Total interaction index: A variance-based sensitivity index for second-order interaction screening

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Abstract

Sensitivity analysis aims at exploring which of a number of variables have an impact on a certain response. Not only are the individual variables of interest but also whether they interact or not. By analogy with the total sensitivity index, used to detect the most influential variables, a screening of interactions can be done efficiently with the so-called total interaction index (TII), defined as the superset importance of a pair of variables. Our aim is to investigate the TII, with a focus on statistical inference. At the theoretical level, we derive its connection to total and closed sensitivity indices. We present several estimation methods and prove the asymptotical efficiency of the Liu and Owen estimator. We also address the question of estimating the full set of TIIs, with a given budget of function evaluations. We observe that with the pick-and-freeze method the full set of TIIs can be estimated at a linear cost with respect to the problem dimension. The different estimators are then compared empirically. Finally, an application is given aiming at discovering a block-additive structure of a function, where no prior knowledge either about the interaction structure or about the blocks is available.

Keywords: Sensitivity analysis, FANOVA decomposition, Sobol indices, High-order interactions, Superset importance, Additive structure

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1. Introduction

Global sensitivity analysis has broad applications in screening, interpretation and reliability analysis [1, 2]. A well-established method is the estimation of Sobol indices which quantify the influence of variables, or groups of variables, on the variability of an output. First-order Sobol indices and closed Sobol indices quantify the single influence of variables or groups of variables [3]. Homma and Saltelli [4] introduced the total sensitivity index which measures the influence of a variable jointly with all its interactions. If the total sensitivity index of a variable is zero, this variable can be removed because neither the variable nor its interactions — at any order — have an influence. Thus the total sensitivity index can be used to detect the essential variables, a procedure often called *screening*.

While screening is a first-order analysis, looking at single variables, we now consider its extension to second-order analysis, by looking at pairs of variables. By analogy with the total sensitivity index, we consider the so-called total interaction index (TII), that measures the influence of a pair of variables together with all its interactions. The TII is a particular case of superset importance, a sensitivity index investigated in Hooker [5] and Liu and Owen [6]. If the TII of a pair of variable $\{X_i, X_j\}$ is zero, then there is no interaction term containing simultaneously X_i and X_j, which leads to the elimination of the pair $\{X_i, X_j\}$ from the list of possible interactions. By analogy with screening, this can be viewed as *interaction screening*. More precisely this is second-order interaction screening, since we consider pairs of variables.

The main benefit of TII is to discover groups of variables that do not interact with each other, without knowing in advance the number of groups, nor their size. To illustrate this, let us consider a short example. Consider the following function , supposed to be unknown, which we want to analyze based on a limited number of evaluations:

$$f(X_1, \dots, X_6) = \cos([1, X_1, X_5, X_3]\,\beta) + \sin([1, X_4, X_2, X_6]\,\gamma),$$

with $X_k \overset{\text{i.i.d.}}{\sim} U[-1, 1]$, $k = 1, \dots, 6$, $\beta = [-0.8, -1.1, 1.1, 1]'$ and $\gamma = [-0.5, 0.9, 1, -1.1]$. If we estimate the common first-order and total sensitivity indices (Figure 1, left), we detect that all variables are active, on their own as well as by interactions, but not which variables are involved in the interactions and by what amount. Now we estimate the TII for each combination of two variables. A convenient way to present the TII is by a graph, where the thickness of the vertex circle represents the first-order index, and the thickness of the edge between two vertices the TII of the two variables. Now the interaction structure, here a partition into two groups, is clearly visible (Figure 1, right).

This interaction structure corresponds to an additive structure of the analyzed function. This can be advantageously exploited for metamodelling (see [7]), and for optimization: The 6-dimensional optimization problem of minimizing f simplifies into two 3-dimensional ones.

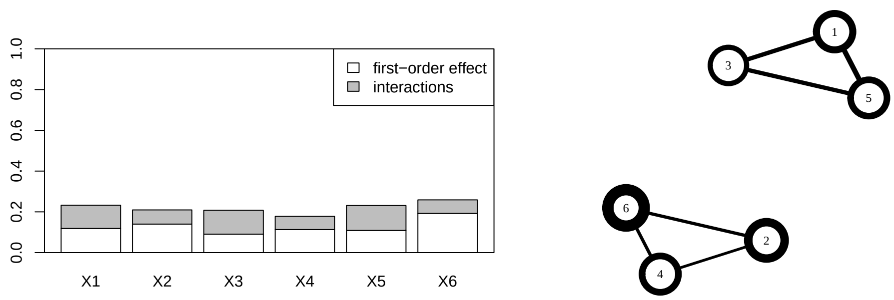

Figure 1: Sensitivity analysis of the example experiment. First-order and total Sobol indices (left), total interaction indices (right).

The aim of our paper is to investigate the TII, with a focus on statistical inference. Our main result is the asymptotical efficiency [8] of the estimator proposed by Liu and Owen [6]. The article is structured as follows. Section 2 presents theoretical results concerning the TII. Several estimation methods are deduced (Section 3), and asymptotical properties of the *method by Liu and Owen* are proved in Section 4. The question of estimating all the TIIs with a given budget of function evaluations is studied in Section 5. Finally the TII is used to recover the block-additive decomposition of a 12-dimensional function. Throughout the paper a capital letter like X_i indicates a single random variable where a lower case letter like x_i indicates a realization of the variable, e.g. a Monte Carlo random sample of the distribution of X_i. A bold letter like $\boldsymbol{X}$ indicates a vector of variables.

2. Theoretical aspects

2.1. A quick overview of FANOVA decomposition and Sobol indices

Assume a set of independent random variables $\boldsymbol{X} = \{X_1, \ldots, X_d\}$, and let ν denote the probability measure of $\boldsymbol{X} = (X_1, ..., X_d)$. Then for any function $f \in L^2(\nu)$, the functional ANOVA decomposition provides a unique decomposition into additive terms

$$f(\boldsymbol{X}) = \mu_0 + \sum_{i=1}^{d} \mu_i(X_i) + \sum_{i<j} \mu_{i,j}(X_i, X_j) + \cdots + \mu_{1,\ldots,d}(X_1, \ldots, X_d). \quad (1)$$

The terms represent first-order effects ($\mu_i(X_i)$), second-order interactions ($\mu_{i,j}(X_i, X_j)$) and all higher-order combinations of input variables. [9] show that the decomposition is unique if all terms on the right hand side of (1) have zero mean

$$\mathrm{E}(\mu_I(\boldsymbol{X}_I)) = 0, \quad I \subseteq \{1, \ldots, d), \quad (2)$$

and the conditional expectations fulfill

$$\begin{aligned}\mathrm{E}(\mu_{i,i'}(X_i X_{i'}) \mid X_i) = \mathrm{E}(\mu_{i,i'}(X_i X_{i'}) \mid X_i') = \mathrm{E}(\mu_{i,i',i''}(X_i X_{i'} X_{i''}) \mid X_i X_{i'}) \\ = \mathrm{E}(\mu_{1,\ldots,n}(X_1 \ldots X_n) \mid X_1 \ldots X_{n-1}) = \cdots = 0, \quad (3)\end{aligned}$$

which implies the orthogonality of all terms in (1).
Generally, due to the independence in $\boldsymbol{X}$ in our framework, the conditional expectation of a functional reduces to

$$\mathrm{E}(h(X_j, X_k) \mid X_j = x_j) = \int h(x_j, x_k)\, d\nu_k(x_k).$$

The decomposition can be obtained by recursive integration

$$\mu_0 = E(f(\boldsymbol{X})),$$

$$\mu_i(X_i) = E(f(\boldsymbol{X})|X_i) - \mu_0,$$

$$\mu_{i,j}(X_i, X_j) = E(f(\boldsymbol{X})|X_i, X_j) - \mu_i(X_i) - \mu_j(X_j) - \mu_0,$$

and more generally

$$\mu_I(\boldsymbol{X}_I) = E(f(\boldsymbol{X})|\boldsymbol{X}_I) - \sum_{I' \subsetneq I} \mu_{I'}(\boldsymbol{X}_{I'}). \quad (4)$$

By computing the variance of (1), a variance decomposition is obtained where each part quantifies the impact of the input variables on the response.

$$D = \mathrm{var}(f(\boldsymbol{X})) = \sum_{i=1}^{d} \mathrm{var}(\mu_i(X_i)) + \sum_{i<j} \mathrm{var}(\mu_{i,j}(X_i, X_j)) \\ + \cdots + \mathrm{var}(\mu_{1,\ldots,d}(X_1, \ldots, X_d)).$$

The individual variances are widely used to define indices which quantify the influence of input variables and their interactions. Divided by the overall variance D they are known as Sobol indices [3]:

$$S_I = \frac{\mathrm{var}(\mu_I(\boldsymbol{X}_I))}{D} = \frac{D_I}{D}. \tag{5}$$

In this paper we follow [5] and [6] and work with the unnormalized versions of the indices since the estimation of the overall variance is equal for all methods that we will consider. There are several extensions to the indices given in (5). The unnormalized total sensitivity index D_I^T [4] of a group of input variable $\boldsymbol{X}_I$, $I \subseteq \{1, \ldots, d\}$, describes the total contribution of the variables including all interactions of any order and is defined by the sum of all partial variances containing at least one of the variables:

$$D_I^T = \sum_{J \cap I \neq \emptyset} D_J. \tag{6}$$

Another way to describe the influence of a group of variables is the unnormalized closed sensitivity index D_I^C, see e.g. [3]. In contrast to total sensitivity indices, interactions with variables not in $\boldsymbol{X}_I$ are not included here, but all effects caused by subsets of it. It is equal to the so-called variance of the conditional expectation (VCE).

$$D_I^C = \mathrm{var}\left(E[f(\boldsymbol{X})|\boldsymbol{X}_I]\right) = \sum_{J \subseteq I} D_J. \tag{7}$$

A way to calculate the closed sensitivity index, sometimes called pick-and-freeze formula, is given by Sobol [3]:

$$D_I^C = E[f(\boldsymbol{X}_I, \boldsymbol{X}_{-I}) f(\boldsymbol{X}_I, \boldsymbol{Z}_{-I})] - \mu_0^2 \tag{8}$$

where $-I$ denotes the relative complement of I with respect to $\{1,\ldots,d\}$, $\boldsymbol{Z}_{-I}$ is an independent copy of $\boldsymbol{X}_{-I}$, and $\mu_0 = E(f(\boldsymbol{X}))$.

In Owen [10] two further ways to the closed sensitivity index are suggested called "'Correlation 1"' and "'Correlation 2"'. They avoid the subtraction of μ_0^2, and the corresponding Monte Carlo estimation attains a greater accuracy for small values of the closed sensitivity indices. Up to two independent copies of X_{-I} are used, denoted by Y_{-I} and Z_{-I}:

$$\begin{aligned} D_I^C &= E(f(\boldsymbol{X})\,(f(\boldsymbol{X}_I,\boldsymbol{Y}_{-I}) - f(\boldsymbol{Y}))) && (9)\\ &= E\left((f(\boldsymbol{X}) - f(\boldsymbol{Z}_I,\boldsymbol{X}_{-I}))\,(f(\boldsymbol{X}_I,\boldsymbol{Y}_{-I}) - f(\boldsymbol{Y}))\right). && (10)\end{aligned}$$

Finally, we obtain from (6) and (7) the well-known relation (see e.g. [11]):

$$D = D_{-I}^C + D_I^T \tag{11}$$

and in particular, with the formula of total variance,

$$\mathrm{var}(U) = \mathrm{E}(\mathrm{var}(U \mid V)) + \mathrm{var}(\mathrm{E}(U \mid V)),$$

one can deduce that the total sensitivity index relatively to I is equal to the expectation of the conditional variance (ECV) relatively to the complementary subset $-I$:

$$D_I^T = \mathrm{E}\left(\mathrm{var}[f(\boldsymbol{X})|\boldsymbol{X}_{-I}]\right). \tag{12}$$

2.2. Total interaction indices

Next we aim at an index which measures the portion of variance of an output explained by two input variables simultaneously, which we call total interaction index (TII). It is equal to the second-order version of the more general superset importance, which was introduced by Liu and Owen [6] for uniform distributions (Υ_u^2) as a measure of importance of interactions and their supersets. It was also investigated in the data-mining framework by Hooker [5] ($\overline{\sigma}_u^2$). It is defined for any subset $u \subseteq \{1,\ldots,d\}$ as

$$\Upsilon_u^2 = \overline{\sigma}_u^2 = \sum_{I \supseteq u} D_I.$$

The TII now is the special case for subsets of size two.

Definition 1. With the notation and assumptions of Section 2.1, the *total interaction index* $\mathfrak{D}_{i,j}$ of two variables X_i and X_j is defined by

$$\mathfrak{D}_{i,j} := \mathrm{var}\left(\sum_{I \supseteq \{i,j\}} \mu_I(\boldsymbol{X}_I)\right) = \sum_{I \supseteq \{i,j\}} D_I. \tag{13}$$

The index can be interpreted analogously to D_i^T, the total sensitivity index of a single variable. Both give the total contribution of the subject – the single variable or the pair of variables – to the output variance including all higher interactions.

It is not difficult to see that the TII is connected to total sensitivity indices, as well as to closed sensitivity indices:

Proposition 1. *The following relations hold:*

$$\mathfrak{D}_{i,j} = D_i^T + D_j^T - D_{i,j}^T, \tag{14}$$
$$\mathfrak{D}_{i,j} = D + D_{-\{i,j\}}^C - D_{-i}^C - D_{-j}^C. \tag{15}$$

Proof. (15) is deduced from (14) using (11). For (14), the proof comes from the identity:

$$\sum_{I \supseteq \{i\} \text{ or } I \supseteq \{j\}} D_I = \sum_{I \supseteq \{i\}} D_I + \sum_{I \supseteq \{j\}} D_I - \sum_{I \supseteq \{i,j\}} D_I.$$

□

As the TII is equal to the superset importance of a pair of indices, another way of computation is given by

Proposition 2. *(Liu and Owen [6])*

$$\mathfrak{D}_{i,j} = \frac{1}{4} E\left[f(X_i, X_j, \boldsymbol{X}_{-\{i,j\}}) - f(X_i, Z_j, \boldsymbol{X}_{-\{i,j\}}) \right.$$
$$\left. - f(Z_i, X_j, \boldsymbol{X}_{-\{i,j\}}) + f(Z_i, Z_j, \boldsymbol{X}_{-\{i,j\}})\right]^2 \tag{16}$$

where Z_i (resp. Z_j) is an independent copy of X_i (resp. X_j).

Proof. In addition to the proof given by Liu and Owen [6], we can give a direct proof connecting (16) to (15). Indeed, when expanding (16), of the 10 resulting terms the 4 squared terms are simply equal to $E(f(\boldsymbol{X})^2) = D + \mu_0^2$. The 6 double products gather two by two, and can be computed using (8):

- $E[f(Z_i, X_j, \boldsymbol{X}_{-\{i,j\}})f(Z_i, Z_j, \boldsymbol{X}_{-\{i,j\}})]$
$= E[f(X_i, X_j, \boldsymbol{X}_{-\{i,j\}})f(X_i, Z_j, \boldsymbol{X}_{-\{i,j\}})] = D^C_{-j} + \mu_0^2$
- $E[f(X_i, Z_j, \boldsymbol{X}_{-\{i,j\}})f(Z_i, Z_j, \boldsymbol{X}_{-\{i,j\}})]$
$= E[f(X_i, X_j, \boldsymbol{X}_{-\{i,j\}})f(Z_i, X_j, \boldsymbol{X}_{-\{i,j\}})] = D^C_{-i} + \mu_0^2$
- $E[f(Z_i, X_j, \boldsymbol{X}_{-\{i,j\}})f(X_i, Z_j, \boldsymbol{X}_{-\{i,j\}})]$
$= E[f(X_i, X_j, \boldsymbol{X}_{-\{i,j\}})f(Z_i, Z_j, \boldsymbol{X}_{-\{i,j\}})] = D^C_{-\{i,j\}} + \mu_0^2$

Finally, combining all the terms gives (15). □

Furthermore, note that Liu and Owen's formula (16) can be viewed as the integration of the second-order interaction index of a 2-dimensional function, obtained by fixing all variables except X_i, X_j. This result, proved below, gives an alternative way to compute the TII, used in [7] and investigated further in Section 3.

Proposition 3. *(Fixing method). For any $x_{-\{i,j\}}$, define $f_{\textit{fixed}}$ as the 2-dimensional function $f_{\textit{fixed}} : (x_i, x_j) \to f(\boldsymbol{x})$ obtained from f by fixing all variables except x_i and x_j. Let $D_{i,j|\boldsymbol{X}_{-\{i,j\}}}$ denote the second-order interaction index of $f_{\textit{fixed}}(X_i, X_j)$, which depends on the fixed variables $\boldsymbol{X}_{-\{i,j\}}$. Then the TII of X_i and X_j is obtained by integrating $D_{i,j|\boldsymbol{X}_{-\{i,j\}}}$ with respect to $\boldsymbol{X}_{-\{i,j\}}$:*

$$\mathfrak{D}_{i,j} = E\left(D_{i,j|\boldsymbol{X}_{-\{i,j\}}}\right). \tag{17}$$

Proof. Since the function f_{fixed} is 2-dimensional, it has only one interaction, which is a second-order one, and coincides with its TII. Hence, this interaction can be computed by applying (16) to f_{fixed}:

$$D_{i,j|\boldsymbol{X}_{-\{i,j\}}} = \frac{1}{4}\mathrm{E}\left[f_{\text{fixed}}(X_i, X_j) - f_{\text{fixed}}(X_i, Z_j) - f_{\text{fixed}}(Z_i, X_j) \right. \\ \left. + f_{\text{fixed}}(Z_i, Z_j)\right]^2.$$

Now one can rewrite the right hand side by using conditional expectations :

$$D_{i,j|\boldsymbol{X}_{-\{i,j\}}} = \frac{1}{4}\mathrm{E}\left[\left[f(X_i, X_j, \boldsymbol{X}_{-\{i,j\}}) - f(X_i, Z_j, \boldsymbol{X}_{-\{i,j\}}) \right.\right.$$
$$\left.\left. -f(Z_i, X_j, \boldsymbol{X}_{-\{i,j\}}) + f(Z_i, Z_j, \boldsymbol{X}_{-\{i,j\}})\right]^2 |\boldsymbol{X}_{-\{i,j\}}\right]. \quad (18)$$

Taking the expectation gives the result. □

3. Estimation methods

In this section, we treat different estimation methods for the computation of the TII. The theoretical expressions (14), (15), and (16) suggest different specific estimation methods. The first two ones rely respectively on RBD-FAST and pick-and-freeze estimation methods. First the underlying FAST method is quickly reviewed. Then these methods are presented together with some remarks on their properties.

3.1. Review of FAST

The Fourier amplitude sensitivity test (FAST) by [12] is a quick method for estimating first-order indices. Sample points of $\boldsymbol{X}$ are chosen such that the indices can be interpreted as amplitudes obtained by Fourier analysis of the function. More precisely the design of N points is such that

$$x_i(s_k) := G_i(\sin(\omega_i s_k)), \quad i = 1, \ldots, d, \ k = 1, \ldots, N, \ s_k = \frac{2\pi(k-1)}{N},$$

with G_i functions to ensure that the sample points follow the distribution of $\boldsymbol{X}$. The set of integer frequencies $\{\omega_1, \ldots, \omega_d\}$ associated with the input variables is chosen as "free of interferences" as possible; *free of interferences up to the order M* means that $\sum_{i=1}^{p} a_i\omega_i \neq 0$ for $\sum_{i=1}^{p} |a_i| \leq M + 1$ [13]. In practice, $M = 4$ or $M = 6$. The Fourier coefficients for each variable can then be numerically estimated by

$$\widehat{A}_\omega = \frac{1}{N}\sum_{j=1}^{N} f(x(s_j))\cos(\omega s_j),$$
$$\widehat{B}_\omega = \frac{1}{N}\sum_{j=1}^{N} f(x(s_j))\sin(\omega s_j),$$

and the first-order indices can be estimated by the sum of the corresponding amplitudes up to the order M:

$$\widehat{D}_i = 2\sum_{p=1}^{M}(\widehat{A}^2_{p\omega_i} + \widehat{B}^2_{p\omega_i}).$$

An estimate of the overall variance is given by the sum of all amplitudes

$$\widehat{D} = 2\sum_{n=1}^{N/2}(\widehat{A}^2_n + \widehat{B}^2_n). \tag{19}$$

3.2. Estimation with RBD-FAST, via total sensitivity indices

The computation of a total sensitivity index of groups of variables is possible with an RBD-FAST method. RBD-FAST is a group of modifications of classical FAST which use random permutations of design points to avoid interferences [14, 11]. To compute the RBD-FAST estimator of the total sensitivity index of a group of variables $\widehat{D}^T_I$, simple frequencies like $\boldsymbol{\omega} = \{1, \ldots, d\}$ are assigned to the variables. Then $N = 2(Md + L)$ design points are generated over a periodic curve where M denotes the fix inference factor (usually 4 or 6) and $L(> 100)$ is a selectable integer number regulating the sample size. The values of the factors in I are then randomly permuted (either differently per factor or identically) and the model is evaluated at the points. The total sensitivity index is estimated by

$$\widehat{D}^T_I = \frac{N}{L}\sum_{p=dM+1}^{N/2}(\widehat{A}^2_p + \widehat{B}^2_p).$$

The estimator corresponding to (14) is then given by

$$\widehat{\mathfrak{D}}_{i,j} = \widehat{D}^T_i + \widehat{D}^T_j - \widehat{D}^T_{i,j}. \tag{20}$$

3.3. Estimation with pick-and-freeze method, via closed sensitivity indices

It is also possible to compute closed sensitivity indices with an RBD-FAST method, which is called *hybrid version* in Mara [11]. But, as in classical FAST, frequencies that are free of interferences are needed. Here to apply (15), the estimation of the closed index D^C_{-i} is necessary which requires a number of $d-1$ free of interference frequencies. Those frequencies are not easy to find, especially for high dimensions. Therefore Monte Carlo integration is considered. Since the required closed indices, D^C_{-i} and $D^C_{i,j}$ are expected to be large, the pick-and-freeze method (8) is more suitable here than the expression in (9). To obtain the closed sensitivity index of a group of variables $\boldsymbol{X}_I$ a large number (n_{pf}) of random numbers from the distribution of $\boldsymbol{X}$ is sampled and another n_{pf} random numbers are sampled for the remaining variables $\boldsymbol{X}_{-I}$. Denote by $x^{*k} = (x^{*k}_I, x^{*k}_{-I})$ and $\boldsymbol{z}^{*k}_{-I}$ these two samples for $k = 1, \dots, n_{\mathrm{pf}}$. The closed sensitivity index of $\boldsymbol{X}_I$ is then estimated by the sample version of (8):

$$\widehat{D}^C_I = \frac{1}{n_{\mathrm{pf}}} \sum_{k=1}^{n_{\mathrm{pf}}} f(\boldsymbol{x}^{*k}_I, \boldsymbol{x}^{*k}_{-I}) f(\boldsymbol{x}^{*k}_I, \boldsymbol{z}^{*k}_{-I}) - \hat{\mu}_0^2, \tag{21}$$

with

$$\hat{\mu}_0 = \sum_{k=1}^{n_{\mathrm{pf}}} f(\boldsymbol{x}^{*k}_I, \boldsymbol{x}^{*k}_{-I}).$$

Consequently, with (15), the corresponding estimator for the TII is given by

$$\widehat{\mathfrak{D}}_{i,j} = \widehat{D} + \widehat{D}^C_{-\{i,j\}} - \widehat{D}^C_{-i} - \widehat{D}^C_{-j}, \tag{22}$$

where $\widehat{D}$ is the estimation of the variance calculated by the sample variance of $(\boldsymbol{x}^{*k}_I, \boldsymbol{x}^{*k}_{-I})$. One may remark that the additional sampling required in the pick-and-freeze method is quite economic here, since we only need the 2 additional samples z^*_i, z^*_j in Equation (21) for the computation of $\widehat{D}^C_{-\{i,j\}}$, $\widehat{D}^C_{-i}$ and $\widehat{D}^C_{-j}$.

3.4. Method by Liu and Owen

Liu and Owen suggest the estimation by Monte Carlo integration of the integral in Proposition 3, similar to the closed sensitivity index estimation in (21). Denote by $\boldsymbol{x}^k$ and $\boldsymbol{z}^k$, $k = 1, \dots, n_{\mathrm{LO}}$, two independent samples of length n_{LO} drawn from ν. Then the TII is estimated by

$$\begin{aligned}\widehat{\mathfrak{D}}_{i,j} = \frac{1}{4} \times \frac{1}{n_{\mathrm{LO}}} \sum_{k=1}^{n_{\mathrm{LO}}} \big[& f(x^k_i, x^k_j, \boldsymbol{x}^k_{-\{i,j\}}) - f(x^k_i, z^k_j, \boldsymbol{x}^k_{-\{i,j\}}) \\ & - f(z^k_i, x^k_j, \boldsymbol{x}^k_{-\{i,j\}}) + f(z^k_i, z^k_j, \boldsymbol{x}^k_{-\{i,j\}}) \big]^2 .\end{aligned} \tag{23}$$

3.5. Positivity and bias of the estimators

With the indices being theoretically non-negative, the estimates should also be non-negative. This holds in any case for the estimator by the *method by Liu and Owen* (23), which is a sum of squares.

The three estimation methods differ in terms of bias.

The *pick-and-freeze method* estimator (22) is unbiased since only direct Monte Carlo integrals (mean estimators) are used as estimators for the conditional expectations.

In the *method by Liu and Owen* (23) the estimator is unbiased, too, because of the direct Monte Carlo integration. This is especially remarkable in combination with positivity. In particular, it implies that when the true value is zero, the estimator is identically to zero as well, which holds indeed:

Proposition 4. *If* $\mathfrak{D}_{i,j} = 0$*, then the estimator is equal to zero:* $\widehat{\mathfrak{D}}_{i,j} \equiv 0$.

Proof. Let us consider the FANOVA decomposition of f (Section 2.1). If $\mathfrak{D}_{i,j} = 0$, then all the terms containing both x_i and x_j vanish. So the decomposition reduces to

$$\begin{aligned} f(\boldsymbol{x}) &= \sum_{i \notin I, j \notin I} \mu_I(x_i, \boldsymbol{x}_{-\{i,j\}}) + \sum_{i \in I, j \notin I} \mu_I(x_i, \boldsymbol{x}_{-\{i,j\}}) + \sum_{i \notin I, j \in I} \mu_I(x_j, \boldsymbol{x}_{-\{i,j\}}) \\ &:= a_0(\boldsymbol{x}_{-\{i,j\}}) + a_i(x_i, \boldsymbol{x}_{-\{i,j\}}) + a_j(x_j, \boldsymbol{x}_{-\{i,j\}}). \end{aligned}$$

Then the four terms in squared brackets in formula (23) add up to zero:

$$\begin{aligned} & f(x_i^k, x_j^k, \boldsymbol{x}_{-\{i,j\}}^k) - f(x_i^k, z_j^k, \boldsymbol{x}_{-\{i,j\}}^k) - f(z_i^k, x_j^k, \boldsymbol{x}_{-\{i,j\}}^k) + f(z_i^k, z_j^k, \boldsymbol{x}_{-\{i,j\}}^k) \\ &= a_i(x_i^k, \boldsymbol{x}_{-\{i,j\}}^k) - a_i(x_i^k, \boldsymbol{x}_{-\{i,j\}}^k) - a_i(z_i^k, \boldsymbol{x}_{-\{i,j\}}^k) + a_i(z_i^k, \boldsymbol{x}_{-\{i,j\}}^k) \\ &+ a_j(x_j^k, \boldsymbol{x}_{-\{i,j\}}^k) - a_j(z_j^k, \boldsymbol{x}_{-\{i,j\}}^k) - a_j(x_j^k, \boldsymbol{x}_{-\{i,j\}}^k) + a_j(z_j^k, \boldsymbol{x}_{-\{i,j\}}^k) = 0 \end{aligned}$$

□

Tissot and Prieur [13] also mention a bias for *RBD-FAST* estimators caused by a random noise in the signal coming from the sampled variables. This bias might be even enhanced here through the use of a combination of *RBD-FAST* estimators.

Remark 1. *Fixing method using 2-dimensional functions.* Proposition 3 showed that the TII can be computed by averaging the second-order interaction of 2-dimensional functions. As second-order interactions depend only on the overall variance and the first-order effects, for which accurate estimators are known, this suggests to estimate the TII based on them. More precisely, one can use the following scheme, proposed in [7], which is a sample version of the TII expression given in Proposition 3.

Let us consider a couple of integers (i, j), with $i < j$. For $k = 1, \ldots, n_{\mathrm{MC}}$, do:

1. Simulate $x^k_{-\{i,j\}}$ from the distribution of $\boldsymbol{X}_{-\{i,j\}}$, that is take a single sample of all variables except X_i and X_j,
2. Create the 2-dimensional function f_{fixed} by fixing f on $x^k_{-\{i,j\}}$:

$$f_{\mathrm{fixed}}(X_i, X_j) = f(x^k_1, \ldots, X_i, \ldots, X_j, \ldots, x^k_d),$$

3. Compute the second-order interaction index of f_{fixed}, denoted $\widehat{D}^k_{i,j|\boldsymbol{X}_{-\{i,j\}}}$, by removing the first-order indices from the overall variance.

Finally, compute the estimator

$$\widehat{\mathfrak{D}}_{i,j} = \frac{1}{n_{\mathrm{MC}}} \sum_{k=1}^{n_{\mathrm{MC}}} \widehat{D}^k_{i,j|\boldsymbol{X}_{-\{i,j\}}}. \tag{24}$$

For step 3, the FAST method can be used, since the computation is both quick, and returns a *positive* value provided that the frequency parameters are free of interferences and that the number of FAST evaluations, denoted n_{FAST}, is large enough. In various analytical simulations the method showed to be less accurate than the *method by Liu and Owen* and thus is not investigated further in this paper.

4. Asymptotic properties of the Liu and Owen estimator

In this section we consider the notion of asymptotical efficiency of van der Vaart [8, Chapter 25], and we show that the *Liu and Owen estimator* (23) is asymptotically efficient to estimate a single total interaction index.

Recalling equation (23) we define the estimator for a pair of input variables $\{X_i, X_j\}$:

$$T_n = \frac{1}{n}\sum_{k=1}^{n} \frac{\left(\Delta_{i,j}^k\right)^2}{4}$$

with

$$\begin{aligned}\Delta_{i,j}^k := f(X_i^k, X_j^k, \boldsymbol{X}_{-\{i,j\}}^k) - f(X_i^k, Z_j^k, \boldsymbol{X}_{-\{i,j\}}^k) - f(Z_i^k, X_j^k, \boldsymbol{X}_{-\{i,j\}}^k) \\ + f(Z_i^k, Z_j^k, \boldsymbol{X}_{-\{i,j\}}^k).\end{aligned}$$

In what follows we assume that $\boldsymbol{X}$ and $\boldsymbol{Z}$ are independent random vectors with probability measure ν and that the $(\Delta_{i,j}^k)^2$ are square integrable.

Proposition 5. *T_n is consistent for $\mathfrak{D}_{\mathrm{i,j}}$*

$$T_n \xrightarrow[n\to\infty]{a.s.} \mathfrak{D}_{\mathrm{i,j}}$$

and asymptotically normally distributed

$$\sqrt{n}\left(T_n - \mathfrak{D}_{\mathrm{i,j}}\right) \xrightarrow[n\to\infty]{d} \mathcal{N}\left(0, \frac{var[(\Delta_{i,j}^1)^2]}{16}\right).$$

Proof. The results are a direct application of the law of large numbers and the central limit theorem, applied to the variables $(\Delta_{i,j}^k)^2$. $\square$

Proposition 6. *T_n is an asymptotically efficient estimator for $\mathfrak{D}_{\mathrm{i,j}}$.*

Proof. Denote $\boldsymbol{\mathcal{X}}_k = (X_j^k, Z_j^k, \boldsymbol{X}_{-\{i,j\}}^k)$, $\mathcal{Z}_k = X_i^k$, $\mathcal{Z}_k' = Z_i^k$ and let g be the function defined over $\mathbb{R}^d \times \mathbb{R}$ by:

$$g(\boldsymbol{a}, b) = f(b, a_1, a_3, \ldots, a_d) - f(b, a_2, a_3, \ldots, a_d)$$

Then we have

$$\Delta_{i,j}^k = g(\boldsymbol{\mathcal{X}}_k, \mathcal{Z}_k) - g(\boldsymbol{\mathcal{X}}_k, \mathcal{Z}_k').$$

Therefore

$$T_n = \frac{1}{n}\sum_{k=1}^{n} \Phi_2(g(\boldsymbol{\mathcal{X}}_k, \mathcal{Z}_k), g(\boldsymbol{\mathcal{X}}_k, \mathcal{Z}_k')),$$

and

$$\mathfrak{D}_{i,j} = \mathrm{E}(\Phi_2(g(\boldsymbol{\mathcal{X}}_1, \mathcal{Z}_1), g(\boldsymbol{\mathcal{X}}_1, \mathcal{Z}_1^{'}))),$$

where Φ_2 is the 2-dimensional function of $\mathbb{R}^2$:

$$\Phi_2(u, v) = \frac{(u - v)^2}{4}.$$

Remark that $\mathcal{Z}_k$ and $\mathcal{Z}_k^{'}$ are independent copies of each other, both independent of $\boldsymbol{\mathcal{X}}_k$, and that Φ_2 is a symmetric function. The result then follows from Lemma 2.6 in Janon et al. [15], with the following change of notation

$$i \leftarrow k,\ \boldsymbol{X} \leftarrow \boldsymbol{\mathcal{X}},\ Z \leftarrow \mathcal{Z},\ Z^{'} \leftarrow \mathcal{Z}^{'},\ f \leftarrow g.$$

□

We conclude this section by remarking that the two last propositions extend to the general superset importance, including the case of the total sensitivity index of one variable.

Proposition 7. *Let $\Upsilon_I = \sum_{J \supseteq I} D_J$ be the superset importance for a set I. Define*

$$T_{I,n} = \frac{1}{n} \sum_{k=1}^{n} \frac{(\Delta_I^k)^2}{2^{|I|}},$$

with $\Delta_I^k = \sum_{J \subseteq I} (-1)^{|I-J|} f(\boldsymbol{Z}_J^k, \boldsymbol{X}_{-J}^k)$.
Then $T_{I,n}$ is asymptotically normal and asymptotically efficient for Υ_I.

Proof. Note that $T_{I,n}$ is the sample version of the formula (10) given by Liu and Owen [6] for Υ_I (with suitable change of notations). The proof of asymptotical normality is thus a direct consequence of central limit theorem. For asymptotical efficiency, the proof relies on similar arguments than Proposition 6:

- When $I = \{i\}$ is a single variable, we have:

  $$\Delta_I^k = f(Z_i^k, \boldsymbol{X}_{-i}^k) - f(X_i^k, \boldsymbol{X}_{-i}^k),$$

  which is of the form $g(\boldsymbol{\mathcal{X}}_k, \mathcal{Z}_k) - g(\boldsymbol{\mathcal{X}}_k, \mathcal{Z}_k^{'})$ with $\mathcal{Z}_k = Z_i^k$, $\mathcal{Z}_k' = X_i^k$, $\boldsymbol{\mathcal{X}}_k = \boldsymbol{X}_{-i}^k$, and $g(\boldsymbol{a}, b) = f(b, \boldsymbol{a})$.

- When $|I| \geq 2$, let choose $i \in I$. Then, by splitting the subsets of I into two parts, depending whether they contain $\{i\}$, we have:

$$\Delta_I^k = \sum_{J \subseteq I - \{i\}} (-1)^{|I-J|} f(\boldsymbol{Z}_J^k, \boldsymbol{X}_{-J}^k) + \sum_{J \subseteq I - \{i\}} (-1)^{|I-(J\cup\{i\})|} f(\boldsymbol{Z}_{J\cup\{i\}}^k, \boldsymbol{X}_{-(J\cup\{i\})}^k)$$

$$= \sum_{J \subseteq I - \{i\}} (-1)^{|I-J|} f(\boldsymbol{Z}_J^k, X_i^k, \boldsymbol{X}_{-(J\cup\{i\})}^k) - \sum_{J \subseteq I - \{i\}} (-1)^{|I-J|} f(\boldsymbol{Z}_J^k, Z_i^k, \boldsymbol{X}_{-(J\cup\{i\})}^k),$$

  which is also of the form $g(\boldsymbol{\mathcal{X}}_k, \mathcal{Z}_k) - g(\boldsymbol{\mathcal{X}}_k, \mathcal{Z}_k')$ with $\mathcal{Z}_k = X_i^k$, $\mathcal{Z}'_k = Z_i^k$, $\boldsymbol{\mathcal{X}}_k = (\boldsymbol{X}_{I-\{i\}}^k, \boldsymbol{Z}_{I-\{i\}}^k, \boldsymbol{X}_{-I}^k)$, and a suitable g, since the second term in the difference is obtained from the first one by exchanging X_i^k and Z_i^k.

The results then derives by applying Lemma 2.6 in Janon et al. [15] to the symmetric function $\Phi_2(u,v) = \frac{(u-v)^2}{2^{|I|}}$, remarking that $\mathcal{Z}_k$ and $\mathcal{Z}_k'$ are independent copies of each other, both independent of $\boldsymbol{\mathcal{X}}_k$. □

5. Estimating the full set of TIIs and application

5.1. Estimating the full set of TIIs

In the previous section, we proved the asymptotical efficiency of the *Liu and Owen estimator* to estimate a single TII. However, in practice one often needs to estimate the full set of $\frac{d(d-1)}{2}$ TIIs corresponding to all pairs of d influential variables. In that case, the strategies that reuse computations are helpful, as shown by Saltelli [16] about closed and total sensitivity indices. Such a strategy is possible for the TIIs with the *pick-and-freeze method* (22):

Proposition 8. *Given two samples of size n drawn independently from the distribution of $(X_1, \ldots, X_d)$, it is possible to compute at the cost of $n(d+1)$ function evaluations one estimate by the pick-and-freeze method for all $\binom{d}{2}$ TIIs. Furthermore:*

- *The same function evaluations can be used to give an estimate of the full set of total sensitivity indices.*
- *With an extra cost of n function evaluations, one can obtain in addition an estimate of the full set of first-order sensitivity indices.*

Proof. From Equation (15), one needs to estimate μ_0 and all the D_{-i}^C and $D_{-\{i,j\}}^C$ for $1 \le i < j \le d$. Now choose the pick-and-freeze method for estimation, and denote by f the function to evaluate and $\boldsymbol{x}^{*k}, \boldsymbol{z}^{*k}$ the two samples ($1 \le k \le n$). Then from Equation (8), all the D_{-i}^C can be estimated by computing $f(\boldsymbol{x}^{*k})$ and the $f(z_i^{*k}, \boldsymbol{x}_{-i}^{*k})$, $1 \le i \le d$. These $n(d+1)$ numbers are enough to give an estimate of μ_0, but also of all the $D_{-\{i,j\}}^C$, as remarked by Saltelli [16]. This is because one can exchange X_i and Z_i independently of the other variables in Equation (8):

$$\begin{aligned} D_{-\{i,j\}}^C + \mu_0^2 &= E[f(X_i, X_j, \boldsymbol{X}_{-\{i,j\}}) f(Z_i, Z_j, \boldsymbol{X}_{-\{i,j\}})] \\ &= E[f(Z_i, X_j, \boldsymbol{X}_{-\{i,j\}}) f(X_i, Z_j, \boldsymbol{X}_{-\{i,j\}})] \end{aligned}$$

The total sensitivity indices are obtained at the same time, thanks to Equations (11) and (5). The last part of the proposition is a direct consequence of Saltelli [16], Theorem 1, and Equations (11) and (15). □

Remark 2. Such strategy does not seem possible for the *Liu and Owen estimator* that requires in addition the evaluation of the $\binom{d}{2}$ $f(z_i, z_j, \boldsymbol{x_{-i,j}}^{(k)})$, for a total cost of $n\left(\binom{d}{2} + d + 1\right)$.

The performance of the estimators presented in Section 3 is now studied in analytical simulations. We consider a global budget of function evaluations N, granted to estimate all the TII. The parameters for each method are chosen in order to match N, since this is supposed to be the most time-consuming part, especially for functions with high complexity. Table 1 summarizes the relation between parameter settings and N. For *RBD-FAST*, when M is fixed (e.g. $M = 6$) then N is determined only by L.

5.1.1. Test functions

In order to study the estimators' performances in different situations we consider three functions with different interaction structures. The first func-

Estimation method	Number of function evaluations
RBD-FAST	$N = \left(\binom{d}{2} + d\right) \times 2(Md + L)$
Pick-and-freeze	$N = (d+1) \times n_{\text{pf}}$
Liu and Owen	$N = (\binom{d}{2} + d + 1) \times n_{\text{LO}}$

Table 1: Number of function evaluations for the three estimators (20), (22) and (24).

tion *function 1* is defined by

$$g(X_1, X_2, X_3, X_4) = \sin(X_1 + X_2) + 0.4\cos(X_3 + X_4),$$
$$X_k \overset{\text{i.i.d.}}{\sim} U[-1,1], \quad k = 1,2,3,4.$$

Its interactions are visibly not higher than second-order, a common situation. As a contrast, the extreme case of a single third-order interaction is applied in *function 2*:

$$g(X_1, X_2, X_3) = X_1 X_2 X_3, \quad X_k \overset{\text{i.i.d.}}{\sim} U[-1,1], \quad k = 1,2,3.$$

As a mixed case the popular g-function [17] is chosen. It is defined by

$$g(X_1, \dots, X_d) = \prod_{k=1}^{d} \frac{|4X_k - 2| + a_k}{1 + a_k}, \quad a_k \geq 0,$$
$$X_k \overset{\text{i.i.d.}}{\sim} U[0,1], \quad k = 1, \dots, d.$$

We choose $d = 6$ and $\boldsymbol{a} = (0, 0, 0, 0.4, 0.4, 5)'$ to create a function that contains high interactions. This is demonstrated by the fact that, analytically, the overall variance with $D = 3.27522$ is much greater than the sum of first and second-order indices equal to 2.06419. For the number of function evaluations we choose around 5 000 evaluations per index (in total $N = \binom{d}{2} \times 5\,000$) and thus set the parameters L, n_{pf}, and n_{LO} according to Table 1. We estimate each index 100 times for all three methods. Calculations are conducted using the R package `fanovaGraph` (see section Acknowledgements and supplementary material). The results can be seen in Figure 2.

5.1.2. Discussion

As expected in Section 3.5, negative results are observed for *RBD-FAST* and the *pick-and-freeze method*, but not for the *method by Liu and Owen*.

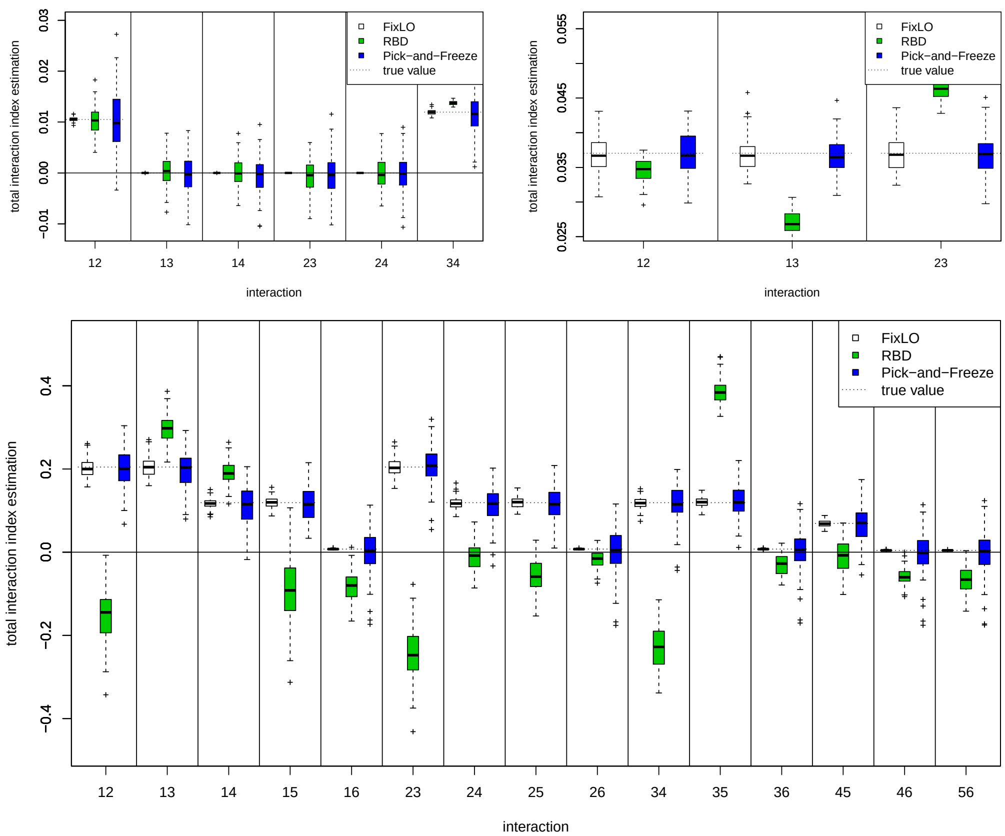

Figure 2: Estimates of the TII by the three estimators (20), (22), and (23) for test functions *1* (top left), *2* (top right) and g-function (bottom).

The *RBD-FAST* estimates show a small variance and seem to be unbiased for *function 1*. But with the presence of higher-order interactions in *function 2* and g-function, estimates are severely biased. One reason for this might be the bias for RBD-FAST methods described in Section 3.5.
The estimates by *pick-and-freeze method* on the other hand appear to be unbiased, but with a larger variance, resulting from the underlying crude Monte Carlo integration.
The *method by Liu and Owen* performs well in terms of bias as expected from Section 3.5. Its variance is very low for *function 1*, higher for *function 2* and varies for the g-function. We observe that the variance is higher

when the pair of variables in question $\{X_i, X_j\}$ is part of interactions of a higher order than second-order. The reason for this lies in the variance of the estimates $\widehat{D}^k_{i,j|\boldsymbol{X}_{-\{i,j\}}}$ in the fixing method (17). For second-order interactions those estimates do not depend on the fixed values $\boldsymbol{X}_{-\{i,j\}}$ and thus vary only slightly, while for higher interactions the estimates should differ with the fixed variables included in the interaction. While this means that the accuracy of the *method by Liu and Owen* strongly depends on the interaction situation, it is still here the best of the estimation methods. This is especially remarkable as the number of Monte Carlo samples n_{LO} is much lower than for the *pick-and-freeze method*, e.g. in dimension 6 it is more than 3 times lower. Moreover the methods' estimates have the desirable property of having a very low variance for total interaction indices that are close to zero (they are even exactly zero for inactive indices as mentioned in Section 3.5). That means that the *method by Liu and Owen* enables a precise detection of inactive interactions, an important task for interaction screening.
Finally notice that the *pick-and-freeze method* may take advantage of the recycling strategy when the number of influential variables d is larger: Its global computational cost is only linear with respect to d.

In simulation studies performed in higher dimensions, however, we did not observe a general superiority of the *pick-and-freeze method*. This may be due to the fact that after [6] "it is numerically better to average squared differences than to take a difference of large squared quantities". Here the *pick-and-freeze method* is indeed taking a linear combination of 4 potentially large squared quantities (15).

5.2. Example of application

In many phenomena it is not rare, that some groups of input variables have a separate influence on the output. In that case, the function of interest is decomposed as a sum of lower dimensional terms. In this section, we illustrate how the TII can be used to recover such decomposition. For instance, let us consider a function:

$$\begin{aligned} f(X_1, \dots, X_{12}) = \frac{1}{10}&(1.3X_1 + 0.7X_2)(0.7X_3 + 1.2X_1) \\ &+ \frac{1}{2}\sin(10(1.3X_2 + 0.8X_4 + 1.2X_5 + 1.4X_6)) \\ &\quad + \frac{2.1X_7 + 1.3X_8 + 0.8X_9}{5|X_7| + 1} + \frac{1}{100}\left(X_{10} + X_{11} + X_{12}\right), \end{aligned}$$

with $X_k \overset{\text{i.i.d.}}{\sim} U[-\pi, \pi], \quad k = 1, \ldots, 12$. It consists of three larger additive terms, two of them intersect in X_2, and three nearly inactive variables X_{10}, X_{11}, X_{12}. Our aim is to recover the decomposition of f into the additive parts. First we estimate the first-order and total sensitivity indices by FAST (section 3.1). The results, normalized by the overall variance for comparison purpose, can be seen in Figure 3 on the left. The values for total sensitivity indices are all very high, so that no variable can be removed. The large differences between standard and total sensitivity indices indicate a strong interaction structure in the function, but the nature of the structure cannot be read from it.

Therefore, in the next step, we estimate total interaction indices. We choose the *method by Liu and Owen* for estimation, but the *pick-and-freeze method* is another reasonable choice, giving similar results. A nice way to visualize the estimated interaction structure is the so called FANOVA graph [7]. In the graph, each vertex represents one input variable and an edge between two vertices indicates the presence of second or higher-order interactions between the variables. Figure 3 on the right shows the FANOVA graph for the application example. The thickness of the edges is proportional to the TII and in addition the thickness of the circles around vertices indicates the first-order indices. The three additive parts are clearly visible, as well as the intersection in X_2. The nearly inactive variables can be detected as single thin vertices.

6. Conclusion

We considered the problem of analyzing the interaction structure of a multivariate function, possibly containing high-order interactions. For this purpose, we investigated the total interaction index (TII), defined as the superset importance of a pair of variables. The TII generalizes variable screening, usually conducted with the total sensitivity index, to interactions, and can be used to discover additive structures.

First, we gave several theoretical expressions of the TII, including connections to total and closed sensitivity indices, and an interpretation as an average of the second-order interaction of a 2-dimensional function obtained by fixing the original one ("fixing method"). The Liu and Owen's [6] formula can be viewed this way.

Then we focused on statistical inference, and considered three estimators deduced from the aforementioned expressions: *RBD-FAST*, *pick-and-freeze*

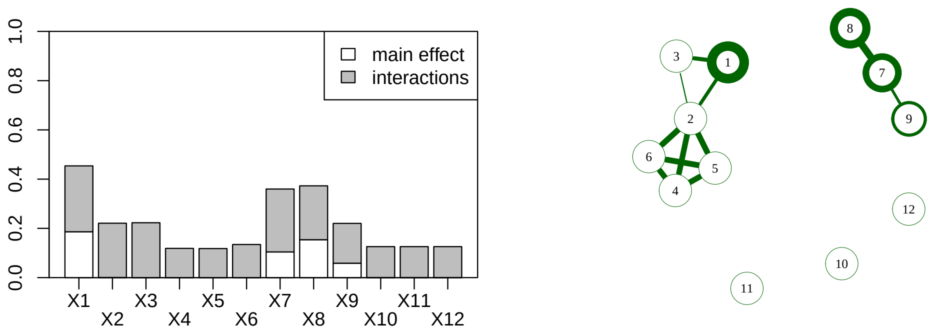

Figure 3: On the left: First-order indices (white) and total sensitivity indices (gray) of the application example, estimated by FAST. On the right: FANOVA-graph for the application example. The thickness of the circles around the vertices represents first-order indices, the thickness of the edges represents total interaction effects.

method and the *method by Liu and Owen*. We proved that the latter has good properties to estimate a single TII: It is both unbiased and positive, and asymptotically efficient. Its asymptotical normality was also derived.

Furthermore, we addressed the question of estimating the full set of TIIs with a given budget of function evaluations. In this case, the *pick-and-freeze method* can give estimates at a linear cost with respect to the problem dimension, while quadratic for the others. However, this is balanced by the lesser accurate estimate, built as a difference of 4 potentially large squared quantities. We investigated the question in an empirical study, showing in particular some results in dimensions up to 6. We observed that the *RBD-FAST estimator* could not be trusted, revealing an unpredictable strong bias with some functions. The *method by Liu and Owen* gave the best results, even in 6 dimensions taking around three times less function evaluations per index than the *pick-and-freeze method* for the same number of overall evaluations. In larger dimensions, our experience is that the *method by Liu and Owen* is still a good competitor.

Finally, we illustrated how the detection of inactive total interactions can be used to recover the decomposition of a complex function by identifying the groups of input variables that have a separate influence on it, without any prior knowledge about the groups. Here the indices were also used to graphically visualize the interaction structure of the function.

Supplementary material

The estimation methods as well as FANOVA graphs have been implemented in the R package `fanovaGraph` (version 1.4), published on the official R website (CRAN). We thank T. Muehlenstaedt for a useful first version of the code, and U. Ligges and O. Mersmann for their relevant advice about programming.

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