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Total interaction indices for the decomposition of functions with high complexity

Jana Fruth · Olivier Roustant · Sonja Kuhnt

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Abstract We consider functions of high complexity that cannot be reduced to main effects and second order interactions. In this context, identifying groups of variables that have no interaction together can be done with the *total interaction* index, which quantifies the total contribution brought by a couple of variables. The aim of the paper is to investigate these indices. At the theoretical level, we show connections with total indices and closed indices, and prove that the total interaction index can be computed by integrating the second interaction of a 2-dimensional function obtained by cutting the original one. Then, we focus on computational issues and compare three different methods on several analytical test functions. The superiority of the so-called fixing method is demonstrated to estimate total interaction indices of low value.

1 Introduction

Let $f(x_1, \dots, x_d)$, $f \in L^2(\Delta, \mu)$ be a highly complex, real-valued function over $\Delta \subset \mathbb{R}^d$. Our aim is to reduce the complexity of f by decomposition to study the structure of the function with regard to sensitivity analysis, optimization, metamodel improvement or graph visualization.

The usual approach to screen a function is to analyse the variance of $f(X)$ where X is a random vector with distribution ν . Sobol indices for the influence of the input variables on the response variance are calculated and only variables with noticeable influence are kept. Sometimes also indices for the influence of interactions between two variables are calculated

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and again only important interactions are retained. Indices for higher interactions however cannot be estimated for computational and cost reasons and so important information is often lost. One way to consider higher interactions is to use so-called total indices of main effects, i. e. indices that contain the influence of an effect including all its interactions. By this, higher order interactions cannot be missed but only main effects can be treated.

We want to go one step further and consider indices that we propose to call *total interaction indices* which originate from Muehlenstaedt et al (2011). Here second order interactions and their higher interactions are considered and thus a deeper insight in the structure of a function can be obtained. In particular, the detection of inactive total interactions can be applied to identify groups of input variables that have no interaction together, which often happens, even for complex phenomena. This allows to recover the structure of a function that is decomposed as a sum of lower-dimensional terms. The paper is structured as follows. Section 2 presents the main theoretical results concerning total interaction indices, after giving a quick overview of FANOVA decomposition and Sobol indices. Then in section 3, three estimation methods are deduced, and compared empirically. Finally in section 4, the total interaction indices are used to recover the block-additive decomposition of a 6-dimensional function as a sum of two 3-dimensional ones.

2 Theoretical aspects

2.1 A quick overview of FANOVA decomposition and Sobol Indices

Assume that the input factors X_1, \dots, X_d are independent random variables, and denote ν the probability measure of $X = (X_1, \dots, X_d)$. Then for any function $f \in L^2(\nu)$, the functional ANOVA decomposition provides a unique decomposition of the function into additive terms

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

The terms represent main effects ($\mu_i(X_i)$), second-order interactions ($\mu_{ij}(X_i, X_j)$) and all higher combinations of input variables. For uniqueness two conditions have to hold (Efron and Stein, 1981):

$$E(\mu_I(X_I)) = 0, \quad I \subseteq \{1, \dots, d\} \quad (1)$$

and

$$E(\mu_{i' i''}(X_{i'} X_{i''}) | X_i) = E(\mu_{i' i''}(X_{i'} X_{i''}) | X_i X_{i'}) = \dots = 0. \quad (2)$$

From (1) and (2) it follows that

$$E(\mu_I(X_I) \mu_{I'}(X_{I'})) = 0, \quad I \neq I'. \quad (3)$$

The decomposition can be obtained by recursive integration:

$$\mu_0 = E(f(X)),$$

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

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

and more generally:

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

By computing the variance, an ANOVA-like variance decomposition is obtained where each part quantifies the impact of the input variables on the response.

$$D = \text{var}(f(X)) = \text{var}(\mu_0) + \sum_{i=1}^d \text{var}(\mu_i(X_i)) + \sum_{i < j} \text{var}(\mu_{ij}(X_i, X_j)) \\ + \dots + \text{var}(\mu_{1, \dots, d}(X_1, \dots, X_d))$$

Those variances are widely used as indices for the influence of input variables and their interactions (Sobol indices). In this paper we only look at the variances and ignore the usual normalizing by the overall variance (D) for the sake of simplicity.

$$D_I = \text{var}(\mu_I(X_I)). \quad (5)$$

There are several extensions to the standard Sobol indices in (5). The total effect index D_i^T (Saltelli et al, 2000) of a single input variable X_i describes the total contribution of the variable including all interactions and is defined by the sum of all indices containing i :

$$D_i^T = \sum_{J \supseteq \{i\}} D_J.$$

It is straightforward to extend this index to groups of variables X_I , for any $I \subseteq \{1, \dots, d\}$, by the sum of all indices containing at least one of the variables:

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

Another way to describe the influence of a group of variables is the closed index D_I^C (see e.g. Mara, 2009). In contrast to total indices, interactions with variables not in 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) and for main effects it matches with the standard Sobol index.

$$D_I^C = \text{var}(E[f(X)|X_I]) = \sum_{J \subsetneq I} D_J. \quad (7)$$

If we define by $-I$ the complementary subset to I ($-I = \{1, \dots, d\} \setminus I$), we obtain from (6) and (7) the well-known relation (see e.g. Mara, 2009):

$$D = D_{-I}^C + D_I^T \quad (8)$$

and in particular, with the formula of total variance, one can deduce that the total index relatively to I is equal to the expectation of the conditional variance (ECV) relatively to the complementary subset $-I$:

$$D_I^T = E(\text{var}[f(X)|X_{-I}]). \quad (9)$$

2.2 Total interaction indices

The total interaction indices measure the portion of variance of an output explained by two input variables simultaneously.

Definition. With the notations and assumptions of section 2.1, the *total interaction* index \mathfrak{D}_{ij} of two variables X_i and X_j is defined by:

$$\mathfrak{D}_{ij} := \text{var} \left(\sum_{I \supseteq \{i,j\}} \mu_I(X_I) \right) = \sum_{I \supseteq \{i,j\}} D_I \quad (10)$$

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

Proposition 1. The following relations hold:

$$\mathfrak{D}_{ij} = D_i^T + D_j^T - D_{i,j}^T \quad (11)$$

$$\mathfrak{D}_{ij} = D + D_{-\{i,j\}}^C - D_{-i}^C - D_{-j}^C \quad (12)$$

Proof (12) is deduced from (11) using (8). For (11), the results come from the identity:

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

The following proposition shows that it is also possible to compute the total interaction indices by integration of second order interactions index of 2-dimensional functions:

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

$$\mathfrak{D}_{ij} = \mathbb{E} \left(D_{i,j|x_{-\{i,j\}}} \right). \quad (13)$$

Remark. Proposition 2 shows the equality between the sensitivity index defined in Muehlenstaedt et al (2011) and the total interaction index (10)

Proof A direct connection of $E\left(D_{i,j|X_{-\{i,j\}}}\right)$ with the definition (10) of total interaction indices can be obtained by considering the FANOVA decomposition of f_{fixed} . This way is detailed in the appendix. However, a simpler approach is to connect the three terms composing the second order interaction of f_{fixed} to the total indices of $f(\mathbf{X})$. Denote respectively by $D_{|X_{-\{i,j\}}}$, $D_{i|X_{-\{i,j\}}}$ and $D_{j|X_{-\{i,j\}}}$ the variance and the main effects of f_{fixed} . Since f_{fixed} is 2-dimensional, there is a unique (second order) interaction, given by:

$$D_{i,j|X_{-\{i,j\}}} = D_{|X_{-\{i,j\}}} - D_{i|X_{-\{i,j\}}} - D_{j|X_{-\{i,j\}}} \quad (14)$$

and thus:

$$E\left(D_{i,j|X_{-\{i,j\}}}\right) = E\left(D_{|X_{-\{i,j\}}}\right) - E\left(D_{i|X_{-\{i,j\}}}\right) - E\left(D_{j|X_{-\{i,j\}}}\right) \quad (15)$$

Consider each term separately:

- The variance of f_{fixed} , first, is given by:

$$D_{|X_{-\{i,j\}}} = \text{var}\left[f(\mathbf{X})|X_{-\{i,j\}}\right]$$

which implies with (9) that:

$$E\left(D_{|X_{-\{i,j\}}}\right) = E\left(\text{var}\left[f(\mathbf{X})|X_{-\{i,j\}}\right]\right) = D_{i,j}^T$$

- For the main effect of f_{fixed} explained by X_i , using (7) or directly the FANOVA decomposition in (4) the index is equal to:

$$\begin{aligned} D_{i|X_{-\{i,j\}}} &= \text{var}\left[E\left[f_{\text{fixed}}(X_i, X_j)|X_i\right]|X_{-\{i,j\}}\right] \\ &= \text{var}\left[E\left[f(\mathbf{X})|X_{-j}\right]|X_{-\{i,j\}}\right] \end{aligned}$$

Now use the total variance formula, conditional to $X_{-\{i,j\}}$:

$$D_{i|X_{-\{i,j\}}} = \text{var}\left[f(\mathbf{X})|X_{-\{i,j\}}\right] - E\left[\text{var}\left[f(\mathbf{X})|X_{-j}\right]|X_{-\{i,j\}}\right]$$

Thus, by integrating w.r. to $X_{-\{i,j\}}$, and using (9) again, we get:

$$\begin{aligned} E\left(D_{i|X_{-\{i,j\}}}\right) &= E\left(\text{var}\left[f(\mathbf{X})|X_{-\{i,j\}}\right]\right) - E\left(\text{var}\left[f(\mathbf{X})|X_{-j}\right]\right) \\ &= D_{i,j}^T - D_j^T \end{aligned}$$

- Similarly, we have: $E\left(D_{j|X_{-\{i,j\}}}\right) = D_{i,j}^T - D_i^T$

Finally, from (15) and (11), we obtain:

$$\begin{aligned} E\left(D_{i,j|X_{-\{i,j\}}}\right) &= D_{i,j}^T - (D_{i,j}^T - D_i^T) - (D_{i,j}^T - D_j^T) \\ &= D_i^T + D_j^T - D_{i,j}^T = \mathfrak{D}_{ij}. \quad \square \end{aligned}$$

3 Estimation methods

In this section, we treat different estimation methods for the computation of total interaction indices. The theoretical expressions (11), (12), (13) suggest three different specific estimation methods, relying respectively on RBD-FAST, Sobol, and FAST estimation methods. Following the method presentations and some remarks on their properties, an empirical comparison of the three estimators is conducted in the end of the section. First the underlying FAST method is quickly reviewed.

3.1 Review of FAST

The Fourier amplitude sensitivity test (FAST) by Cukier et al (1978) is a very efficient method to estimate first order Sobol indices. The sample points of X are chosen so 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

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

with G_i functions to ensure that the sample points follow the distribution of X . The set of integer frequencies $\{\omega_1, \dots, \omega_d\}$ associated to 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 $\sum_{i=1}^p |a_i| \leq M+1$ (Tissot and Prieur, +2011). In practice, $M = 4$ or 6 .

The Fourier coefficients for each variable can then be numerically estimated by

$$A_\omega = \frac{1}{N} \sum_{j=1}^N f(x(s_j)) \cos(\omega s_j),$$

$$B_\omega = \frac{1}{N} \sum_{j=1}^N f(x(s_j)) \sin(\omega s_j).$$

and the main effects' indices can be estimated by the sum of the corresponding amplitudes up to the order M :

$$\widehat{D}_i = 2 \sum_{p=1}^M (A_{p\omega_i}^2 + B_{p\omega_i}^2)$$

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

$$\widehat{D} = 2 \sum_{n=1}^{N/2} (A_n^2 + B_n^2) \quad (16)$$

3.2 The three estimators

3.2.1 Estimation with RBD-FAST, via total indices

The computation of a total index of groups of variables is possible with an RBD-FAST method. RBD-FAST is a group of modifications of classical FAST that use random permutation of design points to avoid interferences (Mara, 2009). To compute the RBD-FAST estimator of the total index of a group of variables \widehat{D}_I^T simple frequencies like $w = \{1, \dots, d\}$ 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 $L (> 100)$ a selectable integer number regulating the sample size. The values of the factors in I are then randomly permuted (either different per factor or the same) and the model is evaluated at the points. The total index is estimated by

$$\widehat{D}_I^T = \frac{N}{L} \sum_{p=dM+1}^{N/2} (A_p^2 + B_p^2)$$

The estimator corresponding to (11) is then given by:

$$\widehat{\mathfrak{D}}_{ij} = \widehat{D}_i^T + \widehat{D}_j^T - \widehat{D}_{\{i,j\}}^T \quad (17)$$

3.2.2 Estimation with Sobol method, via closed indices

It is also possible to compute closed indices with an RBD-FAST method, which is called *hybrid version* in Mara (2009). But, as in classical FAST, frequencies that are free of interferences are needed. Here to apply (12), the estimation of the closed index D_{-i}^C is necessary which requires a number of $d - 1$ free of interference frequencies. Those frequencies are, especially for high dimensions, not easy to find. Therefore another way to obtain closed indices, Monte Carlo integration (Sobol, 1993), is considered. To obtain the closed index of a group of variables X_I a large number (n_{Sobol}) of random numbers from the distribution of X has to be sampled and another n_{Sobol} random numbers are sampled for the remaining variables X_{-I} . Denote by $x^{*k} = (x_I^{*k}, x_{-I}^{*k})$ and z_{-I}^{*k} these two samples for $k = 1, \dots, n_{\text{Sobol}}$. The closed index of X_I is then estimated by

$$\widehat{D}_I^C = \frac{1}{n_{\text{Sobol}}} \sum_{k=1}^{n_{\text{Sobol}}} f(x_I^{*k}, x_{-I}^{*k}) f(x_I^{*k}, z_{-I}^{*k}) - \widehat{\mu}_0^2 \quad (18)$$

with

$$\widehat{\mu}_0 = \sum_{k=1}^{n_{\text{Sobol}}} f(x_I^{*k}, x_{-I}^{*k}).$$

Consequently, with (12), the corresponding estimator for the total interaction index is given by:

$$\widehat{\mathcal{D}}_{ij} = \widehat{D} + \widehat{D}_{-\{i,j\}}^C - \widehat{D}_{-i}^C - \widehat{D}_{-j}^C \quad (19)$$

where \widehat{D} is the estimation of the variance calculated by the sample variance of (x_I^{*k}, x_{-I}^{*k}) . One may remark that the additional sampling required in the Sobol method is quite economic here, since the complementary subsets $-\{i, j\}$, $-\{i\}$ and $-\{j\}$ have a very small size.

3.2.3 Estimation by integrating second order interactions (fixing method)

Following proposition 2, the total interaction index can be computed according to the following scheme:

For $k = 1, \dots, n_{\text{MC}}$, do:

1. Simulate $X_{-\{i,j\}}^{*k}$ from the distribution of $X_{-\{i,j\}}$,
2. Fix all variables out of $\{X_i, X_j\}$ to $X_{-\{i,j\}}^{*k}$, and create the corresponding 2-dimensional function f_{fixed} ,
3. Compute the second order interaction index of f_{fixed} , denoted $\widehat{D}_{i,j|X_{-\{i,j\}}}^k$, by removing the main effects indices to the overall variance as in (14).

Finally, compute the estimator:

$$\widehat{\mathcal{D}}_{ij} = \frac{1}{n_{\text{MC}}} \sum_{k=1}^{n_{\text{MC}}} \widehat{D}_{i,j|X_{-\{i,j\}}}^k \quad (20)$$

This estimation method seems to be greedy, due to the additional loop to simulate $X_{-\{i,j\}}$. On the other hand, only 2-dimensional functions are considered, which allows utilizing efficient techniques to compute the interaction index in step 3. For that purpose, we suggest the FAST method, 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, as we see in the next section.

3.3 Some properties of the three estimators

3.3.1 Positivity

There is no reason why the three estimators (17), (19), (20) should return a positive number. Nevertheless, there is a sufficient condition for the estimator (20) [fixing method]. This comes from the following proposition:

Proposition 3. Let f be a 2-dimensional function, and consider its second order interaction $D_{12} = D - D_1 - D_2$. Denote $\widehat{D}_{12} = \widehat{D} - \widehat{D}_1 - \widehat{D}_2$ its FAST estimate, with the notations of section 3.1. Assume that:

- (i) ω_1 and ω_2 are free of interference up to order $2M$,
 - (ii) $N \geq 2M \times \max(\omega_1, \omega_2)$
- Then $\widehat{D}_{12} \geq 0$.

Proof Denote the sets $W_{\omega_i, M} = \{p\omega_i, p = 1, \dots, M\}$ for $i = 1, 2$, and $W_N = \{1, \dots, N/2\}$. We have:

$$\widehat{D}_{12}/2 = \sum_{n \in W_N} (A_n^2 + B_n^2) - \sum_{n \in W_{\omega_1, M}} (A_n^2 + B_n^2) - \sum_{n \in W_{\omega_2, M}} (A_n^2 + B_n^2)$$

Now, the condition (i) ensures that $W_{\omega_1, M} \cap W_{\omega_2, M} = \emptyset$, while (ii) implies that $W_{\omega_i, M} \subseteq W_N$, for $i = 1, 2$. Hence,

$$\widehat{D}_{12}/2 = \sum_{n \in W_N - (W_{\omega_1, M} \cup W_{\omega_2, M})} (A_n^2 + B_n^2) \geq 0 \quad \square$$

Corollary. It is a direct consequence of proposition 3 that if (i) and (ii) are satisfied, then (20) returns positive values.

Remark In practice, one can use for instance $\omega_1 = 11$, $\omega_2 = 35$ (Mara, 2009), that are free of interferences up to $2M$ for the usual orders $M = 4, 6$; Then the minimal value of N is $2 \times 6 \times \max\{11, 35\} = 420$.

3.3.2 Bias

The three estimation methods differ in terms of bias.

Sobol method (19) The Sobol method estimator is unbiased since only direct Monte Carlo integrals (mean estimators) are used as estimators for the conditional expectations.

Fixing method (20) There are several sources of bias for the FAST estimator of main indices given by Tissot and Prieur (+2011): Interference, aliasing and truncation. However, (i) and (ii) in proposition 3 are stronger than the conditions given by Tissot and Prieur (+2011) to limit the bias due to interferences and aliasing. Furthermore, the bias due to truncation vanishes when n_{FAST} tends to infinity. For that reason one can expect (20) to be only slightly biased.

RBD-FAST (17) Tissot and Prieur (+2011) 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.

3.4 Comparison

<i>RBD-FAST</i>	$N = 2(Md + L) \times \binom{d}{2} + d$
<i>Sobol method</i>	$N = n_{Sobol} \times \left(\binom{d}{2} + d + 1 \right)$
<i>Fixing method</i>	$N = \binom{d}{2} \times n_{MC} \times n_{FAST}$

Table 1 Number of functions evaluations for the three estimators (17), (19) and (20).

The performance of the three estimators shall be studied empirically here. The parameters for each method are chosen in order to match the number of function evaluations N , since this is supposed to be the most time-consuming part, especially for functions with high complexity. We report to table 1 for the relation between parameter settings and N within each of the three methods. For the *Sobol method* the first factor in the MC integration (18) is evaluated only once for all index calculations to keep N low. The addition of 1 in the formula is due to that fact (where d is due to the first and $\binom{d}{2}$ to the second order indices). When we fix M (e.g. $M = 6$) then for *RBD-FAST* N is determined only by L and for *Sobol method* only by n_{Sobol} . For the *fixing method* the number of function evaluation depends on the product of n_{MC} and n_{FAST} . Setting $\omega_1 = 11$ and $\omega_2 = 35$, we chose $n_{FAST} = 500$, which satisfies the condition of proposition 3 and seems sufficient to give reliable estimates, so that only n_{MC} has to be adapted.

The g-function of Sobol is chosen as analytical test function for its high recognition and flexible interaction structure. It is defined by

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

We consider a number of $d = 6$ independent uniformly distributed variables and choose $a = (0, 0, 0, 0.4, 0.4, 5)'$ to have a structure with 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 with 2.06419 (Sobol, 2003). For the number of function evaluations we choose 5000 evaluations for each of the 15 indices (in total: $N = 75\,000$) and thus set the parameters $L = 1\,750$, $n_{Sobol} = 3\,409$ and $n_{MC} = 10$. We estimate each index 100 times for all three methods. The results can be seen in figure 1. As expected in section 3.3.1, negative results can be observed by *RBD-FAST* and the *Sobol method*. Because there is no negative variance, negative values should be treated as zero. The *RBD-FAST* estimates show the smallest variance of the three methods but are severely biased. One reason for this might be the bias for RBD-FAST methods described in section 3.3.2. The estimates by *Sobol method* and *fixing method* however appear almost unbiased but with higher variance, a consequence of crude Monte Carlo integration which is partly applied in the *fixing method* and completely in the *Sobol method*. That explains the better performance of the *fixing method*. Especially for the nearly inactive combinations with variable 6 the variance is very small,

an important property for the task of detecting inactive interactions.

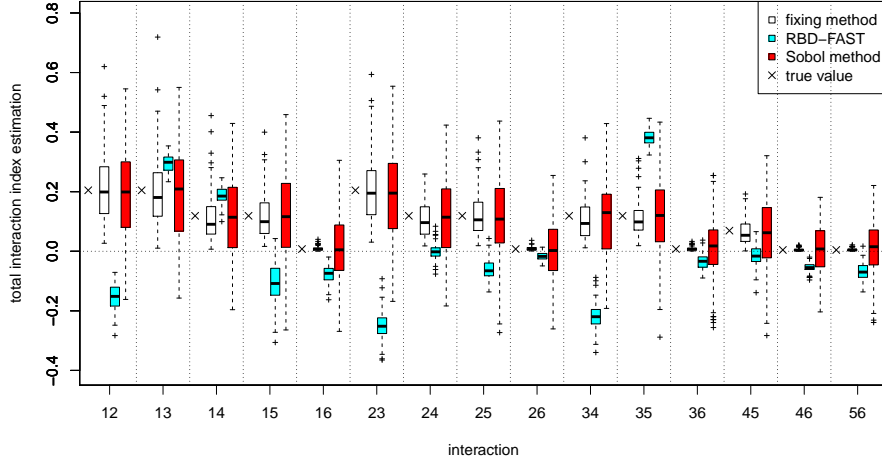


Fig. 1 Estimates of the total interaction indices of the g -function ($d=6$) of the three estimators (17), (19) and (20), $N = 75000$

To get an impression of the influence of the number of evaluations, N , we repeat the example study with the eight times higher value of $N = 600000$. Results can be seen in figure 2. As expected the variances of all three estimates are much reduced, most clearly for the *Sobol method* which also has almost no negative values any more. But its variance is still not smaller than the variance of the *fixing method*. The bias situation as well as the fact that the *fixing method* stands out at detecting inactive interactions remains the same.

4 Example of application

In many phenomena, it is not rare, even for complex ones, 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 total interaction indices can be used to recover such decomposition. For instance, let us consider the function:

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

with $X_k \stackrel{\text{i.i.d.}}{\sim} U[-1, 1]$, $k = 1, \dots, 6$, $\beta = [-0.8, -1.1, 1.1, 1]'$ and $\gamma = [-0.5, 0.9, 1, -1.1]$. Our aim is to recover the decomposition of f into additive parts. First we estimate standard and total indices of the main effects by FAST (section 3.1). The results, divided by the overall variance for comparison purpose, can be seen in table 4. The values for total indices all are very high, so no factor can be removed. The large difference between standard and total indices indicates a strong interaction structure in the function, but the nature of the structure

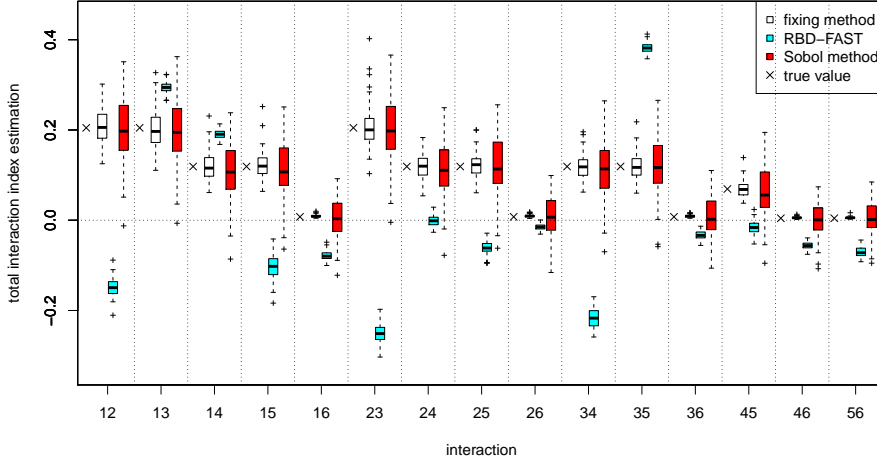


Fig. 2 Estimates of the total interaction indices of the g -function ($d=6$) of the three estimators (17), (19) and (20), $N = 600000$

cannot be read from it.

i	1	2	3	4	5	6
\widehat{D}_i/D	0.11639	0.14049	0.09037	0.11290	0.10862	0.19457
\widehat{D}_i^T/D	0.2326	0.20942	0.20770	0.17768	0.23113	0.25874

Table 2 Standard and total indices for the main effects of the application function

Therefore, in the next step, we want to estimate total interaction indices. On the basis of the results of section 3.4 we chose the *fixing method* for estimation. Results, again divided by the overall variance, are given in table 3.

i	1	1	1	1	1	2	2	
j	2	3	4	5	6	3	4	
$\widehat{\mathcal{D}}_{ij}/D$	0.00010	0.07257	0.00095	0.07876	0.00129	0.00126	0.04609	
i	2	2	3	3	3	4	4	5
j	5	6	4	5	6	5	6	6
$\widehat{\mathcal{D}}_{ij}/D$	0.00119	0.05509	0.00159	0.06399	0.00151	0.00153	0.04241	0.00164

Table 3 Estimates of total interaction indices for function a with $n_{\text{FAST}}=500$ and $n_{\text{MC}} = 50$

A nice way to visualize the estimated interaction structure is the so called FANOVA graph (Muehlenstaedt et al, 2011). In the graph, each vertex represent one input factor and

an edge between two vertices indicates the presence of second or higher order interactions between the factors. The left side of figure 3 shows the FANOVA graph for the application function. The thickness of the edges is proportional to the total interaction indices and in addition the thickness of the circles around vertices indicates the standard indices of main effects. The strong connection between factors 1, 3 and 5 is clearly visible as well as the slightly weaker connection between factors 2,4 and 6. All other values are very low and their analytical counterparts actually are zero. So by thresholding those indices by a reasonable value, e.g. $\delta = 0.01$ an even clearer image of the interaction structure (right side of figure 3) can be visualized and we obtain a decomposition into two additive parts. For more details and examples see Muehlenstaedt et al (2011).

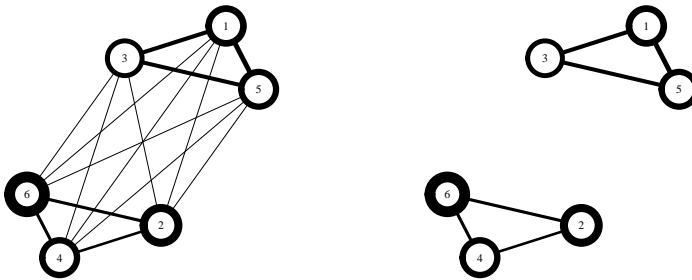


Fig. 3 FANOVA-graph for function a . Left: without thresholding, right: with thresholding at 0.02. The thickness of the circles around the vertices represents main effects, the thickness of the edges represents total interaction effects.

5 Conclusion

In this article total interaction indices were introduced and considered for the decomposition of functions with high order interactions. These indices quantify the contribution of second order interactions of variables and thus indicate decomposition cuts at inactive interactions. Exploiting theoretical connections between different kinds of indices, three methods to estimate total interaction indices were developed, using crude Monte Carlo integrals, RBD-FAST and integrals over the indices of 2-dimensional functions respectively. In empirical comparisons, for the same number of functions evaluations, the last one performed best in terms of bias and variance, especially for inactive interactions whereas the RBD-FAST method revealed a strong bias. 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. Here the indices were also used to graphically visualize the interaction structure of the function.

Further research will address the bias in the RBD-FAST method. The general idea is to apply the technique presented by Tissot and Prieur (+2011) to remove the bias in RBD-FAST

methods. Another main direction is the identification of the threshold cut below which estimates of total interaction indices are assumed to be close enough to zero. Several techniques, such as tests of significance and decision plots, may be considered.

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Appendix - A direct proof of proposition 2.

Another proof of proposition 2 can be obtained by looking at the FANOVA decomposition of f_{fixed} .

Lemma The decomposition below, obtained by gathering terms in the FANOVA decomposition of $f(X)$:

$$f_{\text{fixed}}(X_i, X_j) = \sum_{I \subseteq -\{i,j\}} \mu_I(x_I) + \sum_{I \subseteq -\{i,j\}} \mu_{\{i\} \cup I}(X_i, x_I) + \sum_{I \subseteq -\{i,j\}} \mu_{\{j\} \cup I}(X_j, x_I) + \sum_{I \subseteq -\{i,j\}} \mu_{\{i,j\} \cup I}(X_i, X_j, x_I) \quad (21)$$

is the FANOVA decomposition of $f_{\text{fixed}}(X_i, X_j)$.

The proof of the lemma is reported below. In particular, the second order interaction is given by the last term. Hence, we have by definition:

$$D_{i,j|x_{-\{i,j\}}} = \text{var} \left(\sum_{I \subseteq -\{i,j\}} \mu_{\{i,j\} \cup I}(X_i, X_j, x_I) \right) = \text{var} \left[\sum_{I \subseteq -\{i,j\}} \mu_{\{i,j\} \cup I}(X_i, X_j, X_I) \middle| X_{-\{i,j\}} = x_{-\{i,j\}} \right]$$

And, by integrating with respect to $x_{-\{i,j\}}$:

$$E \left(D_{i,j|x_{-\{i,j\}}} \right) = E \left(\text{var} \left[\sum_{I \subseteq -\{i,j\}} \mu_{\{i,j\} \cup I}(X_i, X_j, X_I) \middle| X_{-\{i,j\}} \right] \right)$$

Now, one can apply the total variance formula,

$$E \left(D_{i,j|x_{-\{i,j\}}} \right) = \text{var} \left(\sum_{I \subseteq -\{i,j\}} \mu_{\{i,j\} \cup I}(X_i, X_j, X_I) \right) - \text{var} \left[E \left(\sum_{I \subseteq -\{i,j\}} \mu_{\{i,j\} \cup I}(X_i, X_j, X_I) \middle| X_{-\{i,j\}} \right) \right]$$

and remark that, using (2), $E(\mu_{\{i,j\} \cup I}(X_i, X_j, X_I) | X_{-\{i,j\}}) = 0$, for any $i, j \notin I$. Finally:

$$\begin{aligned} E(D_{i,j|X_{-\{i,j\}}}) &= \text{var} \left(\sum_{I \subseteq -\{i,j\}} \mu_{\{i,j\} \cup I}(X_i, X_j, X_I) \right) \\ &= \sum_{I \subseteq -\{i,j\}} D_{\{i,j\} \cup I} = \sum_{I \supseteq \{i,j\}} D_I = \mathfrak{D}_{ij}. \quad \square \end{aligned}$$

Proof of the lemma For the sake of simplicity, we denote by μ_0^* , μ_i^* , μ_j^* and μ_{ij}^* the four summands, so that (21) is rewritten as:

$$\begin{aligned} f_{\text{fixed}}(X_i, X_j) &= \mu_0^*(x_{-\{i,j\}}) + \mu_i^*(X_i, x_{-\{i,j\}}) + \mu_j^*(X_j, x_{-\{i,j\}}) \\ &\quad + \mu_{ij}^*(X_i, X_j, x_{-\{i,j\}}) \end{aligned}$$

By uniqueness, it is sufficient to prove that these four terms satisfy the conditions (1) and (2).

– For condition (1), let us show for instance that $\mu_i^*(X_i, x_{-\{i,j\}})$ is centered. We have:

$$E(\mu_i^*(X_i, x_{-\{i,j\}})) = \sum_{I \subseteq -\{i,j\}} E(\mu_{\{i\} \cup I}(X_i, X_I) | X_{-\{i,j\}} = x_{-\{i,j\}})$$

As X_1, \dots, X_d are independent, the conditioning term can be reduced to X_I and thus, applying (2) for the FANOVA of $f(\mathbf{X})$, we obtain:

$$E(\mu_i^*(X_i, x_{-\{i,j\}})) = \sum_{I \subseteq -\{i,j\}} E(\mu_{\{i\} \cup I}(X_i, X_I) | X_I = x_I) = 0$$

The same ideas apply for $\mu_j^*(X_j, x_{-\{i,j\}})$ and $\mu_{ij}^*(X_i, X_j, x_{-\{i,j\}})$.

– For condition (2), it remains to show that $E(\mu_{ij}^*(X_i, X_j, x_{-\{i,j\}}) | X_i) = E(\mu_{ij}^*(X_i, X_j, x_{-\{i,j\}}) | X_j) = 0$. For the first one, for instance, we have:

$$\begin{aligned} &E(\mu_{ij}^*(X_i, X_j, x_{-\{i,j\}}) | X_i) \\ &= \sum_{I \subseteq -\{i,j\}} E(\mu_{\{i,j\} \cup I}(X_i, X_j, X_I) | X_i, X_{-\{i,j\}} = x_{-\{i,j\}}) \\ &= \sum_{I \subseteq -\{i,j\}} E(\mu_{\{i,j\} \cup I}(X_i, X_j, X_I) | X_i, X_I = x_I) \end{aligned}$$

which is null by application of (2) for the FANOVA of $f(\mathbf{X})$. This concludes the proof.

□

References

- Cukier R, Levine H, Shuler K (1978) Nonlinear sensitivity analysis of multiparameter model systems. *Journal of Computational Physics* 26(1):1–42
- Efron B, Stein C (1981) The jackknife estimate of variance. *The Annals of Statistics* 9(3):586–596
- Hoeffding W (1948) A class of statistics with asymptotically normal distributions. *Annals of Mathematical Statistics* 19:293–325
- Mara T (2009) Extension of the rbd-fast method to the computation of global sensitivity indices. *Reliability Engineering & System Safety* 94(8):1274–1281
- Muehlenstaedt T, Roustant O, Carraro L, Kuhnt S (2011) Data-driven Kriging models based on FANOVA-decomposition. To appear in *Statistics & Computing*
- Saltelli A, Chan K, Scott E (2000) *Sensitivity analysis*. Wiley Series in Probability and Statistics
- Saltelli A, Ratto M, Andres T, Campolongo F, Cariboni J, Gatelli D, Saisana M, Tarantola S (2008) *Global Sensitivity Analysis: The Primer*. Wiley-Interscience
- Sobol I (1993) Sensitivity estimates for non linear mathematical models. *Mathematical Modelling and Computational Experiments* 1:407–414
- Sobol I (2003) Theorems and examples on high dimensional model representation. *Reliability Engineering and System Safety* 79:187–193
- Tissot J, Prieur C (+2011) A bias correction method for the estimation of sensitivity indices based on random balance designs