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Sobol-Hoeffding decomposition: bounds and extremes

Olivier Roustant *

Synthesis of works with
F. Barthe, J. Fruth, F. Gamboa, B. Iooss, S. Kuhnt, C. Mercadier and T. Muehlenstaedt

* Mines Saint-Étienne

Seminar of Statistics at IMT Toulouse, 2018 December 11
Outline

1. Sobol-Hoeffding decomposition
   - Definition and ANOVA
   - Supersets and application to screening

2. Computational shortcuts based on derivatives
   - Upper bounds with Poincaré inequalities
   - Lower bounds with geometry

3. Connexion with extremes: the tail dependograph
Part I

Sobol-Hoeffding decomposition
Sobol-Hoeffding decomposition

Framework. \( X = (X_1, \ldots, X_d) \) is a vector of independent input variables with distribution \( \mu_1 \otimes \cdots \otimes \mu_d \), and \( g : \Delta \subseteq \mathbb{R}^d \to \mathbb{R} \) is such that \( g(X) \in L^2(\mu) \).

**Theorem [Hoeffding, 1948, Efron and Stein, 1981, Sobol, 1993]**

There exists a unique expansion of \( g \) of the form

\[
g(X) = g_0 + \sum_{i=1}^{d} g_i(X_i) + \sum_{1 \leq i < j \leq d} g_{i,j}(X_i, X_j) + \cdots + g_{1,\ldots,d}(X_1, \ldots, X_d)
\]

such that \( E[g_I(X_I)|X_J] = 0 \) for all \( I \subseteq \{1, \ldots, d\} \) and all \( J \subsetneq I \).
Sobol-Hoeffding decomposition

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\]

such that \( E[g_I(X_I)|X_J] = 0 \) for all \( I \subseteq \{1, \ldots, d\} \) and all \( J \subsetneq I \). Moreover:

\[
\begin{align*}
g_0 &= E[g(X)] \\
g_i(X_i) &= E[g(X)|X_i] - g_0 \\
g_I(X_I) &= E[g(X)|X_I] - \sum_{J \subsetneq I} g_J(X_J) \quad \text{(recursion)} \\
&= \sum_{J \subseteq I} (-1)^{|I|-|J|} E[g(X)|X_J] \quad \text{(inclusion-exclusion)}
\end{align*}
\]
The non-overlapping condition

\[ \mathbb{E}[g_I(X_I) | X_J] = 0 \quad \text{for all} \quad J \subsetneq I \]

avoids one term to be considered as a more complex one.
Variance decomposition

- The non-overlapping condition
  \[ \mathbb{E}[g_I(X_I)|X_J] = 0 \quad \text{for all} \quad J \subsetneq I \]
  *avoids one term to be considered as a more complex one.*

- It implies that \( g_I(X_I) \) is orthogonal to \( L^2(X_J) \) such that \( J \cap I \subsetneq I \):
  \[
  \mathbb{E}[g_I(X_I)h(X_J)] = \mathbb{E}[\mathbb{E}[g_I(X_I)h_J(X_J)|X_J]] \\
  = \mathbb{E}[h(X_J)\mathbb{E}[g_I(X_I)|X_{J\cap I}]] = 0
  \]
Variance decomposition

- The non-overlapping condition

\[ \mathbb{E}[g_I(X_I) | X_J] = 0 \quad \text{for all} \quad J \subsetneq I \]

*avoids one term to be considered as a more complex one.*

- It implies that \( g_I(X_I) \) *is orthogonal to* \( L^2(X_J) \) *such that* \( J \cap I \subsetneq I \):

\[
\mathbb{E}[g_I(X_I)h(X_J)] = \mathbb{E}[\mathbb{E}[g_I(X_I)h_J(X_J) | X_J]] \\
= \mathbb{E}[h(X_J)\mathbb{E}[g_I(X_I) | X_J \cap I]] = 0
\]

In particular *the decomposition is orthogonal (ANOVA):*

\[
D := \text{Var}(g(X)) = \sum_{I \subseteq \{1, \ldots, d\}} \text{Var}(g_I(X_I))
\]
Orthogonal projections

**Property**
For each $I \subseteq \{1, \ldots, d\}$, the map $\Pi_I : g \mapsto g_I$ is an orthogonal projection.
Orthogonal projections

**Property**

For each $I \subseteq \{1, \ldots, d\}$, the map $\Pi_I : g \mapsto g_I$ is an orthogonal projection

**Proof.**

Using the non-overlapping condition:

- Projection: applying twice the decomposition leaves it unchanged.
- Orthogonality:

\[
\langle \Pi_I g, h \rangle = \mathbb{E}(g_I(X_I)h(X)) = \sum_{J \subseteq \{1, \ldots, d\}} \mathbb{E}(g_I(X_I)h_J(X_J)) = \mathbb{E}(g_I(X_I)h_I(X_I)) = \langle g, \Pi_I h \rangle
\]

since if $J \neq I$, then $I \cap J \subsetneq I$ or $I \cap J \subsetneq J$, thus $\mathbb{E}(g_I(X_I)h_J(X_J)) = 0$. 

Multivariate decompositions with commuting projections

S.-H. dec. is an example of multivariate decompositions obtained with \textit{(a class of) commuting projections} $P_1, \ldots, P_d$ ([Kuo et al., 2010]), here orthogonals:

\[
P_j(g)(x) = \int g(x) d\mu_j(x_j) = \mathbb{E}[g(X)|X_{-j} = x_{-j}]
\]

The non-overlapping condition is written here $P_i(g_I) = 0$ for all $i \in I$. We find again that $\Pi_I$ is an orthogonal projection.
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The form of the decomposition is simply obtained by expansion:

\[
I_d = (P_1 + (I_d - P_1)) \cdots (P_d + (I_d - P_d))
\]
**Multivariate decompositions with commuting projections**

S.-H. dec. is an example of multivariate decompositions obtained with *(a class of) commuting projections* $P_1, \ldots, P_d$ ([Kuo et al., 2010]), here orthogonals:

$$P_j(g)(x) = \int g(x) d\mu_j(x_j) = \mathbb{E}[g(X)|X_{-j} = x_{-j}]$$

The form of the decomposition is simply obtained by expansion:

$$I_d = (P_1 + (I_d - P_1)) \ldots (P_d + (I_d - P_d)) = \sum_{l \subseteq \{1, \ldots, d\}} \prod_{j \notin l} P_j \prod_{k \in l} (I - P_k)$$

The non-overlapping condition is written here $P_i(g_I) = 0$ for all $i \in I$. We find again that $\prod_l$ *is an orthogonal projection*. 

An example: separable functions

Consider \( g(x) = f_1(x_1) \ldots f_d(x_d) \), and denote \( m_j = \mathbb{E}(X_j) \). Then:

\[
\begin{align*}
g_I(x_I) &= \prod_{i \in I} (f_i(x_i) - m_i) \prod_{j \notin I} m_j \\
g_{I}^{\text{tot}}(x) &= \prod_{i \in I} (f_i(x_i) - m_i) \prod_{j \notin I} f_j(x_j)
\end{align*}
\]

**Proof.** The Sobol-Hoeffding decomposition is obtained by expanding:

\[ g(x) = ((f_1(x_1) - m_1) + m_1) \ldots ((f_d(x_d) - m_d) + m_d) \]

For each bracket,

- for \( g_I \), choose \((f_i(x_i) - m_i)\) if \( i \in I \), and \( m_j \) otherwise
- for \( g_{I}^{\text{tot}} \), choose \((f_i(x_i) - m_i)\) if \( i \in I \)
Sensitivity indices

**Sobol indices**

- Partial variances: \( D_I = \text{Var}(g_I(X_I)) \), and **Sobol indices** \( S_I = D_I / D \)

\[
D = \sum_I D_I, \quad 1 = \sum_I S_I
\]

- \( D_{i}^{\text{tot}} = \sum_{J \supseteq \{i\}} D_J \), \( S_{i}^{\text{tot}} = \frac{D_{i}^{\text{tot}}}{D} \) **Total index**

- \( D_{i}^{\text{tot}} = \sum_{J \supseteq \{l\}} D_J \), \( S_{l}^{\text{tot}} = \frac{D_{l}^{\text{tot}}}{D} \) **Total interaction, superset importance**
Sensitivity indices

Sobol indices

- Partial variances: $D_I = \text{Var}(g_I(X_I))$, and Sobol indices $S_I = D_I/D$

$$D = \sum_I D_I, \quad 1 = \sum_I S_I$$

- $D_i^{\text{tot}} = \sum_{J \supseteq \{i\}} D_J$, $S_i^{\text{tot}} = \frac{D_i^{\text{tot}}}{D}$ Total index

- $D_i^{\text{tot}} = \sum_{J \supseteq \{i\}} D_J$, $S_i^{\text{tot}} = \frac{D_i^{\text{tot}}}{D}$ Total interaction, superset importance

Derivative Global Sensitivity Measure (DGSM)

$$\nu_i = \int \left( \frac{\partial g(x)}{\partial x_i} \right)^2 d\mu(x), \quad \nu_I = \int \left( \frac{\partial |I| g(x)}{\partial x_I} \right)^2 d\mu(x)$$
Usage for screening

Assume that:

- \( g \) is continuous on \( \Delta = [0, 1]^d \)
- for all \( i \), the support of \( \mu_i \) contains \([0, 1] \)

**Variable screening**

*If either \( D_i^{\text{tot}} = 0 \) or \( \nu_i = 0 \), then \( X_i \) is non influential*
Usage for screening

Assume that:

- $g$ is continuous on $\Delta = [0, 1]^d$
- for all $i$, the support of $\mu_i$ contains $[0, 1]$

**Variable screening**

*If either $D_{i}^{\text{tot}} = 0$ or $\nu_i = 0$, then $X_i$ is non influential*

**Interaction screening**

*If either $D_{i,j}^{\text{tot}} = 0$ or $\nu_{i,j} = 0$, then $(x_i, x_j) \mapsto g(x)$ is additive*

Total interactions can be visualized on the *FANOVA graph*, where the edge size is proportionnal to the index value.
Illustration on a toy example

8D g-Sobol function, with uniform inputs on $[0, 1]$:

$$g(x) = \prod_{j=1}^{8} \frac{|4x_j - 2| + a_j}{1 + a_j}$$

with $a = c(0, 1, 4.5, 9, 99, 99, 99, 99)$. 
Illustration on a toy example

8D g-Sobol function, with uniform inputs on $[0, 1]$:

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Figure: 1st order analysis (left) and 2nd order analysis (right) with $10^5$ simulated data.
Illustration on a toy example

A 6D block-additive function, with uniform inputs on $[-1, 1]$: 

$$g(x) = \cos([1, x_1, x_2, x_3]^T \beta) + \sin([1, x_4, x_5, x_6]^T \gamma))$$

with $\beta = (-0.8, -1.1, 1.1, 1)^T$ and $\gamma = (-0.5, 0.9, 1, -1.1)^T$. 
Illustration on a toy example

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Figure: 1st order analysis (left) and 2nd order analysis (right) with $10^5$ simulated data
Part II

Upper bounds for Sobol indices
Variance-based and derivative-based measures

- **Usage for screening.**
  
  *If either $D_{i}^{\text{tot}} = 0$ or $\nu_{i} = 0$, then $X_{i}$ is non influential*

- **Advantages / Drawbacks**

<table>
<thead>
<tr>
<th></th>
<th>Computational cost</th>
<th>Interpretability</th>
</tr>
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<tr>
<td>Sobol indices</td>
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<td>+</td>
</tr>
<tr>
<td>DGSM</td>
<td>+</td>
<td>-</td>
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Variance-based and derivative-based measures

- **Usage for screening.**
  
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</tr>
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↓

*Can we use DGSM to do screening based on Sobol indices?*
Poincaré inequality

Poincaré inequality (1-dimensional case)

A distribution $\mu$ satisfies a Poincaré inequality if the energy in $L^2(\mu)$ sense of any centered function is controlled by the energy of its derivative:

For all $h$ in $L^2(\mu)$ such that $\int h(x) d\mu(x) = 0$, and $h'(x) \in L^2(\mu)$:

$$\int h(x)^2 d\mu(x) \leq C(\mu) \int h'(x)^2 d\mu(x)$$

The best constant is denoted $C_P(\mu)$. 
Theorem [Lamboni et al., 2013], [Roustant et al., 2014]

If \( \mu_i \) and \( \mu_j \) admit a Poincaré inequality, then:

\[
D_i \leq D_{i}^{\text{tot}} \leq C(\mu_i)\nu_i, \quad D_{i,j} \leq D_{i,j}^{\text{tot}} \leq C(\mu_i)C(\mu_j)\nu_{i,j}
\]
Upper bounds

Link between total Sobol indices and DGSM

Theorem [Lamboni et al., 2013], [Roustant et al., 2014]

If $\mu_i$ and $\mu_j$ admit a Poincaré inequality, then:

$$D_i \leq D_i^{\text{tot}} \leq C(\mu_i)\nu_i, \quad D_{i,j} \leq D_{i,j}^{\text{tot}} \leq C(\mu_i)C(\mu_j)\nu_{i,j}$$

Proof 1. Denote $g_i^{\text{tot}}(x) := \sum_{J \supseteq \{i\}} g_J(x_J)$. Then:

$$\frac{\partial g(x)}{\partial x_i} = \frac{\partial g_i^{\text{tot}}(x)}{\partial x_i}$$
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If $\mu_i$ and $\mu_j$ admit a Poincaré inequality, then:

$$D_i \leq D^{\text{tot}}_i \leq C(\mu_i) \nu_i, \quad D_{i,j} \leq D^{\text{tot}}_{i,j} \leq C(\mu_i)C(\mu_j) \nu_{i,j}$$

**Proof 1.** Denote $g_{i}^{\text{tot}}(x) := \sum_{J \supseteq \{i\}} g_{J}(x_{J})$. Then:

$$\frac{\partial g(x)}{\partial x_{i}} = \frac{\partial g_{i}^{\text{tot}}(x)}{\partial x_{i}}$$

$$D^{\text{tot}}_i = \text{Var}(g_{i}^{\text{tot}}(x)) = \int (g_{i}^{\text{tot}}(x))^{2} \ d\mu(x)$$

$$\leq C(\mu_i) \int \left(\frac{\partial g_{i}^{\text{tot}}(x)}{\partial x_{i}}\right)^{2} \ d\mu(x) = C(\mu_i) \nu_i$$
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**Proof 2.** Denote $g_{i,j}^{\text{tot}}(x) := \sum_{J \supseteq \{i,j\}} g_J(x_J)$. Then:

$$\frac{\partial^2 g(x)}{\partial x_i \partial x_j} = \frac{\partial^2 g_{i,j}^{\text{tot}}(x)}{\partial x_i \partial x_j}$$
Link between total Sobol indices and DGSM

**Theorem [Lamboni et al., 2013], [Roustant et al., 2014]**

If $\mu_i$ and $\mu_j$ admit a Poincaré inequality, then:

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**Proof 2.** Denote $g_{i,j}^{\text{tot}}(x) := \sum_{J \supseteq \{i,j\}} g_J(x_J)$. Then:

$$\frac{\partial^2 g(x)}{\partial x_i \partial x_j} = \frac{\partial^2 g_{i,j}^{\text{tot}}(x)}{\partial x_i \partial x_j}$$

$$D_{i,j}^{\text{tot}} = \text{Var}(g_{i,j}^{\text{tot}}(x)) = \int (g_{i,j}^{\text{tot}}(x))^2 \, d\mu(x)$$

$$\leq C(\mu_i) \int \left( \frac{\partial g_{i,j}^{\text{tot}}(x)}{\partial x_i} \right)^2 \, d\mu(x)$$

$$\leq C(\mu_i)C(\mu_j) \int \left( \frac{\partial}{\partial x_j} \frac{\partial g_{i,j}^{\text{tot}}(x)}{\partial x_i} \right)^2 \, d\mu(x) = C(\mu_i)C(\mu_j)\nu_{i,j}$$
Getting optimal Poincaré constants on intervals

Assume that $d\mu_1(t)/dt = e^{-V(t)} > 0$ on a bounded interval $[a, b]$. Then, the smallest Poincaré constant $C(\mu_1)$ is obtained by solving a spectral problem:

$$Lf := f'' - V'f' = -\lambda f \quad \text{with} \quad f'(a) = f'(b) = 0$$

Comments.

- For some (rare) pdf, $C(\mu_1)$ can be computed semi-analytically.
- For many other ones, a finite element method can be used.
- Adaptations are possible for unbounded intervals and pdf vanishing at the boundaries.

See technical details in [Roustant et al., 2017].
## Optimal Poincaré constants: Examples

<table>
<thead>
<tr>
<th>pdf</th>
<th>Support</th>
<th>$C_{\text{opt}}$</th>
<th>Form of $f_{\text{opt}}(x)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Uniform</td>
<td>$[a, b]$</td>
<td>$(b - a)^2 / \pi^2$</td>
<td>$\cos \left( \frac{\pi(x-a)}{b-a} \right)$</td>
</tr>
<tr>
<td>$\mathcal{N}(\mu, \sigma^2)$</td>
<td>$\mathbb{R}$</td>
<td>$\sigma^2$</td>
<td>$x - \mu$</td>
</tr>
<tr>
<td>$[r_{n,i}, r_{n,i+1}]$</td>
<td></td>
<td>$1/(n + 1)$</td>
<td>$H_{n+1}(x)$ related to Kummer hypergeom. func.</td>
</tr>
<tr>
<td>$[a, b]$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Db. exp. $e^{-</td>
<td>x</td>
<td>} dx/2$</td>
<td>$\mathbb{R}$</td>
</tr>
<tr>
<td>$[a, b], ab &gt; 0$</td>
<td></td>
<td>$(\frac{1}{4} + \omega^2)^{-1}$</td>
<td>$e^{x/2} \cos(\omega x + \phi)$</td>
</tr>
<tr>
<td>$[a, b], ab \leq 0$</td>
<td></td>
<td>$&gt; (\frac{1}{4} + \omega^2)^{-1}$</td>
<td>$e^{x/2} \times \text{trig. spline}$</td>
</tr>
<tr>
<td>Logistic $\frac{e^x}{(1+e^x)^2} dx$</td>
<td>$\mathbb{R}$</td>
<td>4</td>
<td>$\times$</td>
</tr>
<tr>
<td>$[-1, 1]$</td>
<td></td>
<td>$\approx 0.1729$</td>
<td>linked to Bessel $J_0$</td>
</tr>
</tbody>
</table>

(*) For the truncated Exponential on $[a, b] \subseteq \mathbb{R}^+$, we use $\omega = \pi/(b - a)$

(**) If $a < 0 < b$, the spectral gap is the zero in $]0, \min(\pi/|a|, \pi/|b|)[$ of $x \mapsto \cot(|a|x) + \cot(|b|x) + 1/x$
Optimal Poincaré constants: Examples

Truncated normal distribution – Symmetric case: \( I = [-b,b] \)

**Figure:** Poincaré constant of \( \mu = \mathcal{N}(0, 1) \) truncated on \( I = [-b, b] \), vs \( \mu(I) \)

\( \sigma_I^2 \) : variance of the truncated normal on \( I \) – Black points: Hermite polynomials of even degree.
A case study for global sensitivity analysis

A simplified flood model [Iooss, 2011], [Iooss and Lemaitre, 2015].

1 output: maximal annual overflow (in meters), denoted by $S$:

$$S = Z_v + H - H_d - C_b \quad \text{with} \quad H = \left( \frac{Q}{B K_s \sqrt{\frac{Z_m - Z_v}{L}}} \right)^{0.6}$$

where $H$ is the maximal annual height of the river (in meters).
A case study for global sensitivity analysis

- 8 inputs variables assumed to be independent r.v., with distributions:

<table>
<thead>
<tr>
<th>Input</th>
<th>Description</th>
<th>Unit</th>
<th>Probability distribution</th>
</tr>
</thead>
<tbody>
<tr>
<td>$X_1 = Q$</td>
<td>Maximal annual flowrate</td>
<td>$m^3/s$</td>
<td>Gumbel $G(1013, 558)$, truncated on [500, 3000]</td>
</tr>
<tr>
<td>$X_2 = K_s$</td>
<td>Strickler coefficient</td>
<td>-</td>
<td>Normal $N(30, 8^2)$, truncated on [15, +∞[</td>
</tr>
<tr>
<td>$X_3 = Z_v$</td>
<td>River downstream level</td>
<td>m</td>
<td>Triangular $T(49, 50, 51)$</td>
</tr>
<tr>
<td>$X_4 = Z_m$</td>
<td>River upstream level</td>
<td>m</td>
<td>Triangular $T(54, 55, 56)$</td>
</tr>
<tr>
<td>$X_5 = H_d$</td>
<td>Dyke height</td>
<td>m</td>
<td>Uniform $\mathcal{U}[7, 9]$</td>
</tr>
<tr>
<td>$X_6 = C_b$</td>
<td>Bank level</td>
<td>m</td>
<td>Triangular $T(55, 55.5, 56)$</td>
</tr>
<tr>
<td>$X_7 = L$</td>
<td>River stretch</td>
<td>m</td>
<td>Triangular $T(4990, 5000, 5010)$</td>
</tr>
<tr>
<td>$X_8 = B$</td>
<td>River width</td>
<td>m</td>
<td>Triangular $T(295, 300, 305)$</td>
</tr>
</tbody>
</table>

- **Aim:** To detect unessential $X_i$’s, to quantify the influence of $X_i$’s on $S$, …
A case study for global sensitivity analysis

Figure: The 3 distributions types of the case study, here with mean 0 and variance 1
Results with optimal Poincaré constants

![Diagram showing results with optimal Poincaré constants. The x-axis represents different variables (Q, Ks, Zv, Zm, Hd, Cb, L, B), and the y-axis represents the total Sobol index values. The diagram includes bars indicating Db. exp transport, Optimal bound, and Total Sobol index.](image-url)
Results with optimal Poincaré constants
Part III

Lower bounds for Sobol indices

Ongoing work with F. Gamboa and B. Iooss
Without loss of generality, assume $g_0 = 0$. Define:

$$F_1 = \{ g \in L^2(\mu) \text{ s.t. } g = g_1 \}$$  functions depending exactly on $x_1$

$$F_1^{\text{tot}} = \{ g \in L^2(\mu) \text{ s.t. } g = g_1^{\text{tot}} \}$$  functions depending at least on $x_1$

Notice that $g_1$ and $g_1^{\text{tot}}$ are obtained from $g$ by orthogonal projection

$$g_1 = \Pi_{F_1}(g) = \mathbb{E}[g(X) | X_1 = .]$$

$$g_1^{\text{tot}} = \Pi_{F_1^{\text{tot}}}(g) = g - \mathbb{E}[g(X) | X_2 = ., \ldots, X_d = .]$$

Hence, $D_1 = \|\Pi_{F_1}(g)\|^2$ and $D_1^{\text{tot}} = \|\Pi_{F_1^{\text{tot}}}(g)\|^2$.

Lower bounds of $D_1, D_1^{\text{tot}}$ are obtained by projecting onto subspaces of $F_1, F_1^{\text{tot}}$.
Main result

Let $\phi_1, \ldots, \phi_m$ be orthonormal functions in $F_1^{\text{tot}}$. Then:

$$D_1^{\text{tot}} \geq \sum_{j=1}^{m} \left( \int g(x) \phi_j(x) d\mu(x) \right)^2$$

with equality iff $g$ has the form $g(x) = \sum_{j=1}^{m} \alpha_m \phi_m(x) + h(x_2, \ldots, x_m)$.

If all the $\phi_j$’s belong to $F_1$ then the lower bound is for $D_1$.

Proof.

- $D_1^{\text{tot}} = \| g_1^{\text{tot}} \|^2 = \| \Pi_{F_1^{\text{tot}}} (g) \|^2 \geq \| \Pi_{\phi_1, \ldots, \phi_m} (g) \|^2 = \sum_{j=1}^{m} (\langle g, \phi_j \rangle)^2$

- Equality is when $g_1^{\text{tot}} = \Pi_{\phi_1, \ldots, \phi_m} (g)$, leading to the condition above.

- Same arguments when all the $\phi_j$’s are in $F_1$. 

Tensor-based lower bounds

For all $j$, let $\psi_{j,0} = 1, \psi_{j,1}, \ldots, \psi_{j,n_j-1}$ be orthonormal functions in $L^2(\mu_j)$. Consider tensors, i.e. separable functions:

$$\phi_\ell(x) = \prod_{j=1}^{d} \psi_{j,\ell_j}(x_j)$$

where $\ell = (\ell_1, \ldots, \ell_d)$ is a multi-index.

Let $\mathcal{T}_1 = \{\ell \text{ s.t. } \ell_1 \geq 1\}$, the set of tensors $\phi_\ell$ involving $x_1$. Then:

$$D_1^{\text{tot}}(f) \geq \sum_{\ell \in \mathcal{T}_1} \left( \int f(x) \phi_\ell(x) \nu(dx) \right)^2$$

with equality iff $f$ has the form $f(x) = \sum_{\ell \in \mathcal{T}_1} \alpha_\ell \phi_\ell(x) + g(x_2, \ldots, x_d)$. 
Tensor-based lower bounds

As an illustration, if $\mu_i$ admit the first two moments, denote:

$$\psi_i(x) = (x_i - m_i)/s_i$$

where $m_i$ is the mean and $s_i$ the s.d.

Then $\psi_1, \psi_1 \psi_2, \ldots, \psi_1 \psi_j$ are orthonormal functions of $F_{1}^{\text{tot}}$.

Hence:

$$D_{1}^{\text{tot}} \geq \left( \int g(x) \psi_1(x) d\mu(x) \right)^2 + \sum_{j=2}^{m} \left( \int g(x) \psi_1(x) \psi_j(x) d\mu(x) \right)^2$$

lower bound for $D_1$
Derivative-based lower bounds

All the integrals above can involve derivatives by integrating by part. But this often induce weights; Here is a partial solution to avoid weights.
**Derivative-based lower bounds**

All the integrals above can involve derivatives by integrating by part. But this often induce weights; Here is a partial solution to avoid weights.

Assume that $\mu_j$ is continuous with pdf $p_j \in H^1(\mu_j)$ vanishing at the boundaries but not inside, and such that $p_j' \neq 0$ and $p_j'/p_j \in L^2(\mu_j)$. Denote:

$$Z_j(X_j) = (\ln p_j)'(X_j), \quad I_j = \text{Var}(Z_j(X_j))$$

Then:

$$D_1^{\text{tot}} \geq I_1^{-1} c_1^2 + I_j^{-1} \sum_{j=2}^d I_j^{-1} c_{1,j}^2$$

with

$$c_1 = \int g(x) Z_1(x_1) d\mu(x) = -\int \frac{\partial g(x)}{\partial x_1} d\mu(x)$$

$$c_{1,j} = \int g(x) Z_1(x_1) Z_j(x_j) d\mu(x) = -\int \frac{\partial g(x)}{\partial x_1} Z_j(x_j) d\mu(x) = \int \frac{\partial^2 g(x)}{\partial x_1 \partial x_j} d\mu(x)$$
Derivative-based lower bounds: examples

For normal variables $N(m_j, s_j^2)$:

$$D_1^{\text{tot}} \geq s_1^2 \left( \int \frac{\partial g(x)}{\partial x_1} d\mu(x) \right)^2 + s_1^2 \sum_{j=2}^{d} s_j^2 \left( \int \frac{\partial^2 g(x)}{\partial x_1 \partial x_j} d\mu(x) \right)^2$$

Dist. name | Support | $p$ | $Z$ | $l$
---|---|---|---|---
Normal | $\mathbb{R}$ | \( \frac{1}{s\sqrt{2\pi}} \exp \left( -\frac{1}{2} \frac{(x-m)^2}{s^2} \right) \) | \( -(X - m)/s^2 \) | \( 1/s^2 \)
Laplace | $\mathbb{R}$ | \( \frac{1}{2s} \exp \left( \frac{|x-m|}{s} \right) \) | \( -\text{sgn}(X - m)/s \) | \( 1/s^2 \)
Cauchy | $\mathbb{R}$ | \( \frac{1}{\pi} \frac{s}{(x-x_0)^2+s^2} \) | \( \frac{-2(x-x_0)}{(x-x_0)^2+s^2} \) | \( 1/(2s^2) \)
Improvements on existing works

According to results given in the review [Kucherenko and Iooss, 2017],

- For normal distributions, we improve on:

\[ D_{1}^{\text{tot}} \geq D_{1} \geq s_{1}^{2} \left( \int \frac{\partial g(x)}{\partial x_{1}} d\mu(x) \right)^{2}. \]
Improvements on existing works

According to results given in the review [Kucherenko and Iooss, 2017],

- For normal distributions, we improve on:

  \[ D_1^{\text{tot}} \geq D_1 \geq s_1^2 \left( \int \frac{\partial g(x)}{\partial x_1} d\mu(x) \right)^2. \]

- For uniforms on \([0, 1]\) using the orthonormal function obtained from \(x_1^m\), and an integration by part, we obtain:

  \[ D_1^{\text{tot}} \geq D_1 \geq \frac{2m+1}{m^2} \left( \int (g(1, x_{-1}) - g(x))dx - w_1^{(m+1)} \right)^2 \]

  where \(w_1^{(m+1)} = \int \frac{\partial g(x)}{\partial x_1} x_1^{m+1} dx\). This improves on the known lower bound which has the same form, with the smaller multiplicative constant \(\frac{2m+1}{(m+1)^2}\).
Lower bounds

Improvements on existing works

According to results given in the review [Kucherenko and Iooss, 2017],

- For normal distributions, we improve on:

\[ D_{1}^{\text{tot}} \geq D_{1} \geq s_{1}^{2} \left( \int \frac{\partial g(x)}{\partial x_{1}} d\mu(x) \right)^{2} \]

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where \(w_{1}^{(m+1)} = \int \frac{\partial g(x)}{\partial x_{1}} x_{1}^{m+1} dx\). This improves on the known lower bound which has the same form, with the smaller multiplicative constant \(\frac{2m + 1}{(m+1)^{2}}\).

N.B. Better bounds are obtained by adding orth. funct. of the form \(\psi_{1}\psi_{j}\).
Results on the application

![Bar chart](image)

**Figure:** Results obtained with orth. 1st order pol. tensors $\psi_1, \psi_1\psi_2, \ldots, \psi_1\psi_8$
Results on the application

Figure: Results obtained with orth. 1st order pol. tensors $\psi_1, \psi_1\psi_2, \ldots, \psi_1\psi_8$
When using derivatives and other numerical considerations

We must compute squared integrals $\theta = (\int h(x) d\mu(x))^2$, when $h$ has the form:

$$h_{\text{dir}} = g\phi_1, g\phi_1\phi_j, \ldots,$$

or

$$h_{\text{der}} = \frac{\partial g}{\partial x_i}, \frac{\partial g}{\partial x_j} Z_j, \ldots$$

for centered function $\phi_1, \phi_j, Z_j$. 
When using derivatives and other numerical considerations

We must compute squared integrals $\theta = \left( \int h(x) d\mu(x) \right)^2$, when $h$ has the form:

$$h_{\text{dir}} = g\phi_1, g\phi_1 \phi_j, \ldots,$$

or

$$h_{\text{der}} = \frac{\partial g}{\partial x_i}, \frac{\partial g}{\partial x_j} Z_j, \ldots$$

for centered function $\phi_1, \phi_j, Z_j$.

The sample estimate $\hat{\theta} = \left( \frac{1}{n} \sum_{i=1}^{n} h(X^i) \right)^2$, with $X^1, \ldots, X^n$ i.i.d. $\sim \mu$, verifies:

$$\hat{\theta} \approx \mathcal{N} \left( \theta, \frac{4\theta}{n} \text{Var}_\mu(h) \right)$$

Hence, for one squared integral, using the derivative form can reduce estimation error when $h_{\text{der}}$ is less variable than $h_{\text{dir}}$. 
Partial conclusions

Lower bounds of a (convex comb. of) ANOVA term $g_I$ can be obtained by projection onto subspaces of its ANOVA space $\{g \in L^2(\mu) \text{ s.t. } g = g_I \}$ → Illustrated on main and total effects, but very general!
Lower bounds of a (convex comb. of) ANOVA term $g_I$ can be obtained by projection onto subspaces of its ANOVA space $\{g \in L^2(\mu) \text{ s.t. } g = g_I\}$ → Illustrated on main and total effects, but very general!

Tensors are used to get lower bounds as a sum of squared integrals → Chaos polynomials or more general tensors
Partial conclusions

- Lower bounds of a (convex comb. of) ANOVA term $g_I$ can be obtained by projection onto subspaces of its ANOVA space $\{g \in L^2(\mu) \text{ s.t. } g = g_I\}$
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- Tensors are used to get lower bounds as a sum of squared integrals
  → Chaos polynomials or more general tensors

- Integration by part modify lower bounds into derivative-based forms
  → Specific choices of subspaces remove weights for specific pdfs
Partial conclusions

- Lower bounds of a (convex comb. of) ANOVA term $g_I$ can be obtained by projection onto subspaces of its ANOVA space $\{g \in L^2(\mu) \text{ s.t. } g = g_I\}$
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- Tensors are used to get lower bounds as a sum of squared integrals
  $\rightarrow$ Chaos polynomials or more general tensors

- Integration by part modify lower bounds into derivative-based forms
  $\rightarrow$ Specific choices of subspaces remove weights for specific pdfs

- Using derivative-based inequalities may be useful when the derivative is less variable than the function itself.
Part IV

Tail dependograph

Joint work with C. Mercadier
Multivariate dependence

Denote $F$ a multivariate cdf,

$$F(x) = \mathbb{P}(X_1 \leq x_1, \ldots, X_d \leq x_d)$$

Assume that $F$ is in the domain of attraction of a max-stable distribution $H$ i.e. there exist vector sequences $a_n > 0, b_n$ s.t. for indep. samples $X^1, \ldots, X^n$ of $F$

$$\mathbb{P}\left(\frac{\max_{k=1}^n(X^1_k) - b_{n,1}}{a_{n,1}} \leq x_1, \ldots, \frac{\max_{k=1}^n(X^d_k) - b_{n,d}}{a_{n,d}} \leq x_d\right) \xrightarrow{n \to \infty} H(x)$$
Multivariate dependence

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$$\mathbb{P}\left(\frac{\max_{k=1}^n (X^k_{1}) - b_{n,1}}{a_{n,1}} \leq x_1, \ldots, \frac{\max_{k=1}^n (X^k_{d}) - b_{n,d}}{a_{n,d}} \leq x_d\right) \xrightarrow{n \to \infty} H(x)$$

In the univariate case, $H$ is a generalized extreme value distribution, summarizing the three types Fréchet, Weibull, Gumbel
Multivariate dependence

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$$\mathbb{P} \left( \frac{\max_{k=1}^n (X^k_1) - b_{n,1}}{a_{n,1}} \leq x_1, \ldots, \frac{\max_{k=1}^n (X^k_d) - b_{n,d}}{a_{n,d}} \leq x_d \right) \xrightarrow{n \to \infty} H(x)$$

- In the univariate case, $H$ is a generalized extreme value distribution, summarizing the three types Fréchet, Weibull, Gumbel
- In the multivariate case, the margins are gev, and the multivariate dependence is characterized by a multivariate function
  - extreme value copula, stable tail dependence function, …
Multivariate dependence: stable tail dependence function

Stable tail dependence function (stdf) $\ell$

$$- \log H(x) = \ell(- \log H_1(x_1), \ldots, - \log H_d(x_d))$$

Properties (see e.g. [de Haan and Ferreira, 2006])

- $\ell$ is continuous, convex and homogeneous of order 1
  $\rightarrow$ we can restrict it on $[0, 1]^d$
- $\max(u_1, \ldots, u_d) \leq \ell(u) \leq u_1 + \cdots + u_d$
  Asymptotic dependence
  Asymptotic independence
- $\ell(u) = \lim_{z \to +\infty} z \left(1 - F\left(\frac{F_1^{-1}(u_1/z), \ldots, F_d^{-1}(u_d/z)}{}ight)\right)$
Asymptotic independence and tail dependograph

Let $A, B$ a partition of $\{1, \ldots, d\}$

$X_A$ and $X_B$ are *asymptotically independent* if

$\iff H(x)$ if of the form $H(x) = H_A(x_A)H_B(x_B)$

$\iff \ell(u)$ if of the form $\ell(u) = \ell(u_A) + \ell(u_B)$

$\iff \forall i \in A, \forall j \in B, \ell_{i,j}^{\text{tot}} \equiv 0$
Asymptotic independence and tail dependograph

Let $A, B$ a partition of $\{1, \ldots, d\}$

$X_A$ and $X_B$ are \textit{asymptotically independent}

\[ \iff \quad H(x) \text{ if of the form } H(x) = H_A(x_A)H_B(x_B) \]

\[ \iff \quad \ell(u) \text{ if of the form } \ell(u) = \ell(u_A) + \ell(u_B) \]

\[ \iff \quad \forall i \in A, \forall j \in B, \quad \ell_{i,j}^{\text{tot}} \equiv 0 \]

Thus

\[ X_A \perp \perp_{\infty} X_B \quad \text{if} \quad \text{the FANOVA graph of } \ell \text{ is partitioned by } A \text{ and } B \]

“tail dependograph”
Asymptotic independence and extremal coefficients

The extremal coefficients $\theta_I(\ell)$ are defined by

$$P \left( X_j \leq F_j^{-1}(p), \text{ for all } j \in I \right) = p^{\theta_I(\ell)}$$

Equivalently $\theta_I(\ell) = \ell(1_I)$
Asymptotic independence and extremal coefficients

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Equivalently $\theta_I(\ell) = \ell(1_I)$, and in particular

$$\underbrace{1}_{\text{Asymptotic dependence}} \leq \theta_I(\ell) \leq \underbrace{|I|}_{\text{Asymptotic independence}}$$
Asymptotic independence and extremal coefficients

The extremal coefficients $\theta_I(\ell)$ are defined by

$$\mathbb{P} \left( X_j \leq F_j^{-1}(p), \text{ for all } j \in I \right) = p^{\theta_I(\ell)}$$

Equivalently $\theta_I(\ell) = \ell(1_I)$, and in particular

$$\frac{1}{|I| \ell(1_I)} \leq \theta_I(\ell) \leq \ell(1_I)$$

Hence, $X_i \perp \perp_X \infty X_j$ if $\theta_{i,j}(\ell) = 2$
Illustration: Revealing asymptotic dependence for asymmetric models

Consider a 4-dim. random vector $X$ with standard Gumbel margins, and s.t.d.f. built as a mixture of independence and logistic:

$$
\ell(u) = (1 - w)(u_1 + u_2) + w \left( u_1^{1/\alpha} + u_2^{1/\alpha} \right)^\alpha 
+ (1 - w')(u_3 + u_4) + w' \left( u_3^{1/\alpha'} + u_4^{1/\alpha'} \right)^{\alpha'},
$$

with asymmetric parameters: $(w, \alpha) = (0.2, 0.2)$, $(w', \alpha') = (0.8, 0.83)$. 
Illustration: Revealing asymptotic dependence for asymmetric models

Figure: Tail dependograph (left) and graph representing $2 - \theta_{i,j}$ (right)

→ Both indices recover the asympt. indep. between $(X_1, X_2)$ and $(X_3, X_4)$
→ Asymmetry in tail dependence is more visible on tail dependograph
Inference

The formula $\ell(u) = \lim_{z \to +\infty} z \left( 1 - F \left( F_1^{-1}(u_1/z), \ldots, F_d^{-1}(u_d/z) \right) \right)$ leads to the natural estimator ([Huang, 1992])

$$\hat{\ell}_{k,n}(u) = \frac{n}{k} \left( 1 - \frac{1}{n} \sum_{s=1}^{n} \mathbb{1}\left\{ X_{s}^{(1)} < X_{n-[ku]+1,n}^{(1)}, \ldots, X_{s}^{(d)} < X_{n-[ku_d]+1,n}^{(d)} \right\} \right)$$

$$= \frac{n}{k} \left( 1 - \frac{1}{n} \sum_{s=1}^{n} \mathbb{1}\left\{ u_1 < \tilde{R}_s^{(1)}, \ldots, u_d < \tilde{R}_s^{(d)} \right\} \right)$$

$$= \frac{n}{k} - \frac{1}{k} \sum_{s=1}^{n} \prod_{t=1}^{d} \mathbb{1}\left\{ u_t < \tilde{R}_s^{(t)} \right\}$$

with:

- $X_{1,n}, \ldots, X_{n,n}$: sorted data (asc. order) for coordinate $t$

- $\tilde{R}_s^{(t)} := \frac{n-R_s^{(t)}+1}{k}$, where $R_s^{(t)}$ is the rank of $X_s^{(t)}$ among $X_{1}^{(t)}, \ldots, X_{n}^{(t)}$. 
Inference

Let $\mu = \mu_1 \otimes \cdots \otimes \mu_d$ a measure on $[0, 1]^d$ (without special link with $F$).

As a sum of separable functions, the whole Sobol-Hoeffding decomposition of the stdf estimator can be computed in closed form, and in particular

$$\hat{\ell}_{k,n;\{i,j\}}^{\text{tot}}(u) = -\frac{1}{k} \sum_{s=1}^{n} \prod_{t=1}^{d} \left( 1\{u_t < \tilde{R}_s^{(t)}\} - 1\{t \in \{i,j\}\} \mu_t \left( \tilde{R}_s^{(t)} \right) \right)$$

and the tail dependograph as well

$$D_{\{i,j\}}^{\text{tot}}(\hat{\ell}_{k,n}) = \frac{1}{k^2} \sum_{s=1}^{n} \sum_{s' = 1}^{n} \prod_{t=1}^{d} \left( \mu_t \left( \tilde{R}_s^{(t)} \wedge \tilde{R}_{s'}^{(t)} \right) - 1\{t \in \{i,j\}\} \mu_t \left( \tilde{R}_s^{(t)} \right) \mu_t \left( \tilde{R}_{s'}^{(t)} \right) \right).$$
Inference

As the terms of S.-H. decomposition are obtained by linear operation,

\textit{inference properties of the stdf transfer to its ANOVA terms...}
Inference

As the terms of S.-H. decomposition are obtained by linear operation,

\[ \text{inference properties of the stdf transfer to its ANOVA terms...} \]

Consider the usual assumptions for stdf inference, with corresponding valid sequences \( k = k(n) \). Then, for all \( I \subseteq \{1, \ldots, d\} \),

1. \( \sup_{u_I \in [0,1]^I} |\hat{\ell}_{k,n,I}(u_I) - \ell_I(u_I)| \xrightarrow{\mathbb{P}} 0 \).
2. \( \sqrt{k} \left\{ \hat{\ell}_{k,n,I}(u_I) - \ell_I(u_I) \right\} \xrightarrow{d} Y_{\ell,I}(u_I) \)

where \( Y_{\ell,I} \) is some Gaussian process.
Inference

As the terms of S.-H. decomposition are obtained by linear operation,

\(\textit{inference properties of the stdf transfer to its ANOVA terms...}\)

Consider the usual assumptions for stdf inference, with corresponding valid sequences \(k = k(n)\). Then, for all \(I \subseteq \{1, \ldots, d\}\),

- \(\sup_{u_I \in [0,1]^{|I|}} |\hat{l}_{k,n}(u_I) - l_I(u_I)| \xrightarrow{\mathbb{P}} 0\).
- \(\sqrt{k} \left\{ \hat{l}_{k,n}(u_I) - l_I(u_I) \right\} \xrightarrow{d} Y_{\ell;I}(u_I)\)

where \(Y_{\ell;I}\) is some Gaussian process.

\(\text{... and hence to the tail dependograph}\)

\(\mathbb{D}_I(\hat{l}_{k,n}) \xrightarrow{\mathbb{P}} \mathbb{D}_I(\ell)\)

- If \(\mathbb{D}_I(\ell) > 0\), then \(\mathbb{D}_I(\hat{l}_{k,n})\) is asympt. normal with rate \(\sqrt{k}\)
- If \(\mathbb{D}_I(\ell) = 0\), then \(\mathbb{D}_I(\hat{l}_{k,n})\) is asympt. \(\chi^2\) type with rate \(k\)

(The same is true for \(\mathbb{D}_I^{\text{tot}}\))
Inference

(A piece of intuition about asymptotic distribution)

\[
\hat{\ell}_{k,n;I}(u_I) = \ell_I(u_I) + \frac{1}{\sqrt{k}} Y_{\ell,I}(u_I) + \ldots
\]
Inference

(A piece of intuition about asymptotic distribution)

\[
\hat{\ell}_{k,n;I}(u_I) = \ell_I(u_I) + \frac{1}{\sqrt{k}} Y_{\ell,I}(u_I) + \ldots
\]

- If \(\ell_I \neq 0\),

\[
\int_{D_I(\hat{\ell}_{k,n})} \hat{\ell}_{k,n;I}^2(u_I) d\mu(u) = \int_{D_I(\ell)} \ell_I^2(u_I) d\mu(u) + \frac{1}{\sqrt{k}} \int_{D_I(\ell)} 2 Y_{\ell,I}(u_I) \ell_I(u_I) d\mu(u) + \ldots
\]

\[\text{a Gaussian r.v.}\]
Inference

(A piece of intuition about asymptotic distribution)

\[ \hat{\ell}_{k,n;l}(u_l) = \ell_l(u_l) + \frac{1}{\sqrt{k}} Y_{\ell,l}(u_l) + \ldots \]

- If \( \ell_l \neq 0 \),
  \[ \int_{D_l(\hat{\ell}_{k,n})} \hat{\ell}_{k,n;l}^2(u_l) d\mu(u) = \int_{D_l(\ell)} \ell_l^2(u_l) d\mu(u) + \frac{1}{\sqrt{k}} \int_{D_l(\ell)} 2 Y_{\ell,l}(u_l) \ell_l(u_l) d\mu(u) + \ldots \]
  a Gaussian r.v.

- If \( \ell_l \equiv 0 \),
  \[ \int_{D_l(\hat{\ell}_{k,n})} \hat{\ell}_{k,n;l}^2(u_l) d\mu(u) = 0 + \frac{1}{k} \int_{D_l(\ell)} Y_{\ell,l}^2(u_l) d\mu(u) + \ldots \]
  a \( \chi^2 \) type r.v.
Application on real data


Figure: Estimated tail dependograph: complete, 30 largest values, 9 largest
Application on real data


Figure: Estimated tail dependograph: complete, 30 largest values, 9 largest
Application on real data


**Figure:** Estimated tail dependograph: complete, 30 largest values, 9 largest
Some conclusions

Tail dependograph is a graphical tool to investigate multivariate independence.

- Asymptotic independence is visible by partitions in the graph
- Asymmetric seems to be better visible, compared to extremal coefficients
Some conclusions

Tail dependograph is a graphical tool to investigate multivariate independence.

- Asymptotic independence is visible by partitions in the graph
- Asymmetric seems to be better visible, compared to extremal coefficients
- A natural estimator can be computed analytically
- Inference properties of the stdf transfer to the tail dependograph
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Part V

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