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 \( \nu \):

\[ f : X_1, \ldots, X_d \rightarrow \mathbb{R} \]

2. Sensitivity (Sobol) Indices
- Indices \( D_p \), \( 1 \leq p \leq d \), measure global, model-independent importance of input factors and interactions → factor screening
- Originating from FANOVA (Hoeffding) decomposition

\[ \text{Total index: } D_p = \sum_{k=1}^{p} D_k \text{ and closed index: } D_p = \sum_{k=p+1}^{d} D_k \]

3. Total Interaction Indices
- Indices \( D_{ij} \) measure overall importance of second-order interactions → interaction screening

\[ D_{ij} := \sum_{t \leq 2(\nu_i + \nu_j)} \frac{f(X_{ij})}{2} = \sum_{t \leq 2(\nu_i + \nu_j)} \frac{D_t}{2} \]

4. FANOVA Graph
- Visualization of the interaction structure
- Vertices = variables
- Edge thicknesses = size of total interaction indices
- Introduce by [2]

5. Block-additive Decomposition
Clique of FANOVA graph \( C_1, \ldots, C_{10} \) decompose function into additive parts

\[ f(X_1, \ldots, X_d) = \sum_{i=1}^{10} f_i(X_i) \]

USE FOR:
(i) Improvement of Kriging kernels by block-additive kernels
(ii) Simplification of optimization problems by separate optimizations

\[ \min_{X_i} f(X_i, \ldots, X_d) = \sum_{i=1}^{10} \min_{X_i} f_i(X_i) \]

6. Properties of the Total Interaction Index
- Equal to the superscript importance index for a pair of variables as defined by Liu and Owen [3]
- Relations to Sobol indices

\[ D_{ij} = D_i + D_j - D_0 + D_{ij} \]

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

\[ D_{ij} = E \left( D_{ij}(X_{ij}) \right) \]

7. Estimators for the Total Interaction Index

(i) RBD-FAST estimator (RBD)

\[ \hat{D}_{ij}^{RBD-FAST} = \hat{D}_i + \hat{D}_j - \hat{D}_0 \]

(ii) Sobol estimator (Sobol)

\[ \hat{D}_{ij}^{Sobol} = D + \hat{D}_0 - \hat{D}_i - \hat{D}_j \]

(iii) Fix estimator (FixFast) for \( k = 1, \ldots, m \), \( \hat{D}_0 \)

(a) Simulate \( X_{ij}^{(k)} \) from the distribution of \( X_{ij} \)
(b) Fix all variables except for \( (X_i, X_j) \) to \( X_{ij} \) to create the 2-dimensional function \( f_{\text{2d}} \)
(c) Compute the second order interaction index of \( f_{\text{2d}} \), denoted \( \hat{D}_{ij}^{\text{2d}} \), by FAST, then

\[ \hat{D}_{ij}^{\text{2d}} = \frac{1}{2d} \sum_{k=1}^{d} \hat{D}_{ij}(X_{ij}^{(k)}) \]

(iv) Liu and Owen estimator (Liu-Owen)

\[ \hat{D}_{ij}^{Liu-Owen} = \frac{1}{2} \sum_{k=1}^{d} \left( f_i(x_{ij}^{(k)}) - f_i(x_{ij}^{(k)}) - f_j(x_{ij}^{(k)}) + f_j(x_{ij}^{(k)}) \right)^2 \]

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

9. Empirical Comparisons

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:
  \[ f(x_1, \ldots, x_5) = f_1(x_1, x_3, x_5) + f_2(x_2, x_3, x_4) + f_3(x_1, x_2, x_5) \]

- Kriging kernel adaption: 30 percent reduction in RMSE

Literature

\[ f(x_1, \ldots, x_5) = f_1(x_1, x_3, x_5) + f_2(x_2, x_3, x_4) + f_3(x_1, x_2, x_5) \]