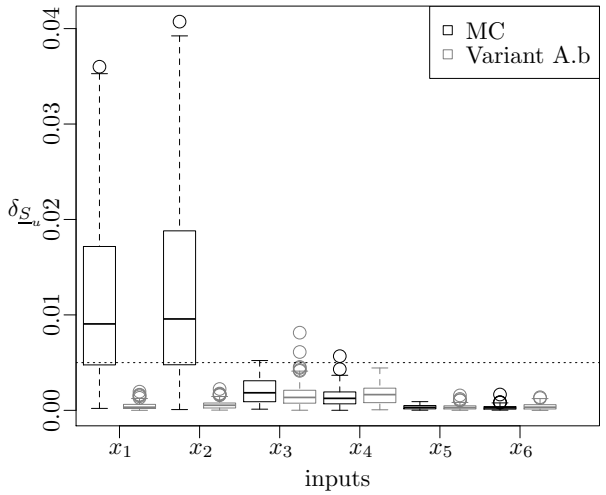
6 Conclusion

When estimating Sobol' indices, the question of how many evaluations must be performed to reach a desired precision is often raised by practitioners. This question is difficult to address mostly because the number of evaluations needed depends on the complexity of the model studied. As such, it is hard to bring out a general rule of thumb.

Table 13 Averaged estimation errors $\delta_{\underline{S}_u}$ and $\delta_{\overline{S}_u}$, and failure rates $r_{\delta_{\underline{S}_u}}$ and $r_{\delta_{\overline{S}_u}}$ for the iid sampling method (Monte Carlo as MC) and Variant *A.b* (qMC).

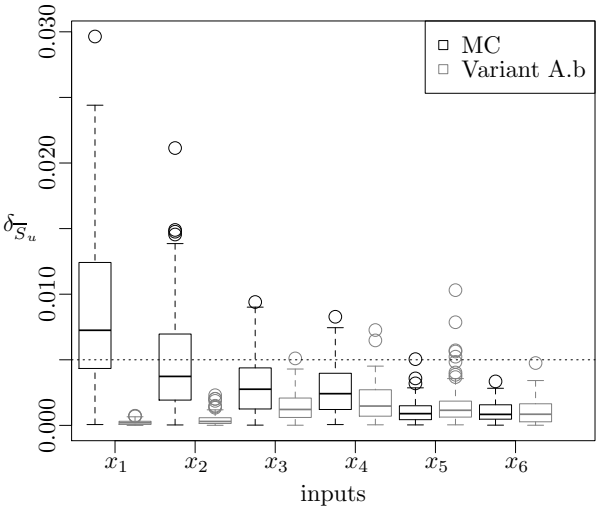
input	procedure	$\delta_{\underline{S}_u}$	$r_{\delta_{\underline{S}_u}}$	$\delta_{\overline{S}_u}$	$r_{\delta_{\overline{S}_u}}$	precision
x_1	qMC	0.0005	0	0.0002	0	0.0344
	MC	0.0116	0.75	0.0086	0.67	
x_2	qMC	0.0006	0	0.0005	0	0.0362
	MC	0.0122	0.74	0.0049	0.37	
x_3	qMC	0.0017	0.02	0.0015	0.01	0.007
	MC	0.0020	0.02	0.0030	0.18	
x_4	qMC	0.0017	0	0.0018	0.02	0.0052
	MC	0.0014	0.01	0.0027	0.11	
x_5	qMC	0.0003	0	0.0016	0.05	0.0012
	MC	0.0003	0	0.0011	0.01	
x_6	qMC	0.0004	0	0.0011	0	0.0012
	MC	0.0003	0	0.0010	0	

Fig. 5 Boxplots of estimation errors $\delta_{\underline{S}_u}$ obtained with both Variant *A.b* and the iid sampling method. The dashed horizontal line marks the tolerance $\varepsilon = 5 \cdot 10^{-3}$.



The sequential estimation procedure proposed in this article offers a practical solution with the construction of an estimator and error bound for Sobol' indices. The number of points is progressively augmented until the error bound becomes lower than a user specified tolerance. The procedure presented combines Sobol' sequences with either Saltelli's strategy to estimate both first-order and total effect indices, or the replication procedure to estimate only first-order indices. Furthermore, we investigated the use of a recent estimator well-suited to the estimation of small first-order indices using quasi-Monte Carlo methods. The efficiency of this estimator, called "Correlation 2", was assessed and highlighted on two test functions and an application. Overall, the variant combining Saltelli's strategy and "Correlation 2" gave the best results, with low failure rates across all indices.

Fig. 6 Boxplots of estimation errors $\delta_{\overline{S}_u}$ obtained with both Variant *A.b* and the iid sampling method. The dashed horizontal line marks the tolerance $\varepsilon = 5 \cdot 10^{-3}$.



The precision of our procedure was also compared to a simpler method based on iid sampling and straightforward confidence intervals. For an identical number of evaluations, our procedure was far more accurate than the iid sampling method. The origin of the discrepancy observed lies in the use of a more robust error bound.

As a future project, the same estimators and algorithms can be designed for rank-1 lattices using the results in [10], and noticing that rank-1 lattices of the same size are also replicated designs of order 1. In addition, in view of the results from [6], one can also include the hybrid error tolerance criterion in these algorithms.

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