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Variance based sensitivity analysis of model output. Design and estimator for the total sensitivity index

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ABSTRACT

Variance based methods have assessed themselves as versatile and effective among the various available techniques for sensitivity analysis of model output. Practitioners can in principle describe the sensitivity pattern of a model $Y = f(X_1, X_2, \ldots, X_k)$ with k uncertain input factors via a full decomposition of the variance V of Y into terms depending on the factors and their interactions. More often practitioners are satisfied with computing just k first order effects and k total effects, the latter describing synthetically interactions among input factors. In sensitivity analysis a key concern is the computational cost of the analysis, defined in terms of number of evaluations of $f(X_1, X_2, \ldots, X_k)$ needed to complete the analysis, as $f(X_1, X_2, \ldots, X_k)$ is often in the form of a numerical model which may take long processing time. While the computational cost is relatively cheap and weakly dependent on k for estimating first order effects, it remains expensive and strictly k-dependent for total effect indices. In the present note we compare existing and new practices for this index and offer recommendations on which to use.

1. Introduction to variance based measures

Sensitivity analysis is the study of how uncertainty in the output of a model (numerical or otherwise) can be apportioned to different sources of uncertainty in the model input factors, factors from now on [30]. Existing regulatory documents on impact assessment recommend the use of quantitative sensitivity analysis [7,21]. Official guidelines insist on the importance of taking factor interactions into account [7,9]. Variance based methods [6,37] are well suited to this task and have asserted themselves among practitioners [28,34].

These methods are the computer experiment equivalent of the experimental design's analysis of the variance of an experimental outcome [1]. Unlike experimental design, where the effects of factors are estimated over levels, variance based methods look at the entire factors distribution, using customarily Monte Carlo methods of various sophistication.

The number of terms in the ANOVA decomposition of the variance of a model with k factors grows as 2^k. For this reason in sensitivity analysis it is customary to compute just two sets of k indices: the k 'first order' effects and the k 'total' effects [11,33]. Until recently both sets of indices were rather expensive to estimate, needing a number of model evaluations strictly depending upon k.

Following the recent development of metamodels, which provide cheap emulators of complex and large computational models, new methods have been proposed to compute sensitivity indices [20,23,43,45]. The computational cost to estimate an emulator is generally k-dependent. This k-dependent cost is mostly linked to the mapping of all possible interactions and much less to the estimation of the main effects. Therefore the computation of main effects by emulators is specially efficient and *weakly* k-dependent. Methods based on meta-modeling and emulators have also been tried to estimate the total sensitivity indices [44,47].

In the present work we do not deal with metamodels, but focus instead on the sample based methods, trying to improve the current best available practice [25].

Variance based methods have a long history in sensitivity analysis. They start with a Fourier implementation in the seventies [6], and have a milestone in the work of Sobol' [37]. The total sensitivity indices have been introduced by Homma and Saltelli [11], although the concept was proposed in [15] (see reviews [10,29,32] or Chapter eight in [27]).

The paper's outline is as follows: Section 2 recalls the basic concepts of variance based measures; Section 3 discusses the Monte Carlo based estimators so far available for the computation of first order and total sensitivity indices. In Section 4 we focus on the total sensitivity index and describe two different designs, 'radial' and 'winding-stairs', for the computation of total indices and compare their economy. Section 5 recalls quasi-random sequences and the concept of discrepancy. A set of numerical experiments is illustrated in Section 6, which also introduces the concept of 'effective dimension'. Section 7 summarizes the relevant results.

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Table 1
Notations used in the text.

Symbol	
N	Sample size
k	Number of factors
X_i	Generic factor
x_{ji}	Generic value for factor X_i taken from row j of X_i
Y	Generic scalar model output equal to $Y = f(X_1, X_2, \ldots, X_k)$
$\mathbf{X}$	$N \times k$ matrix of input factors
$\mathbf{A}$, $\mathbf{B}$	$N \times k$ sample matrices of input factors
$\mathbf{X}_{\sim i}$	$N \times (k-1)$ matrix of all factors but X_i
$\mathbf{A}_{\mathbf{B}}^{(i)}$	Matrix, where column i comes from matrix $\mathbf{B}$ and all other $k-1$ columns come from matrix $\mathbf{A}$
$\mathbf{B}_{\mathbf{A}}^{(i)}$	Matrix, where column i comes from matrix $\mathbf{A}$ and all other $k-1$ columns come from matrix $\mathbf{B}$
$e_{S_{Ti}}(n,k)$	Economy of a design to compute S_{Ti} effects, expressed as elementary effects per run
N_T	Total cost of a sensitivity analysis in terms of model evaluations
$V_{X_i}(\cdot), E_{X_i}(\cdot)$	Variance or mean of argument $(\cdot)$ taken over X_i
$V_{\mathbf{X}_{\sim i}}(\cdot), E_{\mathbf{X}_{\sim i}}(\cdot)$	Variance or mean of argument $(\cdot)$ taken over all factors but X_i

2. Sensitivity indices

Given a model of the form $Y = f(X_1, X_2, \ldots X_k)$, with Y a scalar, a variance based first order effect for a generic factor X_i can be written as (see notations in Table 1):

$$V_{X_i}\left(E_{\mathbf{X}_{\sim i}}(Y \mid X_i)\right) \tag{1}$$

where X_i is the i-th factor and $\mathbf{X}_{\sim i}$ denotes the matrix of all factors but X_i. The meaning of the inner expectation operator is that the mean of Y is taken over all possible values of $\mathbf{X}_{\sim i}$ while keeping X_i fixed. The outer variance is taken over all possible values of X_i. The associated sensitivity measure (first order sensitivity coefficient) is written as:

$$S_i = \frac{V_{X_i}(E_{\mathbf{X}_{\sim i}}(Y \mid X_i))}{V(Y)}. \tag{2}$$

Due to the known identity [18]:

$$V_{X_i}\left(E_{\mathbf{X}_{\sim i}}(Y \mid X_i)\right) + E_{X_i}\left(V_{\mathbf{X}_{\sim i}}(Y \mid X_i)\right) = V(Y). \tag{3}$$

S_i is a normalized index, as $V_{X_i}(E_{\mathbf{X}_{\sim i}}(Y \mid X_i))$ varies between zero and $V(Y)$. $V_{X_i}(E_{\mathbf{X}_{\sim i}}(Y \mid X_i))$ measures the first order (e.g. additive) effect of X_i on the model output, while $E_{X_i}(V_{\mathbf{X}_{\sim i}}(Y \mid X_i))$ is customarily called the residual.

Another popular variance based measure is the total effect index [11,31]:

$$S_{Ti} = \frac{E_{\mathbf{X}_{\sim i}}(V_{X_i}(Y \mid \mathbf{X}_{\sim i}))}{V(Y)} = 1 - \frac{V_{\mathbf{X}_{\sim i}}(E_{X_i}(Y \mid \mathbf{X}_{\sim i}))}{V(Y)}. \tag{4}$$

S_{Ti} measures the total effect, i.e. first and higher order effects (interactions) of factor X_i. One way to visualize this is by considering that $V_{\mathbf{X}_{\sim i}}(E_{X_i}(Y \mid \mathbf{X}_{\sim i}))$ is the first order effect of $\mathbf{X}_{\sim i}$, so that $V(Y)$ minus $V_{\mathbf{X}_{\sim i}}(E_{X_i}(Y \mid \mathbf{X}_{\sim i}))$ must give the contribution of all terms in the variance decomposition which do include X_i.

The decomposition equations describing the variance-based framework are given next. These apply to a square integrable function $Y = f(X_1, X_2, \ldots X_k)$ defined over Ω, the k-dimensional unit hypercube,

$$\Omega = (X \mid 0 \leqslant x_i \leqslant 1;\ i = 1, \ldots, k). \tag{5}$$

We further suppose that the factors are uniformly distributed in $[0, 1]$. The steps of a variance-based framework are as follows:

- Functional decomposition scheme:

$$f = f_0 + \sum_i f_i + \sum_i \sum_{j>i} f_{ij} + \cdots + f_{12\ldots k} \tag{6}$$

where $f_i = f_i(X_i)$, $f_{ij} = f_{ij}(X_i, X_j)$ and so on for a total of 2^k terms, including f_0. Each term is square integrable over Ω. Eq. (6) is known as Hoeffding decomposition. See [1,22] for reviews and [8,24,37] for useful reading. The unicity condition for (6) is granted by [37]:

$$\int_0^1 f_{i_1, i_2, \ldots, i_s}(x_{i_1}, x_{i_2}, \ldots, x_{i_s})\, dx_{i_w} = 0 \tag{7}$$

where $1 \leqslant i_1 < i_2 < \cdots < i_s \leqslant k$ and $i_w \in \{i_1, i_2, \ldots, i_s\}$. The functions $f_{i_1, i_2, \ldots, i_s}$ are obtained from:

$$\begin{aligned} f_0 &= E(Y), \\ f_i &= E_{\mathbf{X}_{\sim i}}(Y \mid X_i) - E(Y), \\ f_{ij} &= E_{\mathbf{X}_{\sim ij}}(Y \mid X_i, X_j) - f_i - f_j - E(Y) \end{aligned} \tag{8}$$

and similarly for higher orders.

- Relation between functions $f_{i_1, i_2, \ldots, i_s}$ and partial variances [37]:

$$\begin{aligned} V_i &= V\left(f_i(X_i)\right) = V_{X_i}\left[E_{\mathbf{X}_{\sim i}}(Y \mid X_i)\right], \\ V_{ij} &= V\left(f_{ij}(X_i, X_j)\right) \\ &= V_{X_i X_j}\left(E_{\mathbf{X}_{\sim ij}}(Y \mid X_i, X_j)\right) - V_{X_i}\left(E_{\mathbf{X}_{\sim i}}(Y \mid X_i)\right) \\ &\quad - V_{X_j}\left(E_{\mathbf{X}_{\sim j}}(Y \mid X_j)\right) \end{aligned} \tag{9}$$

and so on for higher order terms. All terms are linked by:

$$V(Y) = \sum_i V_i + \sum_i \sum_{j>i} V_{ij} + \cdots + V_{12\ldots k}. \tag{10}$$

Dividing both sides of the equation by $V(Y)$, we obtain:

$$\sum_i S_i + \sum_i \sum_{j>i} S_{ij} + \cdots + S_{12\ldots k} = 1. \tag{11}$$

Relations for the second and higher order terms in (9) as well as formula (10) hold if the factors are independent, which is the setting adopted throughout the present work. The case of dependent input factors is not treated in the present paper (see instead [13,31,46,48]).

Note that given the assumption of independence of input factors we may avoid to explicitly include the probability distribution function p_i of factor X_i in the integrals for the estimates of functions in (8). This implies that notation $\int f_i(x_i)\, dx_i$ can be used in place of the more verbose $\int f_i(x_i) p_i(x_i)\, dx_i$, as the factors pdf may be embedded in the function $f_i(x_i)$. Without loss of generality all factors can be conceived as defined in Ω and the mapping from Ω to the actual distribution of X_i is intended to be part of the definition of f.

Indices S_i, S_{Ti} can also be interpreted in terms of expected reduction of variance. This interpretation also holds when the input factors are not independent [31]:

- $V_{X_i}(E_{\mathbf{X}_{\sim i}}(Y \mid X_i))$ is the expected reduction in variance that would be obtained if X_i could be fixed.
- $E_{\mathbf{X}_{\sim i}}(V_{X_i}(Y \mid \mathbf{X}_{\sim i}))$ is the expected variance that would be left if all factors but X_i could be fixed. This holds since $V_{\mathbf{X}_{\sim i}}(E_{X_i}(Y \mid \mathbf{X}_{\sim i}))$ is the expected reduction in variance that would be obtained if all factors but X_i could be fixed.

For this reason Jansen [14] calls $V_{X_i}(E_{\mathbf{X}_{\sim i}}(Y \mid X_i))$ and $E_{\mathbf{X}_{\sim i}}(V_{X_i}(Y \mid \mathbf{X}_{\sim i}))$ top and bottom marginal variances, respectively. For additive models the two terms coincide, as S_{Ti} may be simply viewed as S_i plus all interaction terms including factor X_i.

3. Best practices for the simultaneous computation of S_i and S_{Ti}

We discuss here existing estimators to compute in a single set of simulations both sets of indices S_i and S_{Ti}. By 'simulation' we mean here the computation of an individual value for Y corresponding to a sampled set of k factors $X_1, X_2, \ldots, X_k$.

We imagine to have two independent sampling matrices $\mathbf{A}$ and $\mathbf{B}$, with a_{ji} and b_{ji} as generic elements. The index i runs from one to k, the number of factors, while the index j runs from one to N, the number of simulations. We now introduce matrix $\mathbf{A}_\mathbf{B}^{(i)}$ ($\mathbf{B}_\mathbf{A}^{(i)}$) where all columns are from $\mathbf{A}$ ($\mathbf{B}$) except the i-th column which is from $\mathbf{B}$ ($\mathbf{A}$). S_i can be computed from either the couple of matrices $\mathbf{A}, \mathbf{B}_\mathbf{A}^{(i)}$ or $\mathbf{B}, \mathbf{A}_\mathbf{B}^{(i)}$, e.g.:

$$V_{X_i}\left(E_{\mathbf{X}_{\sim i}}(Y \mid X_i)\right) = \frac{1}{N}\sum_{j=1}^{N} f(\mathbf{A})_j f\left(\mathbf{B}_\mathbf{A}^{(i)}\right)_j - f_0^2 \tag{12}$$

where $(\mathbf{B})_j$ denotes the j-th row of matrix $\mathbf{B}$ [37].

The computation of S_{Ti} proceeds from definition (4), where $V_{\mathbf{X}_{\sim i}}(E_{X_i}(Y \mid \mathbf{X}_{\sim i}))$ is obtained from [11]:

$$V_{\mathbf{X}_{\sim i}}\left(E_{X_i}(Y \mid \mathbf{X}_{\sim i})\right) = \frac{1}{N}\sum_{j=1}^{N} f(\mathbf{A})_j f\left(\mathbf{A}_\mathbf{B}^{(i)}\right)_j - f_0^2. \tag{13}$$

Where do Eqs. (12) and (13) come from? A demonstration is outlined here for Eq. (12) following [12,25]. Applying the known relation $V(Y) = E(Y^2) - E^2(Y)$ to $V_{X_i}(E_{\mathbf{X}_{\sim i}}(Y \mid X_i))$ one obtains:

$$V_{X_i}\left(E_{\mathbf{X}_{\sim i}}(Y \mid X_i)\right) = \int E^2_{\mathbf{X}_{\sim i}}(Y \mid X_i)\, dX_i - \left(\int E_{\mathbf{X}_{\sim i}}(Y \mid X_i)\, dX_i\right)^2.$$

While the latter term above is clearly $(E(Y))^2 \equiv f_0^2$, the former integral can be rewritten by expressing $E^2_{\mathbf{X}_{\sim i}}(Y \mid X_i)$ as an integral in $2(k-1)$ dimensions:

$$\begin{aligned} E^2_{\mathbf{X}_{\sim i}}(Y \mid X_i) &= E_{\mathbf{X}_{\sim i}}(Y \mid X_i) E_{\mathbf{X}_{\sim i}}(Y \mid X_i) \\ &= \iint f(X_1, X_2, \ldots, X_i, \ldots, X_k) \\ &\quad \times f\left(X'_1, X'_2, \ldots, X_i, \ldots, X'_k\right) d\mathbf{X}_{\sim i}\, d\mathbf{X}'_{\sim i} \end{aligned} \tag{14}$$

and

$$\begin{aligned} &\int E^2_{\mathbf{X}_{\sim i}}(Y \mid X_i)\, dX_i \\ &= \iint f(X_1, X_2, \ldots, X_i, \ldots, X_k) \\ &\quad \times f\left(X'_1, X'_2, \ldots, X_i, \ldots, X'_k\right) d\mathbf{X}\, d\mathbf{X}'_{\sim i}. \end{aligned} \tag{15}$$

Eq. (15) is the expectation value over $2k-1$ variables, i.e. $X_1, \ldots, X_k, X'_1, \ldots, X_i, \ldots, X'_k$, of the function $f(X_1, \ldots, X_i, \ldots, X_k)$ $f(X'_1, \ldots, X_i, \ldots, X'_k)$.

This explains the Monte Carlo estimation in Eq. (12). In fact within the product $f(\mathbf{B})_j f(\mathbf{A}_\mathbf{B}^{(i)})_j$ needed to compute S_i (12), the arguments $\mathbf{B}$ and $\mathbf{A}_\mathbf{B}^{(i)}$ have in common the coordinate X_i as in Eq. (15) above. Moving from $(\mathbf{B})_j$ to $(\mathbf{A}_\mathbf{B}^{(i)})_j$ can be seen as a step in the non-X_i direction, i.e. a step along $\mathbf{X}_{\sim i}$ (Fig. 1).

An analogous demonstration can be made for Eq. (13). Consider the product $f(\mathbf{A})_j f(\mathbf{A}_\mathbf{B}^{(i)})_j$ needed to compute S_{Ti} (13). Here the arguments $\mathbf{A}$ and $\mathbf{A}_\mathbf{B}^{(i)}$ have in common the coordinates $\mathbf{X}_{\sim i}$, and can thus be seen as separated by a step in the X_i direction (Fig. 1).

All that is needed to compute both sets of S_i and S_{Ti} for the k factors is the triplet of matrices $\mathbf{A}$, $\mathbf{B}$, $\mathbf{B}_\mathbf{A}^{(i)}$ or alternatively (equivalently) the triplet of matrices $\mathbf{A}$, $\mathbf{B}$, $\mathbf{A}_\mathbf{B}^{(i)}$. As shown in (12) and (13) above, the latter is used in the present work. It can be anticipated that this choice is driven by the use of quasi-random sequences discussed later in this paper (Section 5.1). In a sense that will be clarified later, the points of matrix $\mathbf{A}$, and hence of $\mathbf{A}_\mathbf{B}^{(i)}$, are better distributed than the points of $\mathbf{B}$ and $\mathbf{B}_\mathbf{A}^{(i)}$ when using quasi-random points.

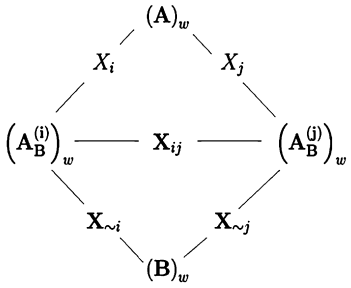

Fig. 1. Row w of matrix $\mathbf{A}$ and row w of matrix $\mathbf{A}_\mathbf{B}^{(i)}$ can be seen as separated by a step in the direction X_i. Likewise row w of matrix $\mathbf{A}_\mathbf{B}^{(i)}$ is separated by row w of matrix $\mathbf{B}$ by a step along the $\mathbf{X}_{\sim i}$ direction. Finally row w of matrix $\mathbf{A}_\mathbf{B}^{(i)}$ and that of $\mathbf{A}_\mathbf{B}^{(j)}$ are separated by a step along $\mathbf{X}_{ij}$, i.e. moving both factors X_i and X_j.

$2 \cdot N$ simulations are needed for computing Y corresponding to matrices $\mathbf{A}, \mathbf{B}$ while $k \cdot N$ simulations are needed to compute Y from matrices $\mathbf{A}_\mathbf{B}^{(i)}$ for all factors. As a result the cost of the analysis is $N \cdot (k+2)$ with N a sufficiently large number (500 or higher). Computing the output for both $\mathbf{A}_\mathbf{B}^{(i)}$ and $\mathbf{B}_\mathbf{A}^{(i)}$ would imply an additional cost of kN simulations.

Estimator (12) for S_i has been improved by [25,41] who proposed:

$$V_{X_i}\left(E_{\mathbf{X}_{\sim i}}(Y \mid X_i)\right) = \frac{1}{N}\sum_{j=1}^{N} f(\mathbf{A})_j \left(f\left(\mathbf{B}_\mathbf{A}^{(i)}\right)_j - f(\mathbf{B})_j\right). \tag{16}$$

In the present paper we suggest a further improvement which uses the triplet $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{A}_\mathbf{B}^{(i)}$ instead of the original formulation which uses $\mathbf{B}$, $\mathbf{A}$ and $\mathbf{B}_\mathbf{A}^{(i)}$. This improvement is related to the use of quasi-Monte Carlo samples as will be discussed in Section 5.1, while the triplet modification would have no impact by using pure Monte Carlo samples. The improvement is supported by simulations carried out in the present work. Details are not reported here since both estimators (12) and (16) for S_i have been outperformed by better practices, as described in [20,45,46]. Other good practices are also available to obtain $E_{\mathbf{X}_{\sim i}}(Y \mid X_i)$ [23,43] which in turn can be used for S_i estimates. These are not reviewed here given the present paper's focus on S_{Ti}.

A numerical improvement of estimator (13) for S_{Ti} has been proposed in [39]:

$$\begin{aligned} &V_{\mathbf{X}_{\sim i}}\left(E_{X_i}(Y \mid \mathbf{X}_{\sim i})\right) \\ &= V(Y) - \frac{1}{N}\sum_{j=1}^{N} f(\mathbf{A})_j \left(f(\mathbf{A})_j - f\left(\mathbf{A}_\mathbf{B}^{(i)}\right)_j\right). \end{aligned} \tag{17}$$

Alternative forms for the estimators of S_i and S_{Ti} are offered by Jansen [14,15] where $V_{X_i}(E_{\mathbf{X}_{\sim i}}(Y \mid X_i))$ needed to compute S_i is obtained from:

$$V_{X_i}\left(E_{\mathbf{X}_{\sim i}}(Y \mid X_i)\right) = V(Y) - \frac{1}{2N}\sum_{j=1}^{N}\left(f(\mathbf{B})_j - f\left(\mathbf{A}_\mathbf{B}^{(i)}\right)_j\right)^2. \tag{18}$$

Jansen's formula for S_{Ti} proceeds via $E_{\mathbf{X}_{\sim i}}(V_{X_i}(Y \mid \mathbf{X}_{\sim i}))$ rather than via $V_{\mathbf{X}_{\sim i}}(E_{X_i}(Y \mid \mathbf{X}_{\sim i}))$ (see Eq. (4)):

$$E_{\mathbf{X}_{\sim i}}\left(V_{X_i}(Y \mid \mathbf{X}_{\sim i})\right) = \frac{1}{2N}\sum_{j=1}^{N}\left(f(\mathbf{A})_j - f\left(\mathbf{A}_\mathbf{B}^{(i)}\right)_j\right)^2. \tag{19}$$

Table 2
Formulas to compute S_i and S_{Ti} (in square brackets the corresponding most representative reference). Formula (b) for S_i uses the triplet $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{A}_\mathbf{B}^{(i)}$ instead of formulation in (16), which uses $\mathbf{B}$, $\mathbf{A}$ and $\mathbf{B}_\mathbf{A}^{(i)}$. Analogously we propose here to compute numerical estimates of (19) using quasi-random numbers in the setting $\mathbf{A}$, $\mathbf{A}_\mathbf{B}^{(i)}$. This leads to (f) which is the *best practice* so far for S_{Ti}.

$V_{X_i}(E_{\mathbf{X}_{\sim i}}(Y\|X_i))$ for S_i	Reference
(a) $\frac{1}{N}\sum_{j=1}^{N} f(\mathbf{A})_j f(\mathbf{B}_\mathbf{A}^{(i)})_j - f_0^2$	'Sobol' 1993' [37]
(b) $\frac{1}{N}\sum_{j=1}^{N} f(\mathbf{B})_j (f(\mathbf{A}_\mathbf{B}^{(i)})_j - f(\mathbf{A})_j)$	[this paper]
(c) $V(Y) - \frac{1}{2N}\sum_{j=1}^{N} (f(\mathbf{B})_j - f(\mathbf{A}_\mathbf{B}^{(i)})_j)^2$	'Jansen 1999' [14]
$E_{\mathbf{X}_{\sim i}}(V_{X_i}(Y \mid \mathbf{X}_{\sim i}))$ for S_{Ti}	
(d) $V(Y) - \frac{1}{N}\sum_{j=1}^{N} f(\mathbf{A})_j f(\mathbf{A}_\mathbf{B}^{(i)})_j + f_0^2$	'Homma 1996' [11]
(e) $\frac{1}{N}\sum_{j=1}^{N} f(\mathbf{A})_j (f(\mathbf{A})_j - f(\mathbf{A}_\mathbf{B}^{(i)})_j)$	'Sobol' 2007' [39]
(f) $\frac{1}{2N}\sum_{j=1}^{N} (f(\mathbf{A})_j - f(\mathbf{A}_\mathbf{B}^{(i)})_j)^2$	'Jansen 1999' [14] and [this paper]

In the following we shall refer to the estimator (17) as 'Sobol' 2007' [39] and to the estimator (19) as 'Jansen 1999'. Table 2 provides all the estimators for S_i and S_{Ti} described so far.

Estimator (f) in Table 2 ('Jansen 1999') has been proved to be more efficient than estimator (d) for total order effects. The proof is Theorem 4 in [38], that compares their variances.

Given that estimator (e) can be easily derived from (d) (by just rewriting $V(Y)$ in (d) as $E(Y^2) - E^2(Y)$ and reordering the terms), it follows that estimator (f), 'Jansen 1999', is also better than (e).

In the present work we propose to use quasi-random numbers in the setting $\mathbf{A}, \mathbf{A}_\mathbf{B}^{(i)}$ to compute S_{Ti} estimates. The best practice for S_{Ti} is thus estimator (f) shown in Table 2. All these conclusions will be tested numerically in Section 6.

Although the quest for better designs and estimators is still active, see e.g. [26], the strategies just described are so far the most efficient to compute a full set of k S_i and S_{Ti} terms based on real function point values, i.e. without using emulators (see Section 1).

The same simulations made for the estimation of the total effects can also be used to estimate $k(k-1)/2$ total effects of pairs of factors, through a straightforward generalization of Jansen's estimator (Fig. 1):

$$E_{\mathbf{X}_{\sim ij}}\left(V_{X_i X_j}(Y \mid \mathbf{X}_{\sim ij})\right) = \frac{1}{2N}\sum_{w=1}^{N}\left(f\left(\mathbf{A}_\mathbf{B}^{(i)}\right)_w - f\left(\mathbf{A}_\mathbf{B}^{(j)}\right)_w\right)^2. \quad (20)$$

This extension is somehow implicit in [25], as therein the main effect of all-factors-but-two is introduced, which is simply the unconditional variance minus $E_{\mathbf{X}_{\sim ij}}(V_{X_i X_j}(Y|\mathbf{X}_{\sim ij}))$, see Eq. (3). Still total effects of couples of factors as computed from Eq. (20) are introduced in the present paper for the first time. These estimates are not independent from those of the total effect for single factors, as all are based on the same simulations.

According to [19] the economy of a method can be defined as the ratio 'effects' versus 'data points'. The best practices described in the present section can generate as many as N individual estimates[1] of S_{Ti} for each of the k, factors. Thus, neglecting the first order indices and the total effect for pairs just described, and using model outputs corresponding to matrices $\mathbf{A}$, $\mathbf{A}_\mathbf{B}^{(i)}$ only (for a total of $N(k+1)$ simulations), an S_{Ti}-specific economy $e_{S_{Ti}}$ can be defined as:

$$e_{S_{Ti}} = \frac{kN}{N(k+1)} \sim 1. \quad (21)$$

[1] An individual estimate is obtained by a single couplet $f(\mathbf{A})_j f(\mathbf{A}_\mathbf{B}^{(i)})_j$, corresponding to two suitably chosen rows of the sampling matrices. A sensitivity index is obtained averaging the N individual estimates.

Table 3
First block of size $q = k+1$ runs for a Monte Carlo simulation for sensitivity analysis. Radial (left-hand) and winding stairs (right-hand) schemes are compared. k X_i steps are generated using either design. N such blocks will be needed for the analysis for a total computation cost of $N_T = N(k+1)$.

Radial sampling	Step	Winding stairs
$a_{1,1}, a_{1,2}, a_{1,3}, \ldots, a_{1,k}$		$a_{1,1}, a_{1,2}, a_{1,3}, \ldots, a_{1,k}$
$b_{1,1}, a_{1,2}, a_{1,3}, \ldots, a_{1,k}$	X_1	$b_{1,1}, a_{1,2}, a_{1,3}, \ldots, a_{1,k}$
$a_{1,1}, b_{1,2}, a_{1,3}, \ldots, a_{1,k}$	X_2	$b_{1,1}, b_{1,2}, a_{1,3}, \ldots, a_{1,k}$
$a_{1,1}, a_{1,2}, b_{1,3}, \ldots, a_{1,k}$	X_3	$b_{1,1}, b_{1,2}, b_{1,3}, \ldots, a_{1,k}$
$\ldots$		$\ldots$
$a_{1,1}, a_{1,2}, a_{1,3}, \ldots, b_{1,k}$	X_k	$b_{1,1}, b_{1,2}, b_{1,3}, \ldots, b_{1,k}$

4. Computational scheme for S_{Ti}

To compute S_{Ti} from formula (f), which represents the best practice so far, the design matrices $\mathbf{A}$ and $\mathbf{A}_\mathbf{B}^{(i)}$ have to be set-up. Different methods may be used. In the following two different designs are compared: the first, called 'radial design', has been firstly presented in [25]; the second, called 'winding design' derives from the method discussed in [14]. The two designs are illustrated in Table 3. Let us focus first on the left-hand side. This shows how – starting from the fist row made of elements from matrix $\mathbf{A}$, a step in the X_1 direction (second row) is generated by drawing a row from the re-sample matrix $\mathbf{A}_\mathbf{B}^{(1)}$, where all entries are from $\mathbf{A}$ but the first which is from $\mathbf{B}$. Likewise the third row is from matrix $\mathbf{A}_\mathbf{B}^{(2)}$, the fourth from $\mathbf{A}_\mathbf{B}^{(3)}$ and so on till the last row is selected from matrix $\mathbf{A}_\mathbf{B}^{(k)}$. In this way k steps have been generated in directions from X_1 to X_k. All steps involve the first point $(a_{1,1}, a_{1,2}, a_{1,3}, \ldots, a_{1,k})$. The entire left-hand side of Table 3 is a block of dimension $q = 1 + k$. A full sensitivity analysis will be composed by N such blocks, the total cost of the analysis being thus $N_T = N(1+k)$. In the following this design, based on Sobol' [37] and Saltelli [25], shall be referred to as 'radial', due to the symmetry of the sampling with respect to the first row in each block.

The right-hand side of Table 3 shows an alternative sampling scheme, derived from 'winding stairs' design originally due to Jansen [14].[2] In this design each row is a step away from the previous row (and not from the first row). With the first two winding stairs rows a step X_1 is generated. A step X_2 is now generated between the second and the third row. Likewise a step X_3 involves rows third and fourth and so on.

Both designs produce k S_{Ti} elementary effects at the cost of $k+1$ runs, and have thus the same economy $e_{S_{Ti}} = \frac{k}{k+1} \sim 1$. In both designs the block is constructed using only a single row of matrices $\mathbf{A}$, $\mathbf{B}$ (Table 3). Note that we have slightly adapted the original winding stairs formulation in using the re-sample matrix $\mathbf{B}$.

In the attempt of improving the design shown in Table 3, we now try to move from a scheme based on just two matrices $\mathbf{A}$, $\mathbf{B}$ of 'sample' and 're-sample' to a scheme with a number n of 're-sample' matrices $\mathbf{B}_1, \mathbf{B}_2, \ldots, \mathbf{B}_n$, with the case $n = 1$ corresponding to the existing practice (Table 3). In this way instead of a single step for e.g. X_1 as shown in Table 3 there will be n such steps.

[2] By way of example the first three rows of an original four-dimensional winding stairs sequence are given below. A single generic sample matrix $\mathbf{X}$ is used. The interested reader might identify in this sequence nine steps of the type $\mathbf{X}_{\sim i}$ and eleven steps of the type X_i. Over longer sequences winding stairs averages to two effects (one S_i and one S_{Ti}) per point

$x_{1,1}, x_{1,2}, x_{1,3}, x_{1,4}$ $x_{1,1}, x_{2,2}, x_{1,3}, x_{1,4}$ $x_{1,1}, x_{2,2}, x_{2,3}, x_{1,4}$ $x_{1,1}, x_{2,2}, x_{2,3}, x_{2,4}$

$x_{2,1}, x_{2,2}, x_{2,3}, x_{2,4}$ $x_{2,1}, x_{3,2}, x_{2,3}, x_{2,4}$ $x_{2,1}, x_{3,2}, x_{3,3}, x_{2,4}$ $x_{2,1}, x_{3,2}, x_{3,3}, x_{3,4}$

$x_{3,1}, x_{3,2}, x_{3,3}, x_{3,4}$ $x_{3,1}, x_{4,2}, x_{3,3}, x_{3,4}$ $x_{3,1}, x_{4,2}, x_{4,3}, x_{3,4}$ $x_{3,1}, x_{4,2}, x_{4,3}, x_{4,4}$.

Table 4
Ten-dimensional Sobol' quasi-random sequence. First eight points.

0.5000	0.5000	0.5000	0.5000	0.5000	0.5000	0.5000	0.5000	0.5000	0.5000
0.2500	0.7500	0.2500	0.7500	0.2500	0.7500	0.2500	0.7500	0.7500	0.2500
0.7500	0.2500	0.7500	0.2500	0.7500	0.2500	0.7500	0.2500	0.2500	0.7500
0.1250	0.6250	0.8750	0.8750	0.6250	0.1250	0.3750	0.3750	0.8750	0.6250
0.6250	0.1250	0.3750	0.3750	0.1250	0.6250	0.8750	0.8750	0.3750	0.1250
0.3750	0.3750	0.6250	0.1250	0.8750	0.8750	0.1250	0.6250	0.1250	0.8750
0.8750	0.8750	0.1250	0.6250	0.3750	0.3750	0.6250	0.1250	0.6250	0.3750
0.0625	0.9375	0.6875	0.3125	0.1875	0.0625	0.4375	0.5625	0.8125	0.6875

In the first row the 'sample' points are always the same, while there are n 're-sample' points instead of just one. The same for the other factors. The dimension of a block is now $q = nk + 1$ runs instead of $q = k + 1$ as in Table 3. The n steps for each factor X_i can be used to compute as many as $\binom{n+1}{2} = n(n+1)/2$ steps of the type X_i, useful to compute S_{Ti} effects. The idea of modifying radial and winding designs with $n > 1$ re-sample points stems from the possibility of increasing the S_{Ti}-specific economy (21), which in the modified design is:

$$e_{S_{Ti}} = \frac{nk(n+1)}{2nk+2} = O(n). \tag{22}$$

A possible drawback of using $n > 1$ is that the $\binom{n+1}{2}$ steps of the type X_i are not independent from one another.

A winding stairs trajectory for $n = 1$ is the same as the 'Morris' trajectory [19], which is used in a screening, semi-quantitative form of sensitivity analysis [4].

Table 3 shows that by design a radial sampling block is mostly populated by points of the 'sample' run, i.e. by elements of **A**, while in winding stairs there is a more balanced use of elements from **A** and **B**. Another useful remark is that for both designs each block is internally balanced (contains the same number of effects S_{Ti} for each factor), so that we can increase the blocks arbitrarily without worrying about the balance of the design. This property is useful when estimating the error in the design. In his original work Sobol' proposes to use Monte Carlo probable error to estimate the error in the computation of the sensitivity indices [37]. In [1] bootstrapping of the elementary effect is suggested instead. The balanced block-based design just described lends itself naturally to an approach based on bootstrapping the blocks themselves (see example in Section 6.3).

5. Exploration of the input factor space

5.1. Using Sobol' quasi-random sequences

Several types of quasi-random (QR) sequences have been suggested by Faure, Niederreiter, Halton, Hammersley, Sobol' and other investigators, see Bratley and Fox [3] for a review of these works.

QR sequences are specifically designed to generate samples of $X_1, X_2, \ldots, X_k$ as uniformly as possible over the unit hypercube Ω.

Unlike random numbers, successive quasi-random points *know* about the position of previously sampled points and fill the gaps between them. For this reason they are also called quasi-random numbers although they are not random at all.

We do not compare the performance of different QR sequences, but limit ourselves for the present work to an updated version of Sobol' QR sequences [35,36] which is characterized by low discrepancy properties (sequence # 8192 by S. Kucherenko [16]).

Sobol's sequences outperform crude Monte Carlo sampling in the estimation of multi-dimensional integrals [40]. The first eight points of a ten-dimensional Sobol's quasi-random sequence are given, as an example, in Table 4.

Matrices **A** and **B** of size (N, k) can be easily generated from a quasi-random sequence of size $(N, 2k)$: **A** is the left half of the quasi-random sequence, and **B** is the right part of it. The following considerations might be of use for practitioners:

1. The uniformity of the quasi-random sequence is linked to the ordered and progressive filling of the space, which is filled, at a given density, every 2^m points ($m = 1, 2, \ldots$). Thus, it would be a mistake to skip rows of the quasi-random matrix.
2. The uniformity of the quasi-random matrix deteriorates as the column index increases, with the first column in Table 4 being the best equidistributed in $[0, 1]$ [42].

The triplet **A**, $\mathbf{A}_\mathbf{B}^{(i)}$ and **B** contains a higher number of *better points*, in the sense of consideration 2 above, with respect to the alternative triplet **A**, $\mathbf{B}_\mathbf{A}^{(i)}$ and **B**. The former triplet is then preferred to compute S_i and S_{Ti}. Based on this argument we would advice practitioners to use formula (b) in Table 2 for S_i, instead of the formula in [41].

5.2. Exploration and discrepancy

Economy in the computation of the indices – as defined by (21) – is not the only consideration needed for a good design. Also important is that the k-dimensional space is explored efficiently. Due to the well-known 'curse of dimensionality', most of the space in a k-dimensional cube is away from the centre[3] and effective designs need to be good at exploring corners and edges. Sobol' sequences are quite effective in multi-dimensional exploration, in that they are characterized by low 'discrepancy' [35,36]. Imagine an hypercube with N points inside. Its theoretical density is hence $d_t = 1/N$. Discrepancy is defined by Sobol' as the maximum deviation between d_t and the point density d_i in an arbitrary hyper-parallelepiped P_i built within the hypercube. The discrepancy D is hence the maximum of this over all possible parallelepipeds.

$$D = \max_{P_i} |d_i - d_t|. \tag{23}$$

In the following comparison of radial and winding stairs, and of $n = 1$ with $n > 1$, these considerations apply:

- There is a natural trade off between exploration and economy: the more we re-use the same point or coordinate, (e.g. by increasing n) the less we explore the hypercube.
- The higher the value of n, the more certain coordinates are repeated at the expenses of others, so small n is more explorative. To make an example, for $k = 3$, and a total of $N_T = 28$ simulations, we can either use seven blocks with $n = 1$ or four blocks with $n = 2$. In the former case $N(1 + 1) = 14$ original points are needed, in the latter $N(1 + 2) = 12$ points are

[3] A way to illustrate the curse of dimensionality is to consider a hypersphere contained into a hypercube and tangent to its faces. The ratio of the volume of the hypersphere to that of the hypercube goes to zero rapidly with increasing the number of dimensions k. For $k = 3$ the ratio is about one half, and becomes 0.002 for $k = 10$.

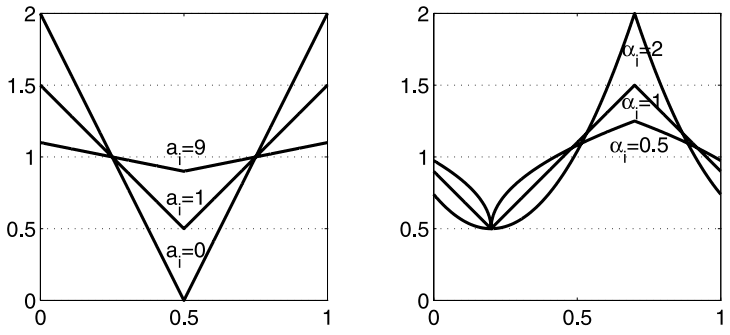

Fig. 2. Left: g_i function for $a_i = 0, 1, 9$. Right: g_i^* function for $a_i = 1$, $\delta_i = 0.3$ and $\alpha_i = 0.5, 1, 2$.

needed. This implies that the average use of a given coordinate is $\frac{28}{14} = 2$ for $n = 1$ and $\frac{28}{12} \sim 2.3$ for $n = 2$, indicating that $n = 1$ is more explorative than $n = 2$.

In summary:

1. The larger n, the less explorative the design.
2. A trade-off between exploration and economy exists but we are unable to judge a-priori if $n > 1$ improves the results of the analysis because of better economy or makes them worse because of poorer exploration.

6. Numerical experiments

The following research questions concerning the estimation of S_{Ti} are tackled here:

1. Which is the best estimator for S_{Ti} between estimators (e) and (f) in Table 2[4]?
2. Which is the best strategy between winding stairs and radial sampling?
3. Is $n > 1$ convenient with either of the above strategies?
4. Is the answer to the questions above dependent upon the typology of the function $f(X_1, X_2, \ldots, X_k)$?

The numerical experiment is based on a set of test cases for which the analytic value of S_{Ti} is available.

6.1. Effective dimensionality

The difficulty of a test case for sensitivity depends upon how many of the k factors have an effect on the output, as well as upon the order and strength of interactions.

The concept of 'effective dimensionality' for sensitivity analysis was introduced by Kucherenko and co-workers [17]. Two measures were proposed by these authors, termed respectively 'truncation' d_t and 'superposition' d_s.

Let $|u|$ be the cardinality of a set of factors u. The effective dimension in the superposition sense d_S is the smallest integer d_S such that:

$$\sum_{0<|u|\leqslant d_S} S_u \geqslant (1-\epsilon). \tag{24}$$

Effective dimension d_S is the order of the highest effect one needs to include in the sum $\sum_{0<|u|\leqslant d_S} S_u$ in order to reach the $(1-\epsilon)$ target.

[4] Estimator (d) of Table 2 has not been included in the numerical experiments because already improved by estimator (e) as shown in [39].

Effective dimension in the truncation sense d_T is the smallest integer such that:

$$\sum_{u\subseteq\{1,2,\ldots d_T\}} S_u \geqslant (1-\epsilon), \tag{25}$$

where u is as above a set of factors. Dimension d_T is the highest number of factors which need to be included in the sum $\sum_{u\subseteq\{1,2,\ldots,d_T\}} S_u$ in order to reach the $(1-\epsilon)$ target. Note that d_T depends on the order of the factors, therefore d_T may be reduced by reordering the factors in decreasing order of importance.

The knowledge of a full set of sensitivity indices S_i and S_{Ti} for the k factors gives a posteriori, i.e. after the sensitivity analysis, a picture of the difficulty of a test case as well as a precise value for d_S and d_T above.

If all the S_i are comparable, this means that there are no non-influential factors, and we a large d_T (25). If there are no interactions, then $d_S = 1$. On the contrary, if $\frac{S_i}{S_{Ti}} \ll 1$ for several factors, that is high interactions, then we have a large d_S (24)). For a discussion see [17].

6.2. Test cases

The mathematical functions used as test cases are given in the following, where all input factors X_i are assumed to be uniformly distributed in the interval $[0, 1]$. Their analytic sensitivity indices are given in Appendix A.

A function which can be used to generate test cases over a wide spectrum of difficulties is Sobol's G function, [1], defined as:

$$G = G(X_1, X_2, \ldots, X_k, a_1, a_2, \ldots, a_k) = \prod_{i=1}^{k} g_i,$$
$$g_i = \frac{|4X_i - 2| + a_i}{1 + a_i} \tag{26}$$

where $a_i \in \Re^+ \ \forall i = 1, \ldots, k$. The typology of the function G is driven by the dimensionality k as well as by the value of the coefficients a_i. Low values of a_i, such as $a_i = 0$, imply an important first order effect (see Fig. 2).

If more than one factor has low a_i's, then high interaction effects will also be present. The worst case for this function is where all a_i's are zero, i.e. all factors are equally important and all factors interact. If only a couple of a_i's are zero and all others are large (e.g. $a_i \geqslant 9$) then we have a relatively easy test case, with just two important factors and a single two-way interaction term. Function G has a singularity in each of its k dimensions corresponding to the points $x_i = \frac{1}{2}$ (Fig. 2). The Sobol' quasi-random sequence starts with such a point (Table 4). For this reason, in order not to give to the tested design an unfair advantage, a modified, shifted, and possibly curved version of G is introduced in this

Table 5
Definition of test cases G^*.

Function name	α_i parameters	a_i parameters
G_1^*	$\alpha_i = 1,\ i = 1, 2, \ldots, 10$	$a_i = (0, 0, 9, 9, 9, 9, 9, 9, 9, 9)$
G_2^*	$\alpha_i = 1,\ i = 1, 2, \ldots, 10$	$a_i = (0, 0.1, 0.2, 0.3, 0.4, 0.8, 1, 2, 3, 4)$
G_3^*	$\alpha_i = 0.5,\ i = 1, 2, \ldots, 10$	$a_i = (0, 0, 9, 9, 9, 9, 9, 9, 9, 9)$
G_4^*	$\alpha_i = 0.5,\ i = 1, 2, \ldots, 10$	$a_i = (0, 0.1, 0.2, 0.3, 0.4, 0.8, 1, 2, 3, 4)$
G_5^*	$\alpha_i = 2,\ i = 1, 2, \ldots, 10$	$a_i = (0, 0, 9, 9, 9, 9, 9, 9, 9, 9)$
G_6^*	$\alpha_i = 2,\ i = 1, 2, \ldots, 10$	$a_i = (0, 0.1, 0.2, 0.3, 0.4, 0.8, 1, 2, 3, 4)$

work (Fig. 2):

$$G^*(X_1, X_2, \ldots, X_k, a_1, a_2, \ldots, a_k, \delta_1, \delta_2, \ldots, \delta_k, \alpha_1, \alpha_2, \ldots, \alpha_k) = \prod_{i=1}^{k} g_i^*, \tag{27}$$

$$g_i^* = \frac{(1+\alpha_i)\cdot|2(X_i+\delta_i - I[X_i+\delta_i]) - 1|^{\alpha_i} + a_i}{1+a_i} \tag{28}$$

where $\delta_i \in [0, 1]$, $\alpha_i > 0$ are shift and curvature parameters respectively, $I[X_i + \delta_i]$ is the integer part of $X_i + \delta_i$, and g_i^* reverts to g_i for $\delta_i = 0$ and $\alpha_i = 1$.

In the test cases that follow the G^* function has been run with $k = 10$. Values for coefficients α_i and a_i are indicated in Table 5. As the sensitivity indices do not depend from coefficients δ_i (see Appendix A) their values are randomly assigned at each Monte Carlo trial.

Function G_1^* is 'easy' in both the sense of (25) and of (24). Function G_2^* is rather 'difficult' in both (25) and (24) sense. Functions G_3^*, G_4^* are a concave version of G_1^*, G_2^*, while functions G_5^*, G_6^* are a convex version of G_1^*, G_2^*.

Another test case used in this work is from [2] and used in [17]; for k factors:

$$K = \sum_{i=1}^{k} (-1)^i \prod_{j=1}^{i} X_j \tag{29}$$

whose analytic S_{Ti} (this work) is given in Appendix A. This function is 'easy' in the sense of (25), i.e. not all factors are equally important, and less easy in the sense of (24) as it has important interactions.

The last test case is from [28]:

$$B = \sum_{i=1}^{m} X_i \cdot \omega_i \tag{30}$$

with $m = 5$, $X \sim N(0, \sigma_X)$, $\omega_i \sim N(0, \sigma_{\omega_i})$, $\{\sigma_{X_i};\ i = 1, \ldots, 5\} = \{1, 1.1, 0.9, 1.2, 0.8\}$, and $\{\sigma_{\omega_i};\ i = 1, \ldots, 5\} = \{0.7, 1.3, 1.4, 0.6, 0.95\}$. This is another ten-dimensional test case, difficult in terms of (25) – all factors are relatively important – and less difficult in terms of (24) – interactions only between couples of X_i, ω_i.

6.3. Simulation results

The numerical experiment involves 50 replicas of the estimation procedure for functions G^*, K and B all tested with 10 total number of parameters. The replicas are obtained differently for different functions.

- For the G^* functions the shift parameters δ_i were randomly selected. This is permitted as the analytical value of S_{Ti} does not depend on δ_i, see Eq. (34) in Appendix A.
- For the K and B functions replicas of matrices **A** and **B** are obtained increasing the row index of Sobol' quasi-random sequence. For example the second replica uses the Sobol' sequence from row $N + 1$ to $2N$; the third from $2N + 1$ to $3N$ and so on.

Table 6
Pairwise simulations discussed in the paper.

'Sobol' 2007' vs 'Jansen 1999'	$\mathbf{A}, \mathbf{A}_\mathbf{B}^{(i)}$ vs $\mathbf{B}, \mathbf{B}_\mathbf{A}^{(i)}$	Radial vs Winding stairs	Radial $n = 1$ and $n > 1$
'Sobol' 2007'	$\mathbf{A}, \mathbf{A}_\mathbf{B}^{(i)}$	Radial	$n = 1$
'Jansen 1999'	$\mathbf{A}, \mathbf{A}_\mathbf{B}^{(i)}$	Radial	$n = 1$
'Jansen 1999'	$\mathbf{B}, \mathbf{B}_\mathbf{A}^{(i)}$	Radial	$n = 1$
'Jansen 1999'	$\mathbf{A}, \mathbf{A}_\mathbf{B}^{(i)}$	Radial	$n = 1$
'Jansen 1999'	$\mathbf{A}, \mathbf{A}_\mathbf{B}^{(i)}$	Winding stairs	$n = 1$
'Jansen 1999'	$\mathbf{A}, \mathbf{A}_\mathbf{B}^{(i)}$	Radial	$n = 1$
'Jansen 1999'	$\mathbf{A}, \mathbf{A}_\mathbf{B}^{(i)}$	Radial	$n > 1$
'Jansen 1999'	$\mathbf{A}, \mathbf{A}_\mathbf{B}^{(i)}$	Radial	$n = 1$

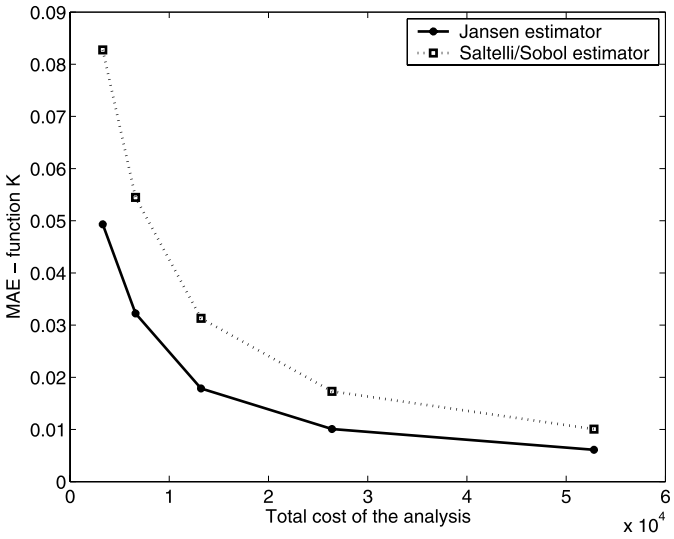

Fig. 3. 'Jansen 1999' estimator vs 'Sobol 2007' estimator for S_{Ti}: best case – K function.

Simulation results are shown in terms of a mean absolute error MAE versus the total cost N_T of the analysis, where MAE is defined as:

$$\text{MAE} = \frac{1}{50}\sum_{j=1}^{50}\sum_{i=1}^{k}\left|\hat{S}_{T_i}(j) - S_{T_i}\right|.$$

Table 6 summarizes our computational experiment which consists of a stepwise, top-down process where two methods (e.g. 'Sobol' 2007' vs 'Jansen 1999' or Radial vs Winding) are compared for all test functions at each step. Not all functions' plots shall be presented. For economy of space, for each conclusion only two functions are given: the one corresponding to the smallest mean absolute error MAE (*best* case) and the one corresponding to the highest (*worst* case). For each step of the computational experiment the two methods compared give the highest and the lowest MAE in correspondence to the same test function. The behaviour of all other test functions must be understood to be in between these two extremes.

'Sobol' 2007' vs 'Jansen 1999' estimator. The new 'Sobol' 2007' estimator [39] for S_{Ti} (17) is compared against that of 'Jansen 1999' [14] (19). Figs. 3 and 4 show respectively the best test case, function K, and the worst one, function G_6^*. Both methods converge at large N_T. Jansen's measure always performs best. As discussed

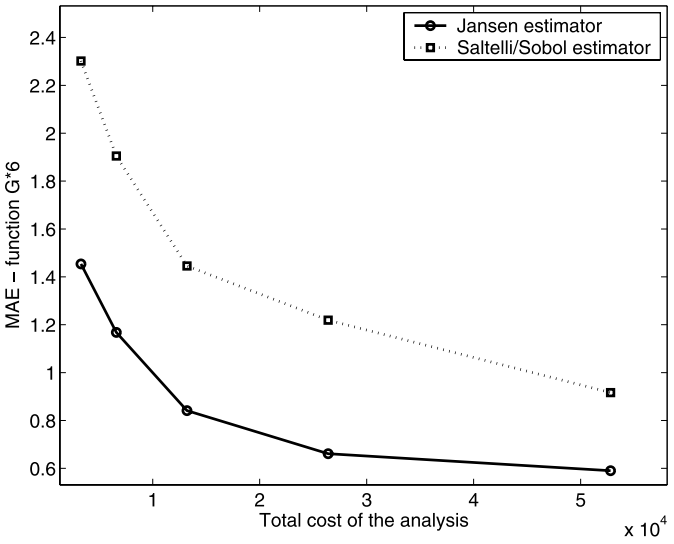

Fig. 4. 'Jansen 1999' estimator vs 'Sobol 2007' estimator for S_{Ti}: worst case – G_6^* function.

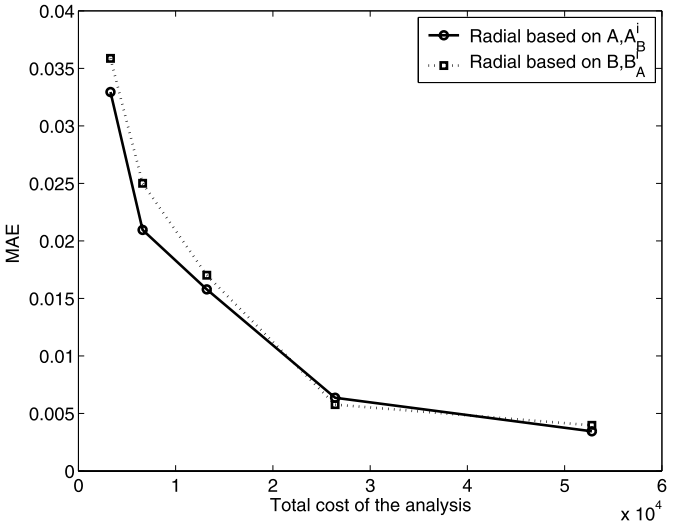

Fig. 5. Comparison of $\mathbf{A}$, $\mathbf{A}_{\mathbf{B}}^{(i)}$ vs $\mathbf{B}$, $\mathbf{B}_{\mathbf{A}}^{(i)}$ in the estimation of S_{Ti}: best case – G_3^* function.

in Section 3, this result is in line with the fact that 'Jansen 1999' estimator is more efficient than 'Sobol' 2007' estimator, as can be derived from [38] (Theorem 4). In the follow up of the experiment the Jansen's estimator has been used.

Comparing A, $\mathbf{A}_{\mathbf{B}}^{(i)}$ with B, $\mathbf{B}_{\mathbf{A}}^{(i)}$. In Figs. 5 and 6 we compare the 'Jansen 1999' estimator coupled to Saltelli 2002 design [25], based on matrices $\mathbf{B}$, $\mathbf{B}_{\mathbf{A}}^{(i)}$, against the same design using matrices $\mathbf{A}$, $\mathbf{A}_{\mathbf{B}}^{(i)}$ for $n = 1$. Both methods converge for large N_T. Best and worst case are for functions G_3^* and G_6^* respectively. The method based on $\mathbf{A}$, $\mathbf{A}_{\mathbf{B}}^{(i)}$ is more often better than $\mathbf{B}$, $\mathbf{B}_{\mathbf{A}}^{(i)}$ and is hence used in the following.

Comparing radial with winding stairs. Figs. 7 and 8 show the best and worst test case, functions K and G_6^* respectively, for the comparison of radial sampling against winding stairs for $n = 1$. Both methods converge. Radial sampling is always better or equal to winding stairs.

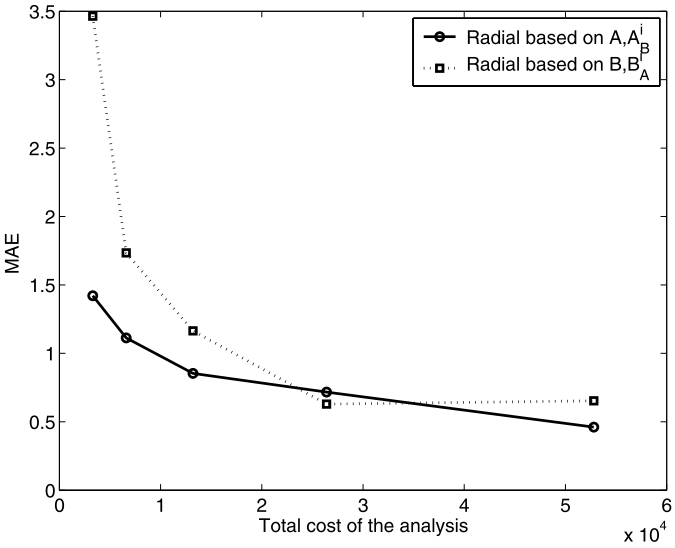

Fig. 6. Comparison of $\mathbf{A}$, $\mathbf{A}_{\mathbf{B}}^{(i)}$ vs $\mathbf{B}$, $\mathbf{B}_{\mathbf{A}}^{(i)}$ in the estimation of S_{Ti}: worst case – G_6^* function.

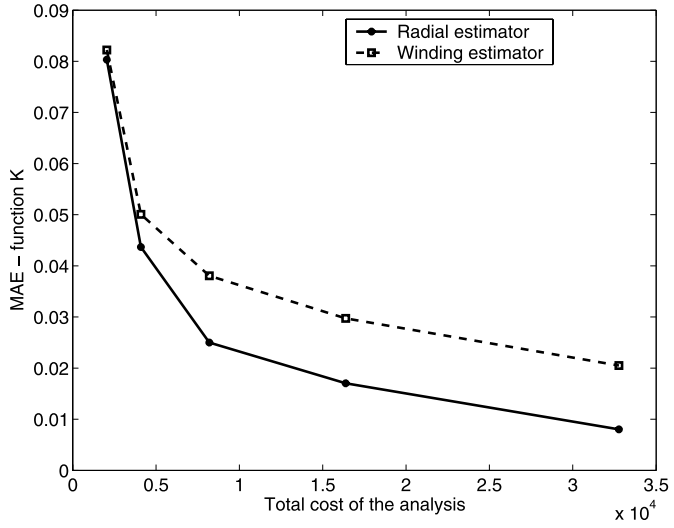

Fig. 7. Radial estimator vs winding stairs estimator for S_{Ti}: best case – K function.

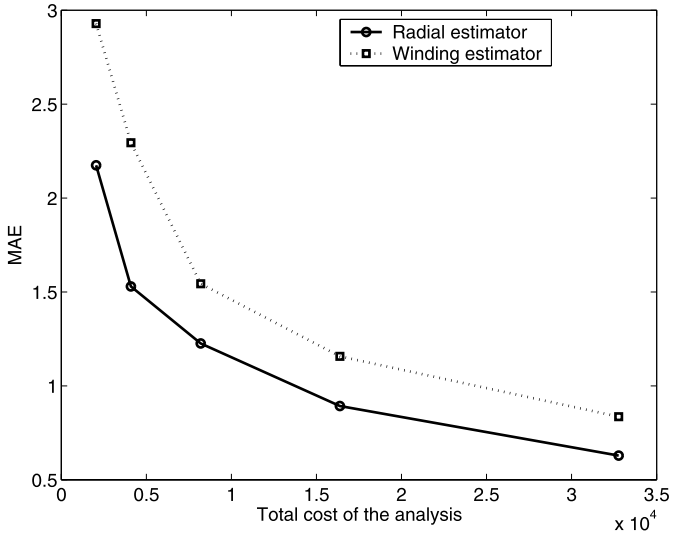

Fig. 8. Radial estimator vs winding stairs estimator for S_{Ti}: worst case – G_6^* function.

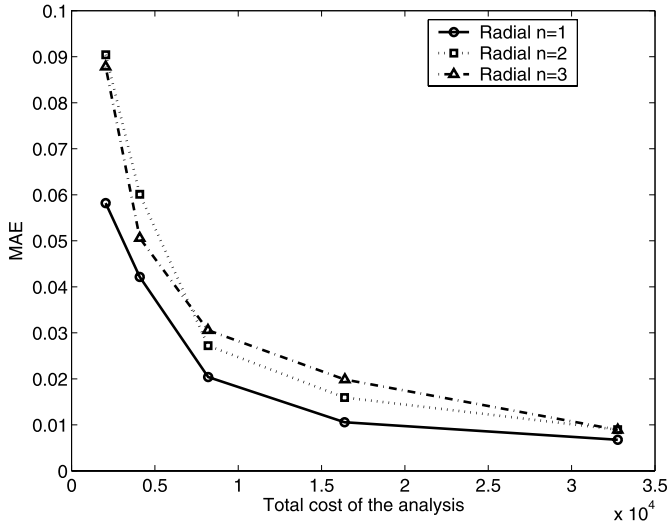

Fig. 9. Radial estimator for S_{Ti} – $n = 1$ vs radial $n = 2$ and $n = 3$: best case – G_3^* function.

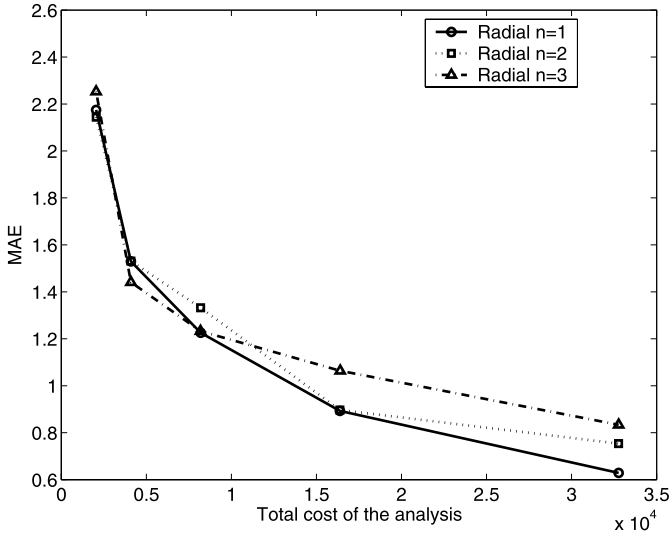

Fig. 10. Radial estimator for S_{Ti} – $n = 1$ vs radial $n = 2$ and $n = 3$: worst case – G_6^* function.

Comparing radial $n = 1$ and $n > 1$. The comparison of $n = 1$ versus $n > 1$ ($n = 2$ and $n = 3$) for radial sampling shows that $n = 1$ is always better than $n > 1$, with constant deterioration of the estimates as n increases. This did not encourage us to test higher values of n. Fig. 9 shows the best case, function G_3^*, while Fig. 10 gives the worst case, function G_6^*. Note that in this case the convergence curves at varying n are obtained by adjusting the value of N, number of blocks, following the rule $N(kn + 1) \equiv N_T$.

Dependence upon the typology of the test function. As seen from Figs. 3–10 the choice of the test function affects the MAE values but not the conclusions so far drawn on the relative merit of the tested algorithms.

All possible combinations of:

- radial sampling versus winding stairs, and
- $n = 1$ versus $n > 1$

have been tested for 'Jansen 1999' estimator and design matrices = $\mathbf{A}, \mathbf{A}_{\mathbf{B}}^{(i)}$. Since outcomes from these analyses confirm the results just described, they are not shown here.

In Section 4 we discussed bootstrapping the blocks to obtain confidence bounds for the sensitivity indices. In Figs. 11 and 12 we show an example of estimation of 90% confidence bounds of total indices for single factors and for pairs of factors based on the B analytic function given in (30).

7. Conclusions

The theory and the computational tools available to compute total sensitivity indices S_{Ti} have been revised. The main motivation for the present work is that previous comparisons of different methods to estimate S_{Ti} were based on incomplete combinations of sampling designs and estimators [5] or a limited set of test functions [25]. In this work a larger set of test functions has been employed reflecting different degrees of linearity, additivity and effective dimension. Further the simulations have been performed over all possible combinations of sampling designs and estimators, although we have not tested alternative quasi-random sequences (Section 5.1).

In conclusion, the present work indicates that the best estimates are obtained using the following choices:

1. Jansen's estimator.
2. Quasi-random number in the $\mathbf{A}$, $\mathbf{A}_{\mathbf{B}}^{(i)}$ configuration.
3. Radial sampling.
4. $n = 1$.

Note that $k + 1$ simulations per block are sufficient to compute all S_{Ti} terms for k factors plus the estimates for the $\frac{k(k-1)}{2}$ total effects for pairs of factors, Eq. (20).

Wishing to compute simultaneously also the S_i one would need one more simulation per block, the extra run corresponding to elements of the matrix $\mathbf{B}$.

While results (1) and (2) above have an analytic justification as described in the text (see Sections 3 and 5), results (3) and (4) are empirical, be they based on a large basis of test functions. These latter findings can be interpreted as a result of the optimality of the points of matrix $\mathbf{A}$ (left-most points of Sobol' quasi-random sequence):

- Radial vs winding stairs: as evident from Table 3, winding stairs design is poorer in $\mathbf{A}$ matrix elements than radial design, hence the poorer performance of winding stairs.
- $n = 1$ vs $n > 1$: similarly to the above, the $n > 1$ approach enriches the design with $\mathbf{B}$ elements reducing the share of $\mathbf{A}$ elements. Further the estimates obtained increasing n are not independent from one another.

The total effect index is a summary sensitivity measure inclusive of interactions effect of any order. According to a recent regulatory document [7] (p. 24): "Sensitivity analysis can be used to explore how the impacts of the options you are analysing would change in response to variations in key parameters and *how they interact*." Similarly a recent guideline for environmental models [9] (p. 55) suggest that: "[SA] methods should preferably be able to deal with a model regardless of assumptions about a model's linearity and additivity, *consider interaction effects among input uncertainties*, [···]."

The present analysis of the best practice available to compute the total sensitivity index is perhaps timely in light of this increased recognition of the importance of accounting for factors' interaction in sensitivity analysis.

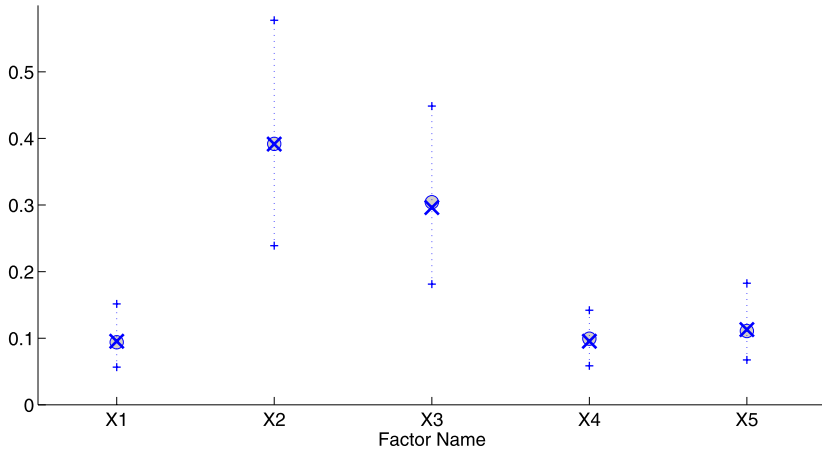

Fig. 11. Total sensitivity indices (circles) and 90% confidence intervals (vertical dashed lines) estimated via Monte Carlo method for factors X_i, $i = 1, \ldots, 5$, of the B function. The crosses indicate the analytic values. Total sensitivity indices for ω_i, $i = 1, \ldots, 5$, are identical to those for X_i, due to the symmetry of the B function. The total indices were estimated using formula (19) with $N = 1000$ as sample size. Monte Carlo confidence intervals were obtained using a sub-sample of size 100 with 10 000 replicas.

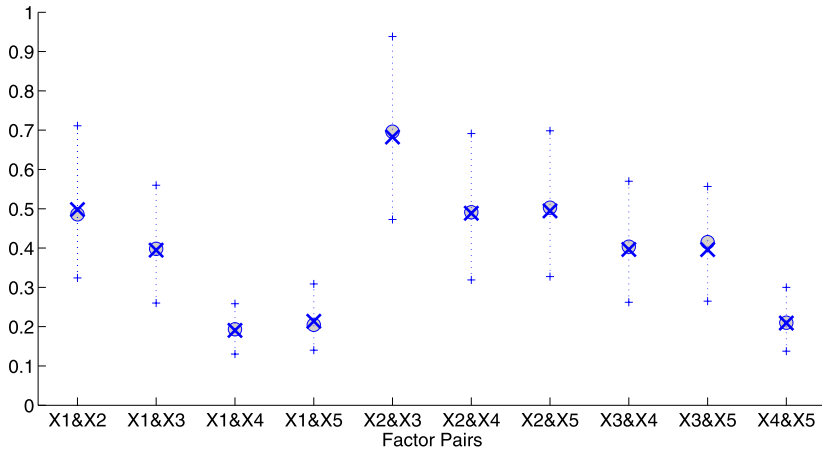

Fig. 12. Total sensitivity indices and 90% confidence intervals estimated via Monte Carlo method for all pairs of factors X_i & X_j of the B function. The crosses indicate the analytic values. Total sensitivity indices for pairs ω_i & ω_j are identical to those for pairs X_i & X_j, given the symmetry of the B function. The total indices were estimated using formula (20) with $N = 1000$ as sample size. Monte Carlo confidence intervals were obtained using a sub-sample of size 100 with 10 000 replicas.

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Appendix A. Analytical test cases

1. G-function

$$G = G(X_1, X_2, \ldots, X_k, a_1, a_2, \ldots, a_k) = \prod_{i=1}^{k} g_i,$$

$$g_i = \frac{|4X_i - 2| + a_i}{1 + a_i} \tag{31}$$

where all input factors X_i are assumed to be uniformly distributed in the interval $[0, 1]$ and $a_i \in \Re^+ \ \forall i = 1, \ldots, k$. The sensitivity indices for G can be obtained analytically from:

$$V_i = V_{X_i}\left(E_{\mathbf{X}_{\sim i}}(Y \mid X_i)\right) = \frac{1/3}{(1 + a_i)^2},$$

$$V\left(E(Y|X_{i_1}, X_{i_2}, \ldots, X_{i_s})\right) = \prod_{j=1}^{s}(1 + V_{i_j}) - 1,$$

$$V_{Ti} = V_i \prod_{j \neq i}(1 + V_j),$$

$$V = \prod_{i=1}^{k}(1 + V_i) - 1. \tag{32}$$

2. G^*-function

$$G^*(X_1, \ldots, X_k, a_1, \ldots, a_k, \delta_1, \ldots, \delta_k, \alpha_1, \ldots, \alpha_k) = \prod_{i=1}^{k} g_i^*,$$

$$g_i^* = \frac{(1 + \alpha_i) \cdot |2(X_i + \delta_i - I[X_i + \delta_i]) - 1|^{\alpha_i} + a_i}{1 + a_i} \tag{33}$$

where all input factors X_i are assumed to be uniformly distributed in the interval $[0, 1]$; $a_i \in \Re^+ \ \forall i = 1, \ldots k$; $\delta_i \in [0, 1]$, $\alpha_i > 0$ are shift and curvature parameters respectively; $I[X_i + \delta_i]$ is the integer part of $X_i + \delta_i$, and g_i^* reverts to g_i for $\delta_i = 0$ and $\alpha_i = 1$.

The mean of each element in the products in the modified G^* function is 1 (as in the standard G function), while its variance is:

$$V_i\left(G^*(X_i, a_i, \alpha_i)\right) = \frac{\alpha_i^2}{(1 + 2\alpha_i)(1 + a_i)^2}. \tag{34}$$

Given (34), the same algorithm as in (32) is then used to compute the analytic full variance decomposition for the estimation tests.

3. K-function

$$K = \sum_{i=1}^{k} (-1)^i \prod_{j=1}^{i} X_j$$

where X_i are uniformly distributed in $[0, 1]$ $\forall i = 1, \ldots, k$.

Analytic S_{Ti} is given by:

$$S_{Ti}(K) = \frac{E(K^2) - E_i - \frac{1}{4}(T_1(i) - 2T_2(i) + T_3(i)) - T_4(i) - T_5(i)}{V(K)} \tag{35}$$

where

$$V(K) = \frac{1}{10}\left(\frac{1}{3}\right)^k + \frac{1}{18} - \frac{1}{9}\left(\frac{1}{2}\right)^{2k} + (-1)^{k+1}\frac{2}{45}\left(\frac{1}{2}\right)^k,$$

$$E(K^2) = \frac{1}{6}\left(1 - \left(\frac{1}{3}\right)^k\right) + \frac{4}{15}\left((-1)^{k+1}\left(\frac{1}{2}\right)^k + \left(\frac{1}{3}\right)^k\right),$$

$$E_i \equiv \frac{1}{6}\left(1 - \left(\frac{1}{3}\right)^{i-1}\right) + \frac{4}{15}\left((-1)^i\left(\frac{1}{2}\right)^{i-1} + \left(\frac{1}{3}\right)^{i-1}\right)$$

and T_1 to T_5 are geometric series whose compact representation is given by:

$$T_1(i) = \frac{1}{2}\left(\frac{1}{3}\right)^{i-2}\left(1 - \left(\frac{1}{3}\right)^{k-i+1}\right),$$

$$T_2(i) = \frac{1}{2}\left(\left(\frac{1}{3}\right)^{i-1} - \left(\frac{1}{3}\right)^k\right),$$

$$T_3(i) = \frac{3}{5}\left(4\left(\frac{1}{3}\right)^{k+1} + (-1)^{i+k}\left(\frac{1}{2}\right)^{k-i-1}\left(\frac{1}{3}\right)^i\right),$$

$$T_4(i) = \frac{1}{5}\left((-1)^{i+1}\left(\frac{1}{3}\right)\left(\frac{1}{2}\right)^{i-3} - 4\left(\frac{1}{3}\right)^i\right),$$

$$T_5(i) = \frac{1}{5}\left((-1)^{k+1}\left(\frac{1}{3}\right)\left(\frac{1}{2}\right)^{k-2} + (-1)^{k+i-1}\left(\frac{1}{3}\right)^i\left(\frac{1}{2}\right)^{k-i-1}\right).$$

4. B-function

$$B = \sum_{i=1}^{m} X_i \cdot \omega_i \tag{36}$$

with $m = 5$, $X \sim N(0, \sigma_X)$, $\omega_i \sim N(0, \sigma_{\omega_i})$, $\{\sigma_{X_i};\ i = 1, \ldots, 5\} = \{1, 1.1, 0.9, 1.2, 0.8\}$, and $\{\sigma_{\omega_i};\ i = 1, \ldots, 5\} = \{0.7, 1.3, 1.4, 0.6, 0.95\}$. For this test case:

$$V(B) = \sum_{i=1}^{m} \sigma_{X_i}^2 \sigma_{\omega_i}^2,$$

$$S_{X_i} = S_{\omega_i} = 0, \quad i = 1, 2, \ldots, m,$$

$$S_{X_i\omega_i} = \frac{\sigma_{X_i}^2 \sigma_{\omega_i}^2}{V(B)}, \quad i = 1, 2, \ldots, m,$$

$$S_{X_i\omega_j} = 0, \quad i \neq j,$$

$$S_{T_{X_i\omega_j}} = S_{X_i} + S_{\omega_j} + S_{X_i\omega_j}$$

so that in this case:

$$S_{T_{X_i\omega_j}} = 0, \quad i \neq j,$$

$$S_{T_{X_i\omega_i}} = S_{X_i\omega_i} = \frac{\sigma_{X_i}^2 \sigma_{\omega_i}^2}{V(B)}.$$

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