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Sobol-Hoeffding decomposition: bounds and extremes

Olivier Roustant ⋆

Synthesis of works with

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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

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

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 $I \subseteq \{1, \dots, d\}$ and all $J \subsetneq I$. Moreover:

$$\begin{aligned}
g_0 &= \mathbb{E}[g(X)] \\
g_i(X_i) &= \mathbb{E}[g(X)|X_i] - g_0 \\
g_I(X_I) &= \mathbb{E}[g(X)|X_I] - \sum_{J \subsetneq I} g_J(X_J) \qquad \text{(recursion)} \\
&= \sum_{J \subseteq I} (-1)^{|I|-|J|} \mathbb{E}[g(X)|X_J] \qquad \text{(inclusion-exclusion)}
\end{aligned}$$

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.

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

$$\begin{aligned} \mathbb{E}[g_I(X_I)h(X_J)] &= \mathbb{E}[\mathbb{E}[g_I(X_I)h_J(X_J)|X_J]] \\ &= \mathbb{E}[h(X_J)\mathbb{E}[g_I(X_I)|X_{J\cap I}]] = 0 \end{aligned}$$

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

$$D := \mathrm{Var}(g(X)) = \sum_{I \subseteq \{1,\dots,d\}} \mathrm{Var}(g_I(X_I))$$

Orthogonal projections

Property

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

Orthogonal projections

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Proof.
Using the non-overlapping condition:

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

$$\begin{aligned} \langle \Pi_I g, h \rangle &= \mathbb{E}(g_I(X_I)h(X)) \\ &= \sum_{J \subseteq \{1,\dots,d\}} \mathbb{E}(g_I(X_I)h_J(X_J)) = \mathbb{E}(g_I(X_I)h_I(X_I)) = \langle g, \Pi_I h \rangle \end{aligned}$$

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 *(a class of) commuting projections* $P_1, \dots, P_d$ ([Kuo et al., 2010]), here orthogonals:

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

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$$I_d \quad = \quad (P_1 + (I_d - P_1)) \dots (P_d + (I_d - P_d))$$

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$$\begin{aligned} I_d &= (P_1 + (I_d - P_1)) \dots (P_d + (I_d - P_d)) \\ &= \sum_{I \subseteq \{1,\dots,d\}} \underbrace{\prod_{j \notin I} P_j \prod_{k \in I} (I - P_k)}_{\Pi_I} \end{aligned}$$

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

An example: separable functions

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

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

Proof. The Sobol-Hoedding decomposition is obtained by expanding:

$$g(x) = ((f_1(x_1) - m_1) + m_1)\dots((f_d(x_d) - m_d) + m_d)$$

For each bracket,

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

Sensitivity indices

Sobol indices

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

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

- $D_i^{\text{tot}} = \sum_{J \supseteq \{i\}} D_J, \qquad S_i^{\text{tot}} = \frac{D_i^{\text{tot}}}{D}$ *Total index*
- $D_I^{\text{tot}} = \sum_{J \supseteq \{I\}} D_J, \qquad S_I^{\text{tot}} = \frac{D_I^{\text{tot}}}{D}$ *Total interaction, superset importance*

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Derivative Global Sensitivity Measure (DGSM)

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

Usage for screening

Assume that:

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

- **Variable screening**
  If either $D_i^{tot} = 0$ or $\nu_i = 0$, then X_i is non influential

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- **Variable screening**
  If either $D_i^{tot} = 0$ or $\nu_i = 0$, then X_i is non influential

- **Interaction screening**
  If either $D_{i,j}^{tot} = 0$ 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 $a = c(0, 1, 4.5, 9, 99, 99, 99, 99)$.

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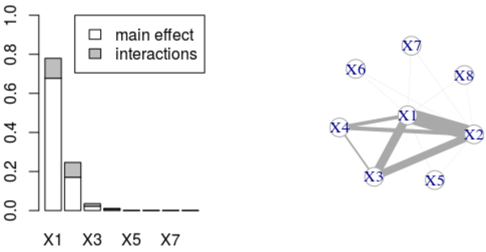

Figure: 1st order analysis (left) and 2nd order analysis (right) with 10^5 simulated data

Illustration on a toy example

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

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

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

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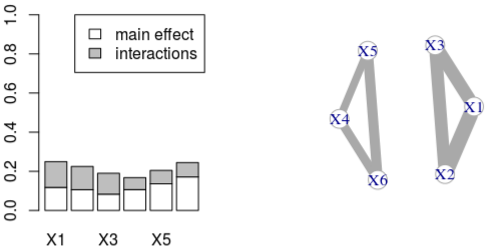

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Part II

Upper bounds for Sobol indices

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**

	Computational cost	Interpretability
Sobol indices	-	+
DGSM	+	-

Variance-based and derivative-based measures

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- **Advantages / Drawbacks**

	Computational cost	Interpretability
Sobol indices	-	+
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$$\downarrow$$

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

Poincaré inequality

Poincaré inequality (1-dimensional case)

A distribution μ 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 $C_{\mathrm{P}}(\mu)$.

Link between total Sobol indices and DGSM

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

If μ_i and μ_j admit a Poincaré inequality, then:

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

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

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

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$$\begin{aligned} D_i^{\text{tot}} = \mathrm{Var}(g_i^{\text{tot}}(x)) &= \int \left(g_i^{\text{tot}}(x)\right)^2 d\mu(x) \\ &\leq C(\mu_i) \int \left(\frac{\partial g_i^{\text{tot}}(x)}{\partial x_i}\right)^2 d\mu(x) = C(\mu_i)\nu_i \end{aligned}$$

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

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$$\begin{aligned} D_{i,j}^{\text{tot}} = \mathrm{Var}(g_{i,j}^{\text{tot}}(x)) &= \int \left(g_{i,j}^{\text{tot}}(x)\right)^2 d\mu(x) \\ &\leq C(\mu_i) \int \left(\frac{\partial g_{i,j}^{\text{tot}}(x)}{\partial x_i}\right)^2 d\mu(x) \\ &\leq C(\mu_i)C(\mu_j) \int \left(\frac{\partial}{\partial x_j} \frac{\partial g_{i,j}^{\text{tot}}(x)}{\partial x_i}\right)^2 d\mu(x) = C(\mu_i)C(\mu_j)\nu_{i,j} \end{aligned}$$

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*:

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

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

pdf	Support	C_{opt}	Form of $f_{\mathrm{opt}}(x)$
Uniform	$[a, b]$	$(b-a)^2/\pi^2$	$\cos\left(\frac{\pi(x-a)}{b-a}\right)$
$\mathcal{N}(\mu, \sigma^2)$	$\mathbb{R}$	σ^2	$x-\mu$
	$[r_{n,i}, r_{n,i+1}]$	$1/(n+1)$	$H_{n+1}(x)$
	$[a, b]$	*related to Kummer*	*hypergeom. func.*
Db. exp. $e^{-\lvert x\rvert}dx/2$	$\mathbb{R}$	4	$\times$
(*)	$[a, b], ab > 0$	$\left(\frac{1}{4}+\omega^2\right)^{-1}$	$e^{x/2}\cos(\omega x+\phi)$
(*, **)	$[a, b], ab \leq 0$	$> \left(\frac{1}{4}+\omega^2\right)^{-1}$	$e^{\lvert x\rvert/2} \times$ *trig. spline*
Logistic $\frac{e^x}{(1+e^x)^2}dx$	$\mathbb{R}$	4	$\times$
Triangular	$[-1, 1]$	≈ 0.1729	*linked to Bessel* J_0

(*) 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 $x \mapsto \mathrm{cotan}(|a|x) + \mathrm{cotan}(|b|x) + 1/x$

Optimal Poincaré constants: Examples

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

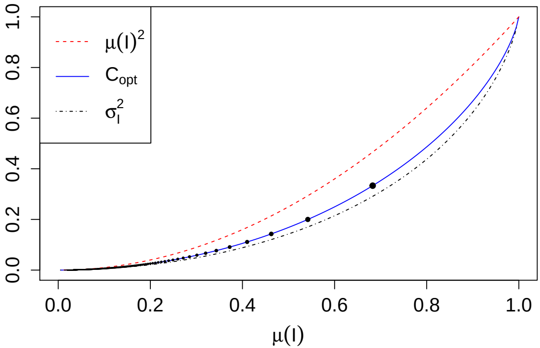
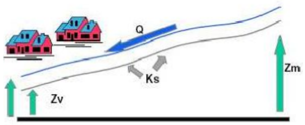


Figure: Poincaré constant of $\mu = \mathcal{N}(0,1)$ truncated on $I = [-b, b]$, vs $\mu(I)$

σ_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:

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

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:

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

- *Aim: To detect unessential X_i's, to quantify the influence of X_i's on S, ...*

A case study for global sensitivity analysis

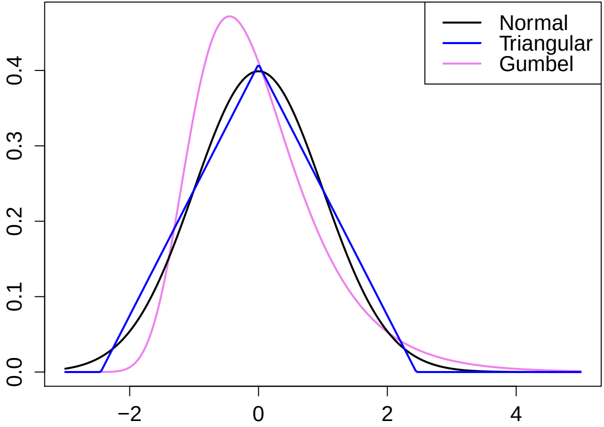
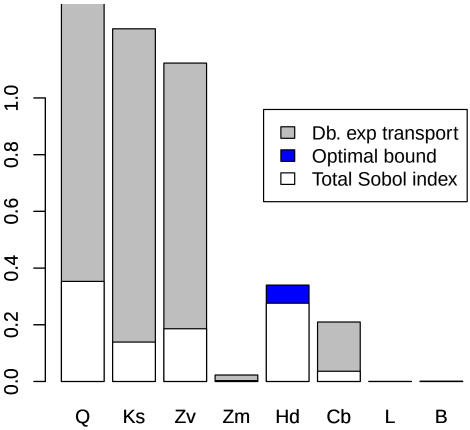


Figure: The 3 distributions types of the case study, here with mean 0 and variance 1

Results with optimal Poincaré constants



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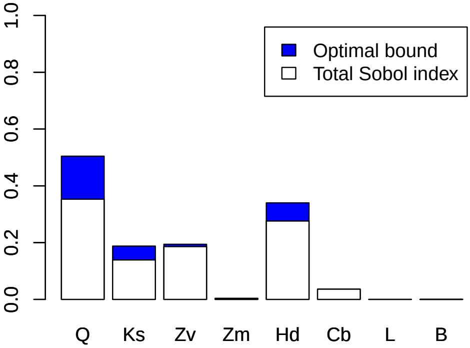

Part III

Lower bounds for Sobol indices

Ongoing work with F. Gamboa and B. Iooss

Principle

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

$$\begin{array}{lcll} F_1 & = & \{g \in L^2(\mu) \text{ s.t. } g = g_1\} & \text{functions } \textit{depending exactly on } x_1 \\ F_1^{\text{tot}} & = & \{g \in L^2(\mu) \text{ s.t. } g = g_1^{\text{tot}}\} & \text{functions } \textit{depending at least on } x_1 \end{array}$$

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

$$\begin{array}{lcl} g_1 & = & \Pi_{F_1}(g) = \mathbb{E}[g(X)|X_1 = .] \\ g_1^{\text{tot}} & = & \Pi_{F_1^{\text{tot}}}(g) = g - \mathbb{E}[g(X)|X_2 = ., \dots, X_d = .] \end{array}$$

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^{tot} are obtained by *projecting onto subspaces* of F_1, F_1^{tot}

Main result

Let $\phi_1, \dots, \phi_m$ be orthonormal functions in F_1^{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 $g(x) = \sum_{j=1}^{m} \alpha_m \phi_m(x) + h(x_2, \dots, x_m)$.

If all the ϕ_j's belong to F_1 then the lower bound is for D_1.

Proof.

- $D_1^{\text{tot}} = \|g_1^{\text{tot}}\|^2 = \|\Pi_{F_1^{\text{tot}}}(g)\|^2 \geq \|\Pi_{\phi_1,\dots,\phi_m}(g)\|^2 = \sum_{j=1}^{m} \left(\langle g, \phi_j \rangle\right)^2$
- Equality is when $g_1^{\text{tot}} = \Pi_{\phi_1,\dots,\phi_m}(g)$, leading to the condition above.
- Same arguments when all the ϕ_j's are in F_1

Tensor-based lower bounds

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

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

where $\underline{\ell} = (\ell_1, \dots, \ell_d)$ is a multi-index.

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

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

with equality iff f has the form $f(x) = \sum_{\underline{\ell} \in \mathcal{T}_1} \alpha_{\ell} \phi_{\underline{\ell}}(x) + g(x_2, \dots, x_d)$.

Tensor-based lower bounds

As an illustration, if μ_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 $\psi_1, \psi_1\psi_2, \dots, \psi_1\psi_j$ *are orthonormal functions of* F_1^{tot}.
Hence:

$$D_1^{\text{tot}} \geq \underbrace{\left(\int g(x)\psi_1(x)d\mu(x)\right)^2}_{\text{lower bound for } D_1} + \sum_{j=2}^{m}\left(\int g(x)\psi_1(x)\psi_j(x)d\mu(x)\right)^2$$

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.

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But this often induce weights; Here is a partial solution to avoid weights.

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

$$Z_j(X_j) = (\ln p_j)'(X_j), \qquad I_j = \mathrm{Var}(Z_j(X_j))$$

Then:

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

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 $N(m_j, s_j^2)$:

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

Dist. name	Support	p	Z	I
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	$\mathbb{R}$	$\frac{1}{2s} \exp\left(\frac{\lvert x-m\rvert}{s}\right)$	$-\mathrm{sgn}(X-m)/s$	$1/s^2$
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:

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

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- 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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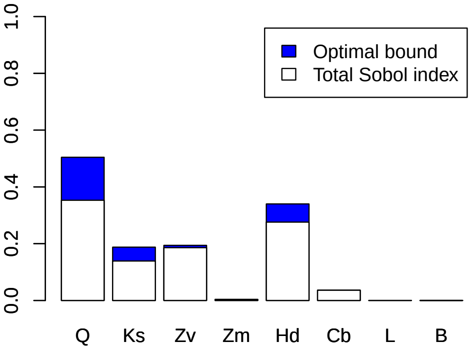
N.B. Better bounds are obtained by adding orth. funct. of the form $\psi_1 \psi_j$.

Results on the application



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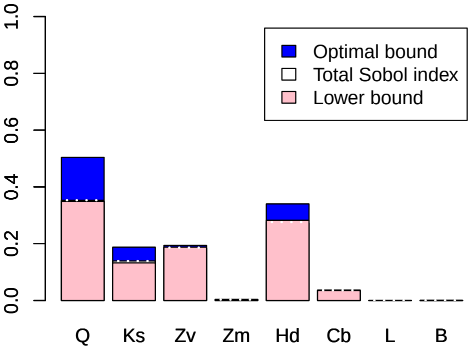

Figure: Results obtained with orth. 1st order pol. tensors $\psi_1, \psi_1\psi_2, \ldots, \psi_1\psi_8$

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:

$$h_{\text{dir}} = g\phi_1, g\phi_1\phi_j, \ldots, \qquad \text{or} \qquad h_{\text{der}} = \frac{\partial g}{\partial x_i}, \frac{\partial g}{\partial x_j} Z_j, \ldots$$

for centered function ϕ_1, ϕ_j, Z_j.

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for centered function ϕ_1, ϕ_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:

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

Hence, for one squared integral, using the derivative form can reduce estimation error when h_{der} is less variable than h_{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* $\{g \in L^2(\mu)$ s.t. $g = g_I\}$

  $\rightarrow$ *Illustrated on main and total effects, but very general!*

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- *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,

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

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 $X^1, \dots, X^n$ of F

$$\mathbb{P}\left(\frac{\max_{k=1}^n(X_1^k) - b_{n,1}}{a_{n,1}} \leq x_1, \dots, \frac{\max_{k=1}^n(X_d^k) - b_{n,d}}{a_{n,d}} \leq x_d\right) \underset{n\to\infty}{\to} H(x)$$

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- 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) ℓ

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

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

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

Asymptotic independence and tail dependograph

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

X_A and X_B are *asymptotically independent*

$$
\begin{aligned}
&\Leftrightarrow \quad H(x) \text{ if of the form } H(x) = H_A(x_A)H_B(x_B) \\
&\Leftrightarrow \quad \ell(u) \text{ 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
\end{aligned}
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Thus

$$X_A \underset{\infty}{\perp\!\!\!\perp} X_B \quad \textit{if} \quad \underbrace{\textit{the FANOVA graph of } \ell}_{\text{“tail dependograph”}} \textit{ is partitioned by A and B}$$

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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Hence,

$$X_i \underset{\infty}{\perp\!\!\!\perp} X_j \quad \text{if} \quad \theta_{i,j}(\ell) = 2$$

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:

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

with asymetric parameters: $(w, \alpha) = (0.2, 0.2), \quad (w', \alpha') = (0.8, 0.83)$.

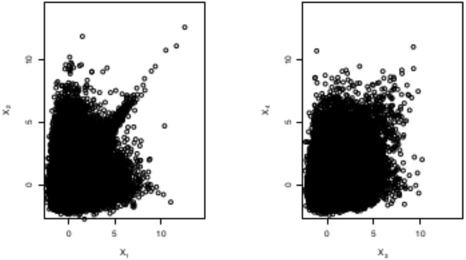
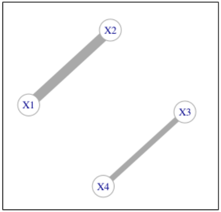


Illustration: Revealing asymptotic dependence for asymmetric models



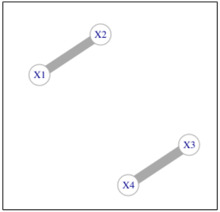


Figure: Tail dependograph (left) and graph representing $2 - \theta_{i,j}$ (right)

$\rightarrow$ Both indices recover the asympt. indep. between (X_1, X_2) and (X_3, X_4)

$\rightarrow$ Asymmetry in tail dependence is more visible on tail dependograph

Inference

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

$$
\begin{aligned}
\hat{\ell}_{k,n}(u) &= \frac{n}{k}\left(1 - \frac{1}{n}\sum_{s=1}^{n} \mathbf{1}\left\{X_s^{(1)} < X^{(1)}_{n-[ku_1]+1,n}, \dots, X_s^{(d)} < X^{(d)}_{n-[ku_d]+1,n}\right\}\right) \\
&= \frac{n}{k}\left(1 - \frac{1}{n}\sum_{s=1}^{n} \mathbf{1}\left\{u_1 < \tilde{R}_s^{(1)}, \dots, u_d < \tilde{R}_s^{(d)}\right\}\right) \\
&= \frac{n}{k} - \frac{1}{k}\sum_{s=1}^{n} \underbrace{\prod_{t=1}^{d} \mathbf{1}\{u_t < \tilde{R}_s^{(t)}\}}_{\text{separable function}}
\end{aligned}
$$

with:

- $X^{(t)}_{1,n}, \dots, X^{(t)}_{n,n}$: 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 $X_1^{(t)}, \dots, X_n^{(t)}$.

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

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

and the tail dependograph as well

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

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

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

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... 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. χ^2 type with rate k

(The same is true for D_I^{tot})

Inference

(A piece of intuition about asymptotic distribution)

$$\hat{\ell}_{k,n;I}(u_I) \quad = \quad \ell_I(u_I) + \frac{1}{\sqrt{k}} Y_{\ell,I}(u_I) + \dots$$

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Application on real data

Dataset: yearly maxima temperatures at 21 French cities during 1946 – 2000.

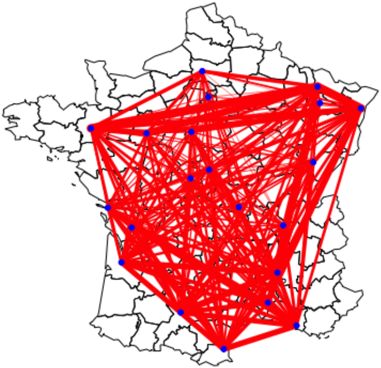

Figure: Estimated tail dependograph: complete, 30 largest values, 9 largest

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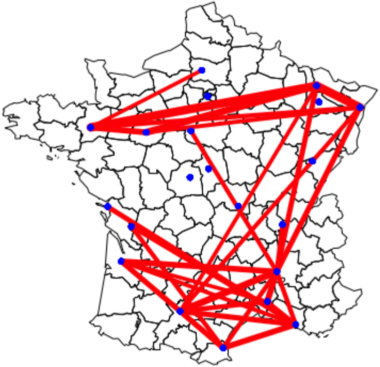

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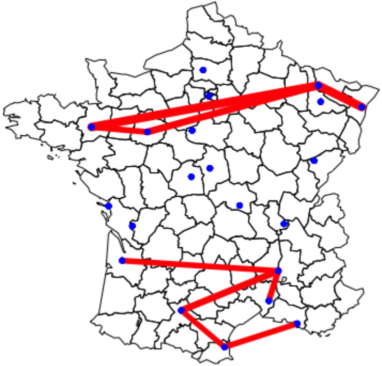

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Tail dependograph is a graphical tool to investigate multivariate independence.

- Asymptotic independence is visible by partitions in the graph
- Asymetric 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

References - Thank you for your attention!

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