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Total Interaction Index: A Variance-based Sensitivity Index for Function Decomposition

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1. Assumptions

Computer experiment or meta model function depending on d independent variables with probability measure ν

$$f : X_1, \dots, X_d \to \mathbb{R}$$

2. Sensitivity (Sobol) Indices

- Indices $\mathbf{D_I}$, $I \subset \{1, \dots, d\}$ measure global, model-independent importance of input factors and interactions → factor screening
- Originating from FANOVA (Hoeffding) decomposition

$$var(f(X)) = var(f_0) + \sum_{i=1}^{d} \underbrace{var(f_i(X_i))}_{\mathbf{D_i}} + \sum_{j<k} \underbrace{var(f_{jk}(X_j, X_k))}_{\mathbf{D_{jk}}} + \dots + \underbrace{var(f_{12\dots d}(X_1, X_2, \dots, X_d))}_{\mathbf{D_{1,2,\dots,d}}}$$

- Extensions:

Total index: $D_I^T = \sum_{J \cap I \neq \emptyset} D_J$ and closed index: $D_I^C = \sum_{J \subseteq I} D_J$

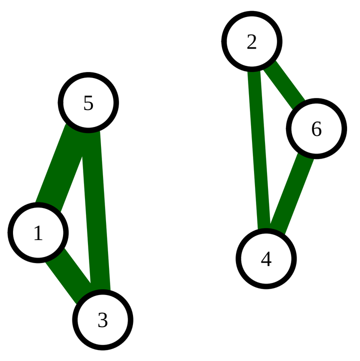
3. Total Interaction Indices

- Indices $\mathfrak{D}_{\mathbf{ij}}$ measure overall importance of second-order interactions → interaction screening

$$\mathfrak{D}_{ij} := var\left(\sum_{I \supseteq \{i,j\}} f_I(X_I)\right) = \sum_{I \supseteq \{i,j\}} D_I.$$

4. FANOVA Graph

- Visualization of the interaction structure
- Vertices = variables
- Edge thicknesses = size of total interaction indices
- Introduced by [2]



5. Block-additive Decomposition

Cliques of FANOVA graph $C_1, \dots, C_l$ decompose function into additive parts

$$f(X_1, \dots, X_d) = \sum_{i=1}^{l} f_{C_i}(X_{C_i})$$

USE FOR:

(i) Improvement of Kriging kernels by block-additive kernels

(ii) Simplification of optimization problems by separate optimizations

$$\min_{x_1,\dots,x_d} f(x_1, \dots, x_d) = \sum_{i=1}^{l} \min_{x_{C_i}} f_{C_i}(x_{C_i})$$

6. Properties of the Total Interaction Index

- Equal to the superset importance index for a pair of variables as defined by Liu and Owen [3]
- Relations to Sobol indices

$$\mathfrak{D}_{ij} = D_i^T + D_j^T - D_{i,j}^T$$
$$\mathfrak{D}_{ij} = D + D^C_{-\{i,j\}} - D^C_{-i} - D^C_{-j}$$

- Can also be derived by integration of second order indices of 2-dimensional functions (fixing method)

$$\mathfrak{D}_{ij} = E\left(D_{ij|X_{-\{ij\}}}\right)$$

with $D_{ij|X_{-\{ij\}}}$ the second order index of the function f fixed to all variables but X_i and X_j

7. Estimators for the Total Interaction Index

(i) RBD-FAST estimator (RBD)

$$\widehat{\mathfrak{D}}^{\text{RBD-FAST}}_{ij} = \widehat{D}_i^T + \widehat{D}_j^T - \widehat{D}_{\{i,j\}}^T,$$

with $\widehat{D}_I^T$ RBD-FAST estimator by [4] for the total index of a group of indices

(ii) Sobol estimator (Sobol)

$$\widehat{\mathfrak{D}}^{\text{Sobol}}_{ij} = \widehat{D} + \widehat{D}^C_{-\{i,j\}} - \widehat{D}^C_{-i} - \widehat{D}^C_{-j},$$

with $\widehat{D}^C_{-\{i,j\}}$ pick-freeze estimator for the closed index of a group of indices by [5]

(iii) Fixing estimator (FixFast) for $k = 1, \dots, n_{\text{MC}}$ do

(a) Simulate $X^{*k}_{-\{i,j\}}$ from the distribution of $X_{-\{i,j\}}$,

(b) Fix all variables except for $\{X_i, X_j\}$ to $X^{*k}_{-\{i,j\}}$ to create the 2-dimensional function f_{fixed},

(c) Compute the second order interaction index of f_{fixed}, denoted $\widehat{D}^k_{ij|X_{-\{ij\}}}$, by FAST, then

$$\widehat{\mathfrak{D}}^{\text{fix}}_{ij} = \frac{1}{n_{\text{MC}}} \sum_{k=1}^{n_{\text{MC}}} \widehat{D}^k_{ij|X_{-\{ij\}}}.$$

(iv) Liu and Owen estimator (FixLO)

$$\widehat{\mathfrak{D}}^{\text{LO}}_{ij} = \frac{1}{4} \times \frac{1}{n_{\text{LO}}} \sum_{k=1}^{n_{\text{LO}}} \left[f(x^k_i, x^k_j, x^k_{-\{i,j\}}) - f(x^k_i, z^k_j, x^k_{-\{i,j\}}) - f(z^k_i, x^k_j, x^k_{-\{i,j\}}) + f(z^k_i, z^k_j, x^k_{-\{i,j\}})\right]^2,$$

with x^k and z^k, $k = 1, \dots, n_{\text{LO}}$ two independent Monte Carlo samples drawn from ν

8. Derivation of Properties of Liu and Owen Estimator

- Unbiased, non-negative
- Identically zero in case of true inactive interaction, due to the differences in the squared term
- **Proposition.** $\widehat{\mathfrak{D}}^{\text{LO}}_{ij}$ is asymptotically normal distributed and asymptotically efficient for $\mathfrak{D}_{ij}$

Proof. The asymptotic normal distribution follows directly from the central limit theorem.

For the proof of the asymptotic efficiency, write $\widehat{\mathfrak{D}}^{\text{LO}}_{ij} = T_n = \frac{1}{n}\sum_{k=1}^{n} \frac{\left(\Delta^k_{i,j}\right)^2}{4}$, denote $\mathcal{X}_k = (X^k_j, Z^k_j, X^k_{-\{i,j\}})$, $\mathcal{Z}_k = X^k_i$, $\mathcal{Z}'_k = Z^k_i$, and let g be the function defined over $\mathbb{R}^d \times \mathbb{R}$ by

$$g(\mathbf{a}, b) = f(b, a_1, a_3, \dots, a_d) - f(b, a_2, a_3, \dots, a_d).$$

Then

$$\Delta^k_{i,j} = g(\mathcal{X}_k, \mathcal{Z}_k) - g(\mathcal{X}_k, \mathcal{Z}'_k).$$

Therefore

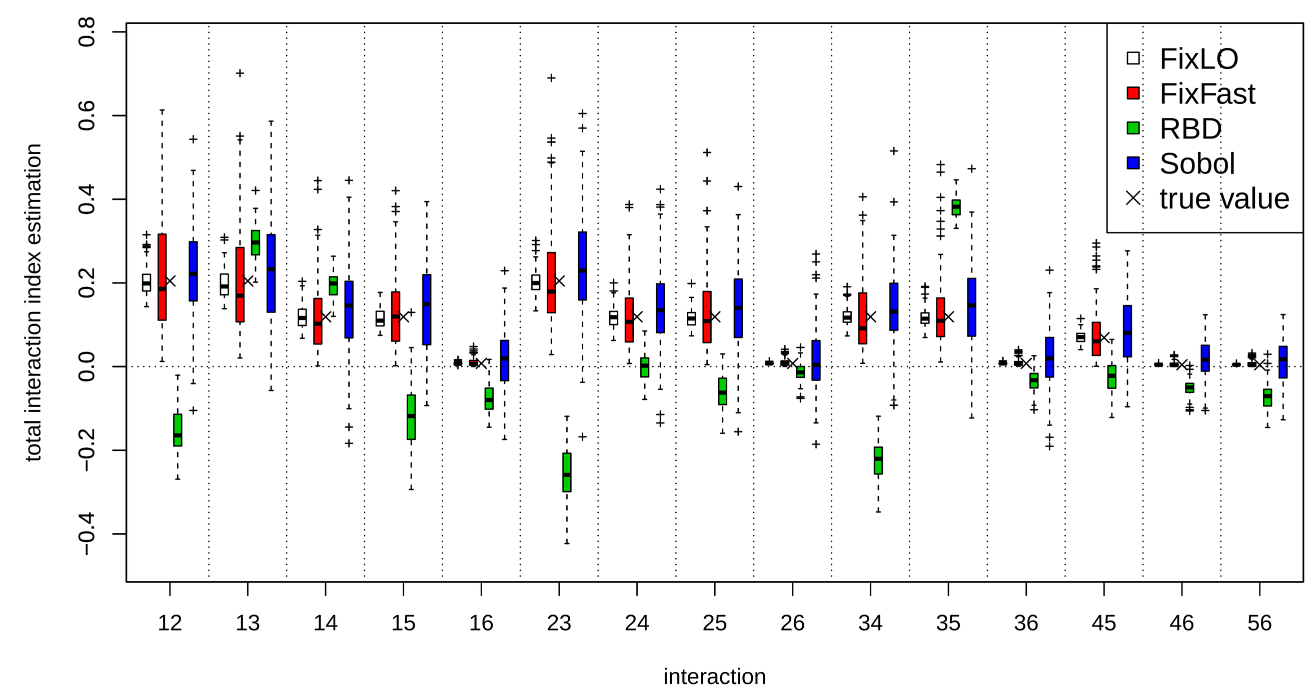
$$T_n = \frac{1}{n} \sum_{k=1}^{n} \Phi_2(g(\mathcal{X}_k, \mathcal{Z}_k), g(\mathcal{X}_k, \mathcal{Z}'_k)) \text{ and } \mathfrak{D}_{i,j} = E(\Phi_2(g(\mathcal{X}_1, \mathcal{Z}_1), g(\mathcal{X}_1, \mathcal{Z}'_1)))$$

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 $\mathcal{X}_k$, and that Φ_2 is a symmetric function. The result then follows from Lemma 2.6 in [6], with the following change of notation $i \leftarrow k$, $X \leftarrow \mathcal{X}$, $Z \leftarrow \mathcal{Z}$, $Z' \leftarrow \mathcal{Z}'$, $f \leftarrow g$. □

9. Empirical Comparisons

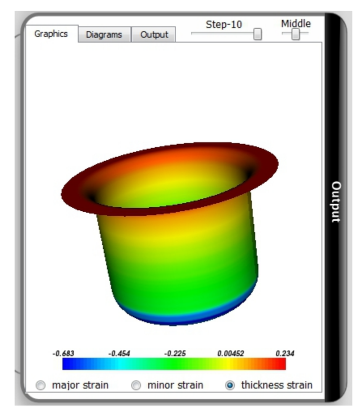
Test function: g-function [5] with $d = 6$ and $\boldsymbol{a} = (0, 0, 0, 0.4, 0.4, 5)'$ defined by

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



10. Application to Sheet Metal Forming

Computer simulation of 2D sheet metal forming process [7]

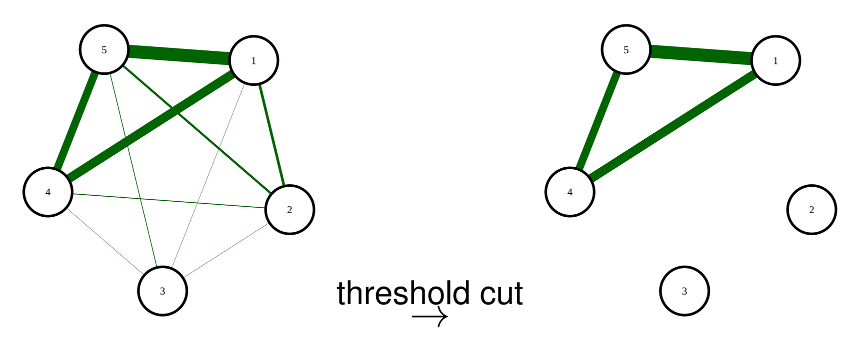


5 input variables:

- 3 material parameters
- blank holder force
- friction

output: minimal thickness strain

- Estimation of total interaction indices by Liu and Owen estimator, visualization in FANOVA graph:



- Block-additive decomposition: $f(x_1, \dots, x_5) = f_{145}(x_1, x_4, x_5) + f_2(x_2) + f_3(x_3)$
- Kriging kernel adaption: 30 percent reduction in RMSE

Literature

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[8] Fruth, J.; Mühlenstädt, T.; Roustant, O. (2012): fanovaGraph: Building Kriging models from FANOVA graphs. R package version 1.3.