



Sensitivity analysis

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Context

We consider

$$Y = f(\underline{X})$$

- f is a **model** (scientific simulation software, symbolic function ...)
- $\underline{X} = (X_1, \dots, X_d)$ is the set of **uncertain parameters** modeled by a multivariate distribution of dimension d
- Y is the **feature of interest** evaluated by the model, supposed here to be scalar.

Why sensitivity analyses ?

The main objectives of sensitivity analyses may be :

- ① **remove some variables** which are not influential on the feature of interest, within a context of high dimension,
- ② **prioritize variables** in order to prioritize modeling efforts : we need a *relative* quantification
- ③ **quantify the impact of a variable** : we need an *exact* quantification

Sensitivity : several notions

Several features can quantify the dependence.

Sensitivity = Dispersion = Variance

If we agree that the **variance is a good way to quantify the dispersion**, sensitivity analyses aim at determining the most important contributors to the variance of Y .

We use the **conditional expectation** $\mathbb{E}(Y|X_i) = Y_i^*$ which is the random variable function of X_i which approximates Y the best in the least square sense :

$$Y_i^* = \operatorname{argmin}_g \mathbb{E}([Y - g(X_i)]^2)$$

No constraint on the nature of the link between Y and X_i .

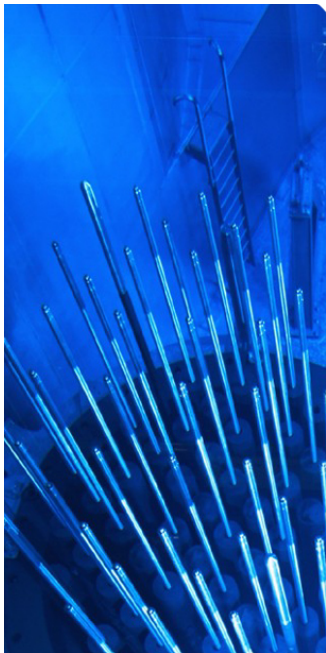
We want to compare **$\operatorname{Var}(Y_i^*)$** to **$\operatorname{Var}(Y)$** :

- ① in the case of independent variables : **Sobol indices**,
- ② in the case of dependent variables : importance factors (**Taylor decomposition variance**), **ANCOVA indices**.

Sensitivity = Distance to the independence

If Y and X_i are strongly correlated, the copula of (Y, X_i) is *far away* from the independent copula.

The **Csiszar divergence measures** enable to quantify that *distance*.



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Sobol Indices

Variance decomposition

Generally, if $Y = f(\underline{X})$ and X with **independent components**, then we can decompose the variance as follows :

$$\text{Var}(Y) = \sum_i \text{Var}(\mathbb{E}(Y|X_i)) + \sum_{i \neq j} \text{Var}(\mathbb{E}(Y|X_i, X_j)) + \cdots + \underbrace{\text{Var}(\mathbb{E}(Y|X_1, \dots, X_n))}_{=0} \quad (1)$$

Sobol Indices

The **Sobol indices of order k** quantifies the part of the variance of Y explained by the variance of $(X_{i_1}, \dots, X_{i_k})$:

$$S_{i_1, \dots, i_k} = \frac{\text{Var}(\mathbb{E}(Y|X_{i_1}, \dots, X_{i_k}))}{\text{Var}(Y)} \quad (2)$$

The **total Sobol indices of order k** quantifies the part of the variance of Y explained by the groups containing the inputs $(X_{i_1}, \dots, X_{i_k})$:

$$S_{i_1, \dots, i_k}^T = \frac{\sum_I \text{Var}(\mathbb{E}(Y|X_I))}{\text{Var}(Y)}, \quad \{i_1, \dots, i_k\} \subset I \subset \{1, \dots, n\} \quad (3)$$

The Hoeffding decomposition

The decomposition (1) of the variance of Y comes from the functional Hoeffding decomposition.

Hoeffding decomposition of a function integrable on $[0, 1]^n$

If f is integrable on $[0, 1]^n$, it admits an unique decomposition which writes :

$$f(x_1, \dots, x_n) = f_0 + \sum_{i=1}^{i=n} f_i(x_i) + \sum_{1 \leq i < j \leq n} f_{i,j}(x_i, x_j) + \dots + f_{1,\dots,n}(x_1, \dots, x_n) \quad (4)$$

where $f_0 = \text{cst}$ and the other functions are mutually orthogonal with respect to the Lebesgue measure on $[0, 1]^n$:

$$\int_0^1 f_{i_1, \dots, i_s}(x_{i_1}, \dots, x_{i_s}) f_{j_1, \dots, j_k}(x_{j_1}, \dots, x_{j_k}) d\underline{x} = 0 \quad (5)$$

as soon as $(i_1, \dots, i_s) \neq (j_1, \dots, j_k)$.

Sobol indices

How can we use this result for $Y = f(\underline{X})$ with \underline{X} a random vector ?

How can we use this result

We would like to decompose f according to Hoeffding decomposition ...but :

① **The inputs of f are not in $[0, 1]^n$** : generally, $Y = f(\underline{X})$ where \underline{X} is defined on \mathbb{R} .

⇒ If we note

$$\underline{U} = (F_1(X_1), \dots, F_n(X_n))^t = \phi^{-1}(\underline{X}) \quad (6)$$

then \underline{U} has uniform marges and its copula is the same as \underline{X} , then **we can use the Hoeffding decomposition on $f \circ \phi$** .

① **Are the Sobol indices w.r.t. the U_i the same as those w.r.t. the X_i ?**

⇒ If $\underline{U} = \psi(\underline{X})$ where ψ is a diffeomorphism and $Y = f(\underline{X})$ then :

$$\mathbb{E}(Y|\underline{U}) = \mathbb{E}(Y|\underline{X}) \quad (7)$$

As a matter of fact : $\mathbb{E}(Y|\underline{U}) = \mathbb{E}(Y|\psi(\underline{X}))$ is the orthogonal projection in a L_2 sens of Y on the space generated by $\psi(\underline{X})$, which is the same as the one generated by \underline{X} , thus the equality of the random variables (7).
As the transformation ϕ (6) acts component by component, ($U_i \leftrightarrow X_i$) then we have :

$$\text{Var} \left(\mathbb{E} \left(Y | U_{i_1}, \dots, U_{i_k} \right) \right) = \text{Var} \left(\mathbb{E} \left(Y | X_{i_1}, \dots, X_{i_k} \right) \right) \quad (8)$$

then **the equality of the Sobol indices w.r.t. the U_i and to the X_i** .

Sobol indices

Probabilistic interpretation of the Hoeffding decomposition

Let's suppose, without loss of generality, that the X_i are in $[0, 1]$. Then, using the Hoeffding decomposition (4), we have :

$$Y = f(\underline{X}) = f_0 + \sum_{i=1}^{i=n} f_i(X_i) + \sum_{1 \leq i < j \leq n} f_{i,j}(X_i, X_j) + \cdots + f_{1,\dots,n}(X_1, \dots, X_n) \quad (9)$$

The orthogonal condition (5) of the f_{i_1, \dots, i_k} w.r.t. the Lebesgue measure on $[0, 1]^n$ can be interpreted as an expectation calculus if the X_i are independent.

⇒ We suppose now that the X_i are **independent**.

Conclusion : Y can be decomposed as :

$$Y = f(\underline{X}) = Z_0 + \sum_{i=1}^{i=n} Z_i + \sum_{1 \leq i < j \leq n} Z_{i,j} + \cdots + Z_{1, \dots, n} \quad (10)$$

where $Z_0 = \text{cst}$ et $Z_{i_1, \dots, i_s} \perp Z_{j_1, \dots, j_k}$ (ie $\mathbb{E}(Z_{i_1, \dots, i_s} \cdot Z_{j_1, \dots, j_k}) = 0$).

Sobol indices

Calculus of the Sobol indices

From the probabilistic decomposition (10), we calculate $\mathbb{E}(Y)$ and $\text{Var}(Y)$:

$$\left\{ \begin{array}{l} \mathbb{E}(Y) = Z_0 + \sum_{i=1}^{i=n} \underbrace{\mathbb{E}(Z_i)}_{=0 \text{ since } \perp Z_0} + \sum_{1 \leq i < j \leq n} \underbrace{\mathbb{E}(Z_{i,j})}_{=0 \text{ since } \perp Z_0} + \cdots + \underbrace{\mathbb{E}(Z_1, \dots, n)}_{=0 \text{ since } \perp Z_0} \\ \mathbb{E}(Y^2) = \sum_{I \neq J} \underbrace{\mathbb{E}(Z_I Z_J)}_{=0 \text{ since } \perp \text{ the } Z_I} + \sum_I \mathbb{E}(Z_I^2) \sum_I \mathbb{E}(Z_I^2) \end{array} \right.$$

$$\Rightarrow \text{Var}(Y) = \sum_{i=1}^{i=n} V_i + \sum_{1 \leq i < j \leq n} V_{i,j} + \cdots + V_{1,\dots,n} \quad (11)$$

where $V_{i_1, \dots, i_k} = \text{Var}(Z_{i_1, \dots, i_k}) = \text{Var}(f_{i_1, \dots, i_k}(X_{i_1}, \dots, X_{i_k}))$.

An example

Data base analysis of aerodynamical coefficients

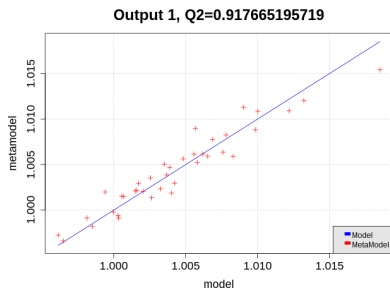
Data

- We focus on a black box from \mathbb{R}^{24} into \mathbb{R}^{12}
- We only know that function through a data base of size $n = 377$
- We have no information on the distribution followed by the input vector
- The objective is to identify, for each output component, the most influential inputs
- We only show the analysis on the first component.

How to proceed ?

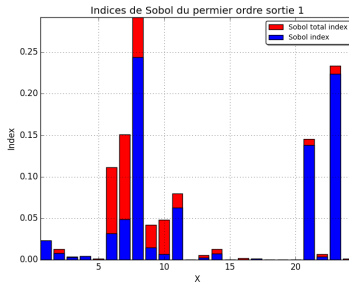
- We tested the independence hypothesis of the input using the Spearmann coefficients : we can't reject the hypothesis with a level 95%
- We built a meta model between the output and the inputs, using the penalized chaos polynomial expansion : the model is built from 90% of the data base and tested on the remaining 10%
- We exploit the model to calculate the Sobol indices (total and of order 1).

Quality of the meta-model



Model validation

Sobol indices



Input contributions to the variance of the output

We notice that it seems important to keep the inputs 6, 7, 8, 11, 21 et 23, and it is very likely that we can remove the inputs 3, 4, 5, 12, 13, 15, 16, 17, 18, 19, 20, 22 et 24 from the study. Doing that, we divided by 2 at least the input dimension.

Historical measures

Sobol indices were introduced by Sobol in 2001 ([Sobol2001]). But sensitivity indices were already existing ! :

- SRC, SRRC indices
- Pearson, Spearmann, PCC, PRCC indices
- importance factors from the *Taylor decomposition*

When the components X_i are independent, these indices are exactly particular cases of Sobol indices.

If the model f is linear w.r.t. the X_i : SRC

If $Y = \alpha_0 + \sum_i \alpha_i X_i$, with X_i independent, then we define the **Standard Regression Coefficient (SRC)** :

$$SRC(X_i) = \frac{\alpha_i^2 \text{Var}(X_i)}{\text{Var}(Y)} \quad (12)$$

Then SRC is the **Sobol indice** of order 1 of X_i : $SRC(Y/X_i) = S(Y/X_i)$.

If the model f is linear w.r.t. the X_i : Pearson

If $Y = \alpha_0 + \sum_i \alpha_i X_i$, then we define the **Pearson correlation** between Y and X_i as :

$$\rho(Y, X_i) = \frac{\text{cov}[Y, X_i]}{\sqrt{\text{Var}(X_i) \text{Var}(Y)}} = \frac{\mathbb{E}([Y - \mathbb{E}(Y)][X_i - \mathbb{E}(X_i)])}{\sqrt{\text{Var}(X_i) \text{Var}(Y)}} \quad (13)$$

Moreover, if the X_i are independent, we show that :

$$\rho(Y, X_i) = \frac{\alpha_i \text{Var}(X_i)}{\sqrt{\text{Var}(X_i) \text{Var}(Y)}} \implies (\rho(Y, X_i))^2 = SRC(X_i) = S(Y/X_i)$$

Historical measures

If the model $rank(f)$ is linear w.r.t. the $rank(X_i)$: **SRRC**

If $Y = f(\underline{X})$ with X_i **independent**, with $\underline{U} = (F_1(X_1), \dots, F_n(X_n))^t = \phi^{-1}(\underline{X})$, we have $Z = F_Y(Y) = F_Y \circ f \circ \phi(\underline{U})$.

If we assume **in addition** that

$$Z = \alpha_0 + \sum_i \alpha_i U_i \quad (14)$$

then we define the **Standard Rank Regression Coefficient (SRRC)** :

$$SRRC(Y/X_i) = SRC(Z/U_i) = \frac{\alpha_i^2 \text{Var}(U_i)}{\text{Var}(Z)} = S(Z/U_i)$$

Then **SRRC** is a **Sobol indice** of order 1 calculated on the ranks of X_i and Y .

If the model $rang(f)$ is linear w.r.t. the ranks $rang(X_i)$: **Spearman**

If we assume that (14), we define the **rank Spearman correlation** between Y and X_i as :

$$\rho_S(Y, X_i) = \rho(F_Y(Y), F_i(X_i))$$

As previously, we show that in the case of **independent variables** :

$$(\rho_S(Y, X_i))^2 = SRRC(Y/X_i) = SRC(Z/U_i) = S(Z/U_i)$$

Historical measures

Importance factors from the *Taylor decomposition* have been defined in metrology first where :

- $Y = f(\underline{X})$
- \underline{X} is a gaussian vector with independent components with **low variation coefficient** ($\sigma/\mu \ll 1$)

$\Rightarrow f$ is linearised at $\mathbb{E}(\underline{X})$

Taylor approximation of order 1 at $\mathbb{E}(\underline{X})$

$Y = f(\underline{X})$ is approximated by its **Taylor approximation of order 1 at $\mathbb{E}(\underline{X})$** :

$$Y = f[\mathbb{E}(\underline{X})] + \langle \nabla f[\mathbb{E}(\underline{X})], \underline{X} - \mathbb{E}(\underline{X}) \rangle = f[\mathbb{E}(\underline{X})] + \sum_i [X_i - \mathbb{E}(X_i)] \left. \frac{\partial f}{\partial X_j} \right|_{\mathbb{E}(\underline{X})} \quad (15)$$

Under the **assumption of a linear model at $\mathbb{E}(\underline{X})$** , and **independent X_i** , we have :

$$\text{Var}(Y) = \sum_i \left(\left. \frac{\partial f}{\partial X_j} \right|_{\mathbb{E}(\underline{X})} \right)^2 \text{Var}(X_i) \quad (16)$$

We define the **importance factor of X_i** :

$$FI(X_i) = \left(\left. \frac{\partial f}{\partial X_j} \right|_{\mathbb{E}(\underline{X})} \right)^2 \frac{\text{Var}(X_i)}{\text{Var}(Y)} = SRC(Y/X_i) = S(Y/X_i)$$

The *FI* are Sobol indices of order 1.

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Taylor decomposition

In the case of dependent X_i , we **take into account the covariance matrix only** in order to calculate :

- the importance factors from the Taylor decomposition
- the ANCOVA indices

Taylor decomposition

$Y = f(\underline{X})$ is approximated by its **Taylor approximation of order 1 at $\mathbb{E}(\underline{X})$** :

$$Y = f[\mathbb{E}(\underline{X})] + \langle \underline{\nabla} f[\mathbb{E}(\underline{X})], \underline{X} - \mathbb{E}(\underline{X}) \rangle = f[\mathbb{E}(\underline{X})] + \sum_i [X_i - \mathbb{E}(X_i)] \left. \frac{\partial f}{\partial X_i} \right|_{\mathbb{E}(\underline{X})} \quad (17)$$

Under the **assumption of a linear model at $\mathbb{E}(\underline{X})$** , we have :

$$\text{Var}(Y) = {}^t \underline{\nabla} f[\mathbb{E}(\underline{X})] \cdot \underline{\underline{\text{Cov}}}[\underline{X}] \cdot \underline{\nabla} f[\mathbb{E}(\underline{X})] = \sum_{i,j} \left. \frac{\partial f}{\partial X_i} \right|_{\mathbb{E}(\underline{X})} \text{Cov}[X_i, X_j] \cdot \left. \frac{\partial f}{\partial X_j} \right|_{\mathbb{E}(\underline{X})} \quad (18)$$

We define the **importance factor of X_i** as :

$$FI(X_i) = \frac{\left(\sum_j \left. \frac{\partial f}{\partial X_j} \right|_{\mathbb{E}(\underline{X})} \text{Cov}[X_i, X_j] \right) \left. \frac{\partial f}{\partial X_i} \right|_{\mathbb{E}(\underline{X})}}{\text{Var}(Y)} \quad (19)$$

ANCOVA indices

The **ANCOVA** (ANalysis of COVariance) method, is a variance-based method generalizing the ANOVA (ANalysis Of VAriance) decomposition for models with correlated input parameters (see [Caniou2012]). It is based on the Hoeffding decomposition of f that writes :

$$Y = f(x_1, \dots, x_n) = f_0 + \sum_{U \subset \{1, n\}} f_U(\underline{X}_U) \quad (20)$$

where U is a non empty set of indices in $\{1, n\}$. Thus $f_U(\underline{X}_U)$ is the combined contribution of X_U to Y .

Definition

The total part of variance of Y due to \underline{X}_U writes :

$$S_U = \frac{\text{Cov}(Y, f_U(\underline{X}_U))}{\text{Var}(Y)} = S_U^1 + S_U^2$$

where

$$\begin{cases} S_U^1 &= \frac{\text{Var}(f_U(\underline{X}_U))}{\text{Var}(Y)} \\ S_U^2 &= \frac{\text{Cov}\left(f_U(\underline{X}_U), \sum_{V|V \cap U = \emptyset} f_V(\underline{X}_V)\right)}{\text{Var}(Y)} \end{cases}$$

S_U^1 is the contribution to $\text{Var}(Y)$ of \underline{X}_U .

S_U^1 is the contribution to $\text{Var}(Y)$ of \underline{X}_U through its correlation to the other variables.

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Csiszar Divergence

Principle : The sensitivity of Y w.r.t. X_i is no more defined as the part of the variance of Y due to the variance of X_i . We use a notion of distance between the real dependence between Y and X_i , and the independence. We assume that Y and X_i are scalar to ease the notations of this presentation.

Indices based on the Csiszar divergence

In [Borgonovo2016] and [DaVeiga2013], the authors compare the distribution of (X_i, Y) , with pdf $p_{X_i, Y}$ to the product distribution of X_i and Y (which assumes the independence), with pdf $p_Y \otimes p_{X_i}$. They define some sensitivity indices based on the **Csiszar divergence** D_f as :

$$S_i^f = D_f(p_{Y \otimes X_i} \| p_{(Y, X_i)})$$

We show that this indice :

- depends on the whole distribution and not on its first moments only
- is independent of the margins (and then of the scale of the components)

This indice depends on the copula only as it can be written as :

$$S_i^f = D_f(\Pi \| c_{(Y, X_i)})$$

Recall : The copula of (X, Y) is the same as the copula of $(f(X), g(Y))$ if f and g are some increasing functions.

In particular, we can consider the uniform margins with $f = F_X$ et $g = F_Y$.

CsiszarDivergence

Définition

([Csiszar1963]) Let P and Q be two probability measures defined on the space Ω and f a convex positive function defined at least on \mathbb{R}^+ such that $f(1) = 0$.

The f -Csiszár divergence of Q w.r.t. P is defined as :

- If P and Q are absolutely continuous w.r.t. the Lebesgue measure dx , with pdf p and q , and if $P \ll Q$, then :

$$D_f(P||Q) = \int_{\Omega} f\left(\frac{p(x)}{q(x)}\right) q(x) dx \in [0, +\infty] \quad (21)$$

- If P and Q are absolutely continuous w.r.t. the counting measure defined on the $(x_k)_{k \in \mathbb{N}}$ (Dirac) and if $P \ll Q$, then :

$$D_f(P||Q) = \sum_{k=0}^{\infty} f\left(\frac{p(x_k)}{q(x_k)}\right) q(x_k) \quad (22)$$

Recall : $P \ll Q$ means $q(x) = 0 \implies p(x) = 0$

Examples

Name	Formula	Generator $f(u)$	$f(0) + f^*(0)$
Total Variation	$\frac{1}{2} \int p(x) - q(x) dx$	$\frac{1}{2} u - 1 $	1
Kullback-Liebler	$\int p(x) \log \frac{p(x)}{q(x)} dx$	$-\log u$	∞
Hellinger (square)	$\int \left(\sqrt{p(x)} - \sqrt{q(x)} \right)^2 dx$	$(\sqrt{u} - 1)^2$	2
Chi-2 Pearson	$\int \frac{(p(x) - q(x))^2}{p(x)} dx$	$(u - 1)^2$	∞

where $f^* : u \mapsto uf(1/u)$ the function *-conjugate of f

Properties

- Unicity : $\forall(P, Q), D_{f_1}(P||Q) = D_{f_2}(P||Q) \Leftrightarrow \exists c \in \mathbb{R}, f_1(u) - f_2(u) = c(u - 1)$
 - The divergences D_{f_1} and D_{f_2} quantify the gaps between the distributions exactly the same way when f_1 and f_2 differ from a linear function of $(u - 1)$
 - The divergences based on Kullback-Liebler and Hellinger are different
- Symetry : $\forall(P, Q), D_f(P||Q) = D_{f^*}(Q||P)$ and $\forall(P, Q), D_{f^*}(P||Q) = D_f(P||Q) \Leftrightarrow \exists c \in \mathbb{R}, f^*(u) - f(u) = c(u - 1)$
- Range : $0 = f(1) \leq D_f(P||Q) \leq f(0) + f^*(0)$
- Convexity : $\forall \lambda \in [0, 1], D_f(\lambda P_1 + (1 - \lambda)P_2 || \lambda Q_1 + (1 - \lambda)Q_2) \leq \lambda D_f(P_1 || Q_1) + (1 - \lambda)D_f(P_2 || Q_2)$

Csiszar Divergence

The sensitivity indice writes :

$$S_i^f = D_f(\Pi \| c_{(Y, X_i)}) = \int_{[0,1]^2} f\left(\frac{1}{c_{X_i, Y}(u, v)}\right) c_{X_i, Y}(u, v) \, dudv = \int_{[0,1]^2} f^*\left(c_{X_i, Y}(u, v)\right) \, dudv$$

How to interpret these indices ?

- If $Y \perp X_i$ then $S_i^f = 0$ (equivalence if f is strictly convex). In that case, X_i can be removed from the study since it has no impact on Y .
- If $Y = f(X_i)$ then $S_i^f = f(0) + f^*(0)$.

The characterisation of the range of the indices is the main result for the dependence analysis.

Methodology and numeric issues

Works are in progress on the following challenges :

- **how to interpret the value of the indice ?** $S_i^f = 0.8$: if Sobol indice, it means that 80% of the variance of Y is explained by the variance of X_i ... but what if Csiszar divergence ?
- **which f to consider ?** If $S_i^f > S_j^f$, do we still have $S_i^g > S_j^g$? Answer : no... thus, the hierarchisation depends on f . We have to *adapt* f to the needs of the study. For example, if $c(x_i, y)$ is low in some particular zones, we take a f which increases the gaps to 1 in that zone. We need to build a know-how !
- **how to estimate a copula density $c_{(Y, X_i)}$:** $\hat{S}_i^f = S_i^f(\hat{c}) \implies$ use of the Bernstein copula ?
- **how to create independence tests** based on an estimation of S_i^f , according to f ? : under the independence assumption, which confidence interval do we have on the values of \hat{S}_i^f ?

Csiszar Divergence - Independence Test

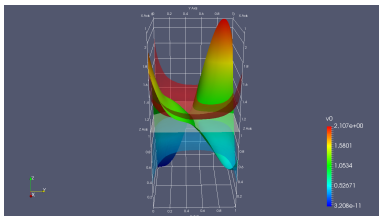
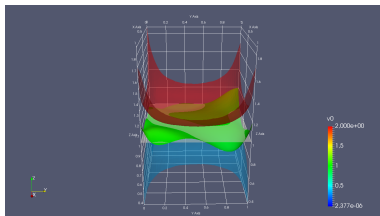
Proposition 1

How to proceed :

- ① On the sample k of (x_i, y) of size n , generated under the independence assumption between x_i and y , we build the copula density $\hat{c}_k(x_i, y)$ of (x_i, y) thanks to the Bernstein copula ;
- ② We repeat Step 1 N times : we draw, at any point (x_i, y) , the quantile 5% and 95% of the values of $\hat{c}_k(x_i, y)$, $1 \leq k \leq N$;
- ③ We build **90% confidence domain** point by point.

From the new sample to be tested, we build the copula density : if it goes out of the confidence domain, then we reject the independence assumption.

Example : Copula of (X_{19}, Y_1) (left) and of (X_8, Y_1) (right)



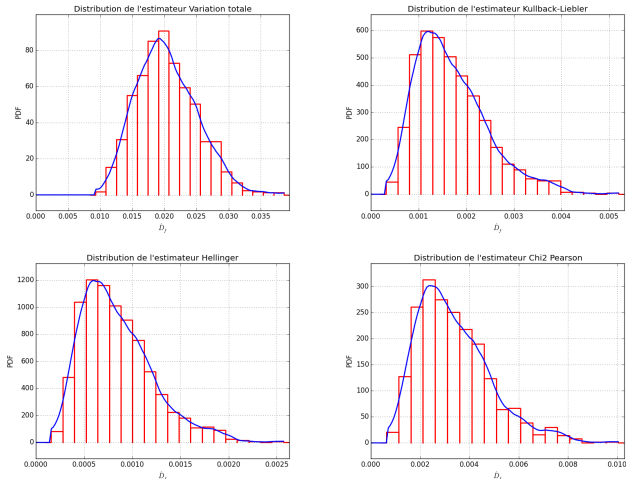
These graphs show that we can't reject the assumption that Y_1 is independent from X_{19} , while Y is clearly highly dependent on X_8 .

Csiszar Divergence - Independence Test

Proposition II

According to the previous procedure, we calculate $\hat{S}_i^f = S_i^j(\hat{c})$ for each f and we determine a distribution of \hat{S}_i^f and a confidence interval under the independence assumption.

Example : Estimation of sensitivity indices, $n = 1000$, $N = 10^4$.



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Références I



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