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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 $g : \Delta \subseteq \mathbb{R}^d \rightarrow \mathbb{R}$ 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

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 \( g(X) \in L^2(\mu) \).


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 \( J \subsetneq I \). Moreover:

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

- The non-overlapping condition

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

*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 \( g_I(X_I) \text{ is orthogonal to } L^2(X_J) \) 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

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

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= \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 $\mathbb{E}(g_I(X_I)h_J(X_J)) = 0$. 
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:

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

$$I_d = (P_1 + (I_d - P_1)) \cdots (P_d + (I_d - P_d))$$
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:

$$I_d = (P_1 + (I_d - P_1)) \cdots (P_d + (I_d - P_d))$$

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

The non-overlapping condition is written here $P_i(g_I) = 0$ for all $i \in I$. We find again that $\prod_I$ 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** $S_I = D_I/D$

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

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

- $D_{I}^{\text{tot}} = \sum_{J \supseteq \{I\}} D_J$, \quad $S_{I}^{\text{tot}} = \frac{D_{I}^{\text{tot}}}{D}$  \quad **Total interaction, superset importance**
**Sensitivity indices**

**Sobol indices**

- Partial variances: \( D_l = \text{Var}(g_l(X_l)) \), and **Sobol indices** \( S_l = D_l/D \)

\[
D = \sum_l D_l, \quad 1 = \sum_l S_l
\]

- Total index

\[
D_{i}^{\text{tot}} = \sum_{J \supseteq \{i\}} D_J, \quad S_{i}^{\text{tot}} = \frac{D_{i}^{\text{tot}}}{D}
\]

- Total interaction, superset importance

\[
D_{i}^{\text{tot}} = \sum_{J \supseteq \{l\}} D_J, \quad S_{i}^{\text{tot}} = \frac{D_{i}^{\text{tot}}}{D}
\]

**Derivative Global Sensitivity Measure (DGSM)**

\[
\nu_i = \int \left( \frac{\partial g(x)}{\partial x_i} \right)^2 d\mu(x), \quad \nu_l = \int \left( \frac{\partial^{|l|} g(x)}{\partial x_l} \right)^2 d\mu(x)
\]
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 $[0, 1]$:

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

with $a = c(0, 1, 4.5, 9, 99, 99, 99, 99)$.  

**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

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

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

with $\beta = (-0.8, -1.1, 1.1, 1)^{\top}$ and $\gamma = (-0.5, 0.9, 1, -1.1)^{\top}$.

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>
</thead>
<tbody>
<tr>
<td>Sobol indices</td>
<td>-</td>
<td>+</td>
</tr>
<tr>
<td>DGSM</td>
<td>+</td>
<td>-</td>
</tr>
</tbody>
</table>
Variance-based and derivative-based measures

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

- **Advantages / Drawbacks**

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<td>-</td>
</tr>
</tbody>
</table>

↓

*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:

$$D_i \leq D_i^{\text{tot}} \leq C(\mu_i)\nu_i,$$

$$D_{i,j} \leq D_{i,j}^{\text{tot}} \leq C(\mu_i)C(\mu_j)\nu_{i,j}.$$
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:

\[
\frac{\partial g(x)}{\partial x_i} = \frac{\partial g_i^{\text{tot}}(x)}{\partial x_i}
\]
Link between total Sobol indices and DGSM

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

$$\frac{\partial g(x)}{\partial x_i} = \frac{\partial g_i^{\text{tot}}(x)}{\partial x_i}$$

$$D_i^{\text{tot}} = \text{Var}(g_i^{\text{tot}}(x)) = \int (g_i^{\text{tot}}(x))^2 d\mu(x) \leq C(\mu_i) \int \left( \frac{\partial g_i^{\text{tot}}(x)}{\partial x_i} \right)^2 d\mu(x) = C(\mu_i)\nu_i$$
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Theorem [Lamboni et al., 2013], [Roustant et al., 2014]

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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></td>
<td>$[r_{n,i}, r_{n,i+1}]$</td>
<td>$1 / (n + 1)$</td>
<td>$H_{n+1}(x)$</td>
</tr>
<tr>
<td></td>
<td>$[a, b]$</td>
<td></td>
<td>related to Kummer hypergeom. func.</td>
</tr>
<tr>
<td>Db. exp. $e^{-</td>
<td>x</td>
<td>} dx/2$</td>
<td>$\mathbb{R}$</td>
</tr>
<tr>
<td>(*)</td>
<td>$[a, b], ab &gt; 0$</td>
<td>$(\frac{1}{4} + \omega^2)^{-1}$</td>
<td>$e^{x/2} \cos(\omega x + \phi)$</td>
</tr>
<tr>
<td>(***)</td>
<td>$[a, b], ab \leq 0$</td>
<td>$&gt; (\frac{1}{4} + \omega^2)^{-1}$</td>
<td>$e^{</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>Triangular</td>
<td>$[-1, 1]$</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 $x \mapsto \cotan(|a|x) + \cotan(|b|x) + 1/x$
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 $\mu(I)$

$\sigma^2_I$ : 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 [looss, 2011], [looss and Lemaitre, 2015].

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

$$S = Z_v + H - H_d - C_b$$

with

$$H = \left( \frac{Q}{BK_s \sqrt{\frac{Z_m - Z_v}{L}}} \right)^{0.6}$$

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 $\mathcal{G}(1013, 558)$, truncated on [500, 3000]</td>
</tr>
<tr>
<td>$X_2 = K_s$</td>
<td>Strickler coefficient</td>
<td>-</td>
<td>Normal $\mathcal{N}(30, 8^2)$, truncated on [15, $+\infty$]</td>
</tr>
<tr>
<td>$X_3 = Z_v$</td>
<td>River downstream level</td>
<td>m</td>
<td>Triangular $\mathcal{T}(49, 50, 51)$</td>
</tr>
<tr>
<td>$X_4 = Z_m$</td>
<td>River upstream level</td>
<td>m</td>
<td>Triangular $\mathcal{T}(54, 55, 56)$</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 $\mathcal{T}(55, 55.5, 56)$</td>
</tr>
<tr>
<td>$X_7 = L$</td>
<td>River stretch</td>
<td>m</td>
<td>Triangular $\mathcal{T}(4990, 5000, 5010)$</td>
</tr>
<tr>
<td>$X_8 = B$</td>
<td>River width</td>
<td>m</td>
<td>Triangular $\mathcal{T}(295, 300, 305)$</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
Results with optimal Poincaré constants

![Graph showing optimal bounds and total Sobol indices for various variables (Q, Ks, Zv, Zm, Hd, Cb, L, B).]
Part III

Lower bounds for Sobol indices

Ongoing work with F. Gamboa and B. Iooss
Principle

Without loss of generality, assume $g_0 = 0$. Define:

\[
\begin{align*}
F_1 &= \{ g \in L^2(\mu) : g = g_1 \} \quad \text{functions depending exactly on } x_1 \\
F_{1}^{\text{tot}} &= \{ g \in L^2(\mu) : g = g_{1}^{\text{tot}} \} \quad \text{functions depending at least on } x_1
\end{align*}
\]

Notice that $g_1$ and $g_{1}^{\text{tot}}$ are obtained from $g$ by orthogonal projection

\[
\begin{align*}
  g_1 &= \Pi_{F_1}(g) = \mathbb{E}[g(X)|X_1 = .] \\
  g_{1}^{\text{tot}} &= \Pi_{F_{1}^{\text{tot}}}(g) = g - \mathbb{E}[g(X)|X_2 = ., \ldots , X_d = .]
\end{align*}
\]

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 $F_{1,\text{tot}}^t$.

Hence:

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

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 \( p_j \in \mathcal{H}^1(\mu_j) \) 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:

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

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 $N(m_j, s^2_j)$:

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

<table>
<thead>
<tr>
<th>Dist. name</th>
<th>Support</th>
<th>$p$</th>
<th>$Z$</th>
<th>$l$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Normal</td>
<td>$\mathbb{R}$</td>
<td>$\frac{1}{s \sqrt{2\pi}} \exp \left( -\frac{1}{2} \frac{(x-m)^2}{s^2} \right)$</td>
<td>$-(X - m)/s^2$</td>
<td>$1/s^2$</td>
</tr>
<tr>
<td>Laplace</td>
<td>$\mathbb{R}$</td>
<td>$\frac{1}{2s} \exp \left( \frac{</td>
<td>x-m</td>
<td>}{s} \right)$</td>
</tr>
<tr>
<td>Cauchy</td>
<td>$\mathbb{R}$</td>
<td>$\frac{1}{\pi} \frac{s}{(x-x_0)^2+s^2}$</td>
<td>$\frac{-2(x-x_0)}{(x-x_0)^2+s^2}$</td>
<td>$1/(2s^2)$</td>
</tr>
</tbody>
</table>
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 \(\frac{2m+1}{(m+1)^2}\).
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N.B. Better bounds are obtained by adding orth. funct. of the form \(\psi_1 \psi_j\).
Results on the application

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

![Diagram showing lower bounds and optimal bounds for various variables. The x-axis represents different variables (Q, Ks, Zv, Zm, Hd, Cb, L, B), and the y-axis represents values from 0.0 to 1.0. The diagram includes bars representing total Sobol indices and lower bounds, with blue indicating optimal bounds.]

**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:

\[
h_{\text{dir}} = g\phi_1, g\phi_1\phi_j, \ldots, \quad \text{or} \quad h_{\text{der}} = \frac{\partial g}{\partial x_i}, \frac{\partial g}{\partial x_j} Z_j, \ldots
\]

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

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

- Integration by part modify lower bounds into derivative-based forms. 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 independent samples $X_1, \ldots, X^n$ of $F$

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

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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 $F$

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

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

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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 $X_1^n, \ldots, X_n^n$ of $F$

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

- 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 gevd, 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

- \( \ell(u) = \lim_{z \to +\infty} z \left( 1 - F \left( F_1^{-1}(u_1/z), \ldots, F_d^{-1}(u_d/z) \right) \right) \)
Asymptotic independence and tail dependograph

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

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

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

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

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

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

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

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\]

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

Thus

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

\[\text{“tail dependograph”}\]
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 $\theta_I(\ell) = \ell(1_I)$
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$$1 \leq \theta_I(\ell) \leq |I|$$

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

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

Asymptotic dependence

Asymptotic independence

Hence,

$$
X_i \perp \perp X_j \text{ if } \theta_{i,j}(\ell) = 2
$$
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: $(w, \alpha) = (0.2, 0.2)$, $(w', \alpha') = (0.8, 0.83)$. 

\[ \text{Illustration: Revealing asymptotic dependence for asymmetric models} \]
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])

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

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

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

with:

- \( X_1^{(t)}, \ldots, X_n^{(t)} \): 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

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

and the tail dependograph as well

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

As the terms of S.-H. decomposition are obtained by linear operation, inference properties of the stdf transfer to its ANOVA terms...
Inference

As the terms of S.-H. decomposition are obtained by linear operation, 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 $I \subseteq \{1, \ldots, d\}$,

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

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 $I \subseteq \{1, \ldots, d\}$,

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

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

\textit{... and hence to the tail dependograph}

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

(The same is true for $D_{I}^{\text{tot}}$)
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)

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

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

\[
\int \hat{\ell}^2_{k,n,l}(u_l) d\mu(u) = \int \ell^2_l(u_l) d\mu(u) + \frac{1}{\sqrt{k}} \int 2Y_{\ell,l}(u_l)\ell_l(u_l) d\mu(u) + \ldots
\]

\[ D_{l}(\hat{\ell}_{k,n}) \]
\[ D_{l}(\ell) \]
\[ a \text{ Gaussian r.v.} \]
**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 \( \ell_I \neq 0 \),

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

\[ D_I(\hat{\ell}_{k,n}) \]

\[ D_I(\ell) \]

a Gaussian r.v.

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

\[ \int \hat{\ell}_{k,n;I}^2(u_I) d\mu(u) = 0 + \frac{1}{k} \int Y_{\ell,I}^2(u_I) d\mu(u) + \ldots \]

\[ D_I(\hat{\ell}_{k,n}) \]

\[ D_I(\ell) \]

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
Acknowledgements

Part of this research was conducted within the frame of the Chair in Applied Mathematics OQUAIDO, gathering partners in technological research (BRGM, CEA, IFPEN, IRSN, Safran, Storengy) and academia (CNRS, Ecole Centrale de Lyon, Mines Saint-Etienne, University of Grenoble, University of Nice, University of Toulouse) around advanced methods for Computer Experiments.
Part V

References - Thank you for your attention!


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