Estimation of moment independent importance measures using a copula and maximum entropy framework

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Pierre Derennes
Jérôme Morio (ONERA), Florian Simatos (ISAE)

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UNIVERSITÉ TOULOUSE III PAUL SABATIER
Université de Toulouse
ONERA
THE FRENCH AEROSPACE LAB
isae
Institut Supérieur de l'Aéronautique et de l'Espace

Context

Example: estimation of launch vehicle booster first phase fallout zone

- **Data:** meteorological conditions, launch vehicle mass, trajectory angle etc.
- **Computation code:** trajectory simulator.
- **Observation:** distance between the theoretical fallout position and the estimated one (due to uncertainty propagation).

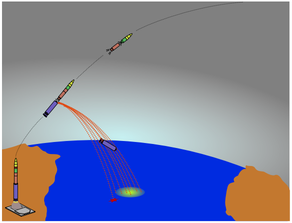
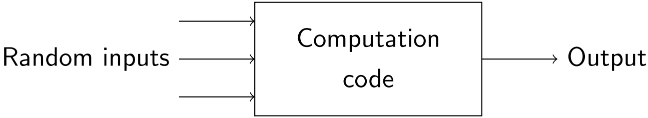
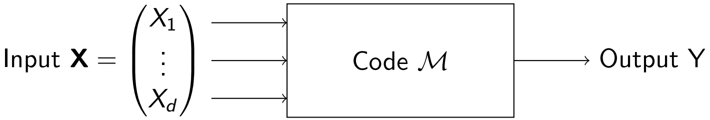


Figure: Illustration scheme of a launch vehicle first stage fallout phase [Derennes et al., 2019].



Sensitivity analysis

- **Goal:** identify and rank the input with respect to their impact on the output model.
- **Why ?**
  - Reduce the output uncertainty by reducing the uncertainty of the most influential inputs.
  - Improve the knowledge of the physical phenomenon.
  - Simplify the model.
- **Notations:**



Sobol's indices

Influence of the input X_i ?

Assumption: The inputs X_i are independent.

Goal: appreciate the contribution of the variable X_i to the variance of the model response Y.

Total variance theorem:

$$\mathbb{V}\mathrm{ar}[Y] = \mathbb{V}\mathrm{ar}[\mathbb{E}[Y|X_i]] + \mathbb{E}[\mathbb{V}\mathrm{ar}[Y|X_i]] \ .$$

First order Sobol's index:

$$\boxed{S_i = \frac{\mathbb{V}\mathrm{ar}\left(\mathbb{E}\left[Y|X_i\right]\right)}{\mathbb{V}\mathrm{ar}\left(Y\right)} \in [0,1]}$$

Total effect index:

$$\boxed{S_{Ti} = \frac{\mathbb{E}\left[\mathbb{V}\mathrm{ar}\left(Y|\mathbf{X}_{\sim i}\right)\right]}{\mathbb{V}\mathrm{ar}\left(Y\right)} \in [0,1]}$$

Borgonovo's indices

Influence of the input X_i ?

Assumption: the couple (X_i, Y) admits a probability density function (PDF) $f_{X_i,Y}$ with respect to Lebesgue measure.

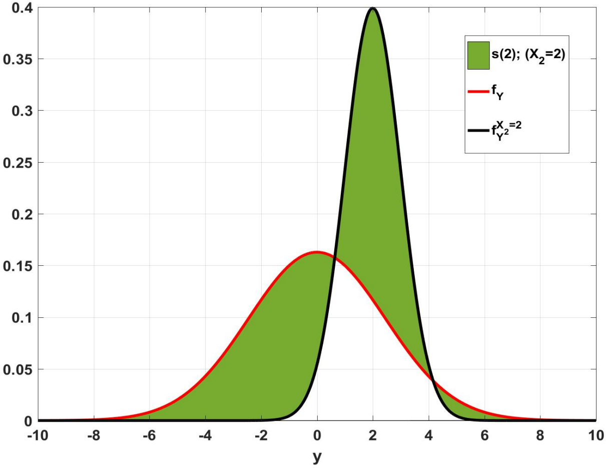
$\Rightarrow$ Random variables X_i, Y and Y conditioned on $X_i = x_i$ admit PDFs denoted by f_{X_i}, f_Y and $f_Y^{X_i=x_i}$ respectively.

Shift of densities:

$$s(x_i) = \left\| f_Y - f_Y^{X_i=x_i} \right\|_{L^1(\mathbb{R})} = \int \left| f_Y(y) - f_Y^{X_i=x_i}(y) \right| dy \ .$$

Geometric meaning of the shift

Example: $Y = X_1 + X_2$ where $X_1 \sim N(0,1)$ and $X_2 \sim N(0,5)$.



Definition of Borgonovo's importance measures

Borgonovo's importance measure [Borgonovo, 2007] of Y with respect to the input X_i:

$$\boxed{\delta_i = \frac{1}{2}\mathbb{E}[s(X_i)] \in [0,1]}$$

For a strict group of inputs $I \subset \{1, \dots, d\}$:

$$\delta_I := \frac{1}{2}\mathbb{E}\left[s(\mathbf{X}_I)\right] \quad \text{with} \quad s(\mathbf{x}_I) = \left\| f_Y - f_Y^{\mathbf{X}_I=\mathbf{x}_I} \right\|_{L^1(\mathbb{R})} .$$

Borgonovo's importance measures

$$\delta_i = \frac{1}{2}\mathbb{E}[s(X_i)]$$

Properties:

- $\delta_i = 0 \Leftrightarrow Y$ and X_i are independent.
- $I \subset J \Rightarrow \delta_I \leq \delta_J$.
- Monotonic transformation invariant.

Advantages:

- Suitable in the case of correlated inputs.
- No assumption on the model (the funtion $\mathcal{M}$ may be nonlinear).
- Consider the entire distribution of the output.

... **But not easy to compute !**

δ_i see as an expectation

$$\delta_i := \frac{1}{2}\mathbb{E}\left[s(X_i)\right], \; s(x_i) = \left\| f_Y - f_Y^{X_i=x_i} \right\|_{L^1(\mathbb{R})} .$$

Double loop method

$$\delta_i \approx \frac{1}{2N}\sum_{n=1}^{N} s(X_i^n), \; \{X_i^n\}_{n=1}^{N} \overset{\text{i.i.d}}{\sim} f_{X_i} ,$$

$$\approx \frac{1}{2N}\sum_{n=1}^{N} \hat{s}(X_i^n), \; \hat{s}(X_i^n) = \left\| \hat{f}_Y - \hat{f}_Y^{X_i=X_i^n} \right\|_{L^1(\mathbb{R})} .$$

Estimation of the output PDF f_Y and conditional PDFs $f_Y^{X_i=X_i^n}$ by Kernel Density Estimation (KDE) procedure.

Drawback

Budget: $N + d \times N^2$ calls to the model to get all δ-sensitivity measures.

δ_i see as measure of dependence

$$\delta_i = \frac{1}{2} \left\| f_Y f_{X_i} - f_{Y,X_i} \right\|_{L^1(\mathbb{R}^2)}$$

Importance Sampling estimation [Derennes et al., 2018]

$$\delta_i = \frac{1}{2} \int \frac{f_Y f_{X_i} - f_{Y,X_i}}{g} g := \frac{1}{2} \int hg = \frac{1}{2} \mathbb{E}\left[h(\mathbf{U})\right], \ \mathbf{U} \sim g \ .$$

$$\delta_i \approx \frac{1}{2} \mathbb{E}\left[\hat{h}(\mathbf{U})\right], \ \hat{h} = \frac{\hat{f}_Y f_{X_i} - \hat{f}_{Y,X_i}}{g} \ .$$

$\hat{f}_Y$, $\hat{f}_{Y,X_i}$: Gaussian kernel estimators.

Only N calls to the model to get all δ-sensitivity measures.

Drawback

Gaussian KDE may be inefficient in the case of bounded support or heavy tailed distributions.

δ_i see as measure of dependence

$$\delta_i = \frac{1}{2} \| f_Y f_{X_i} - f_{Y,X_i} \|_{L^1(\mathbb{R}^2)}$$

Nataf transformation based method [Zhang et al., 2014]

$$\mathbf{R}_i = (r_i(X_i), r_y(Y)) = \left(\Phi^{-1}(F_{X_i}(X_i)), \Phi^{-1}(F_Y(Y))\right) .$$

Very few calls to the model to get all δ-sensitivity measures.

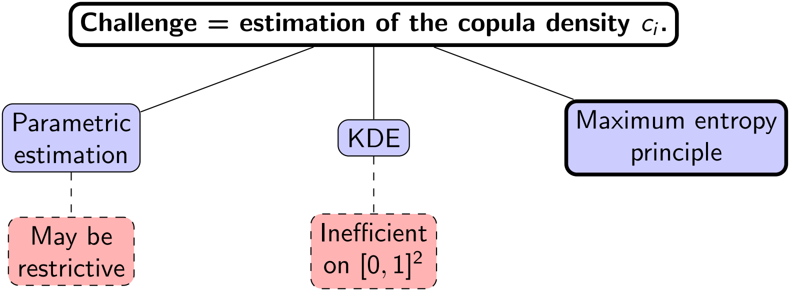
Drawback: strong assumptions are needed

- Inputs variables X_i are independent.
- $\mathbf{R}_i$ is assumed to be a Gaussian vector.

Copula representation of δ_i

$$\delta_i = \frac{1}{2} \int_{[0,1]^2} |c_i(u,v) - 1| \, dudv$$

c_i: PDF of the pair $(U_i, V) := (F_{X_i}(X_i), F_Y(Y))$.



Maximum entropy principle

Stochastic source

$$\mathbf{Z} \sim \mathbf{b}(\mathbf{p}), \ \mathbf{p} \in [\mathbf{0}, \mathbf{1}].$$

Entropy = amount of 'information'

$$H(Z) := H(p) = -p\log(p) - (1-p)\log(1-p).$$

Receptor

$$\mathbf{p} = ?$$

Available information: $Z \in \{0, 1\}$.

More 'reasonnable' assumption:

$$p = \frac{1}{2} = \text{Argmax } H(p).$$

Maximum entropy principle

Goal:

Estimate the PDF $f_{\mathbf{Z}}$ of an d-dimensional real valued random variable $\mathbf{Z}$.

Entropy: $H(f_{\mathbf{Z}}) = -\int_{\mathbb{R}^d} f_{\mathbf{Z}}(\mathbf{z}) \log(f_{\mathbf{Z}}(\mathbf{z})) d\mathbf{z}$.

Constraints: $S \subset \mathbb{R}^d$ and $\mathbb{E}[g(\mathbf{Z})] = \mathbf{b} \in \mathbb{R}^n$, $g : \mathbb{R}^d \to \mathbb{R}^n$.

Maximum entropy (ME) estimator:

$$\begin{cases} \hat{f}_{\mathbf{Z}} = \underset{f \in L^1(S, \mathbb{R}^+)}{\text{Argmax}} \; H[f] \\ \text{s.t. } \int_S g(\mathbf{z}) f(\mathbf{z}) d\mathbf{z} = \mathbf{b} \end{cases} .$$

$$\hat{f}_{\mathbf{Z}}(\mathbf{z}) \propto \mathbb{1}_S(\mathbf{z}) e^{-\langle \Lambda^*, g(\mathbf{z}) \rangle_{\mathbb{R}^n}} ,$$

where Λ^*, called *Lagrange multipliers*, is the unique solution of the following convex optimization problem

$$\underset{\Lambda \in \mathbb{R}^n}{\text{Argmin}} \; \langle \Lambda, \mathbf{b} \rangle_{\mathbb{R}^n} + \log \left(\int_S e^{-\langle \Lambda, g(\mathbf{z}) \rangle_{\mathbb{R}^n}} d\mathbf{z} \right) .$$

ME estimation of c_i - choice of constraints

Facts (dimension one): let Z be a real random variable supported in $S \subset [0, +\infty[$.

• The distribution of Z is uniquely characterized by an infinite sequence of distinct Fractional Moments (FMs) [Lin, 1992].

• Let us consider a sequence of FMs with equispaced exponents $\{\alpha_k := \frac{k\alpha^*}{m}\}_{k=1}^{m}$. The associated ME estimator, i.e,

$$\hat{f}_m^{\mathrm{ME}}(z) \propto \mathbb{1}_S(z) \exp\left(-\sum_{k=1}^{m} \lambda_k z^{\alpha_k}\right) ,$$

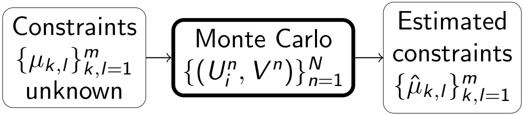
converges to the true distribution of Z as the number of constraints m tends to $+\infty$ [Novi Inverardi and Tagliani, 2003].

Constraints on $(U_i, V) = m^2$ FMs of the product $U_i V$

$$\mu_{k,l} := \mathbb{E}\left[U_i^{\alpha_k} V^{\alpha_l}\right] , \ \ k, l = 1, \ldots, m ,$$

with equispaced exponents $\alpha_k := \frac{k\alpha^*}{m}$.

ME estimation of c_i - estimation of constraints



Compromise between parameters N and m.

For a fixed sample size N, the ME estimator associated to estimated constraints $\{\hat{\mu}_{k,l}\}_{k,l=1}^{m}$ will tend to empirical distribution:

$$\frac{1}{N}\sum_{n=1}^{N}\delta_{(U_i^n, V^n)} \ .$$

= overlearning !

Proposed estimation scheme - Step 1.

Example:

$$Y = \prod_{i=1}^{4} X_i, \text{ with } X_i \overset{\text{i.i.d}}{\sim} L(0,1) \; .$$

- Generate $\{\mathbf{X}^n\}_{n=1}^{N} \overset{\text{i.i.d}}{\sim} f_{\mathbf{X}}$, with $\mathbf{X}^n := (X_1^n, ..., X_d^n)$.

Proposed estimation scheme - Step 1.

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- Obtain N observations of the model by $Y^n = \mathcal{M}(\mathbf{X}^n)$.

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- Compute

$$U_i^n := F_{X_i}(X_i^n) \ \text{ and } \ V^n := \hat{F}_Y(Y^n) \ .$$

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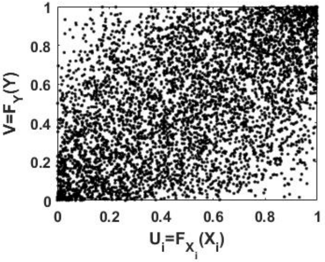
$N = 5,000$



Estimation of constraints

Step 1. $\Rightarrow \{(U_i^n, V^n)\}_{n=1}^N$.

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Estimation of constraints

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Step 2.

- Consider $\alpha_1 < \ldots < \alpha_m$.
- Approximate associated FMs $\{\mu_{k,l} = \mathbb{E}[U_i^{\alpha_k} V^{\alpha_l}]\}_{k,l=1}^m$ by

$$\mu_{k,l} \approx \hat{\mu}_{k,l} = \frac{1}{N} \sum_{n=1}^{N} (U_i^n)^{\alpha_k} (V^n)^{\alpha_l}, \;\; k,l = 1, \ldots, m.$$

Estimation of constraints

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Example: $m = 3$; $(\alpha_1, \alpha_2, \alpha_3) = (\frac{2}{3}, \frac{4}{3}, 2)$; $N = 5,000$.

$$\begin{pmatrix} \hat{\mu}_{1,1} & \hat{\mu}_{1,2} & \hat{\mu}_{1,3} \\ \hat{\mu}_{2,1} & \hat{\mu}_{2,2} & \hat{\mu}_{2,3} \\ \hat{\mu}_{3,1} & \hat{\mu}_{3,2} & \hat{\mu}_{3,3} \end{pmatrix} = \begin{pmatrix} 0.3901 & 0.2902 & 0.2314 \\ 0.2920 & 0.2230 & 0.1810 \\ 0.2340 & 0.1818 & 0.1493 \end{pmatrix}.$$

Computation of Lagrange multipliers

Step 2. $\Rightarrow \{\hat{\mu}_{k,l}\}_{k,l=1}^{m}$.

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Step 3.

Find the minimizer $(\lambda^*_{k,l})$ of the following **convex function**:

$$(\lambda_{k,l}) \mapsto \sum_{k,l=1}^{m} \lambda_{k,l}\hat{\mu}_{k,l} + \log\left(\int_{[0,1]^2} \exp\left(-\sum_{k,l=1}^{m} \lambda_{k,l} u^{\alpha_k} v^{\alpha_l}\right) dudv\right) .$$

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Example: $m = 3$; $(\alpha_1, \alpha_2, \alpha_3) = (\frac{2}{3}, \frac{4}{3}, 2)$; $N = 5,000$.

$$\begin{pmatrix} \lambda^*_{1,1} & \lambda^*_{1,2} & \lambda^*_{1,3} \\ \lambda^*_{2,1} & \lambda^*_{2,2} & \lambda^*_{2,3} \\ \lambda^*_{3,1} & \lambda^*_{3,2} & \lambda^*_{3,3} \end{pmatrix} = \begin{pmatrix} -56.6595 & 147.0305 & -82.2763 \\ 150.8583 & -422.3447 & 257.2539 \\ -88.0923 & 265.3930 & -172.4986 \end{pmatrix} .$$

ME Estimation of the copula density c_i

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Step 4. Estimate the density copula c_i by

$$\hat{c}_i(u,v) \propto \mathbb{1}_{[0,1]^2}(u,v) \exp\left(- \sum_{k,l=1}^m \lambda^*_{k,l} u^{\alpha_k} v^{\alpha_l} \right) .$$

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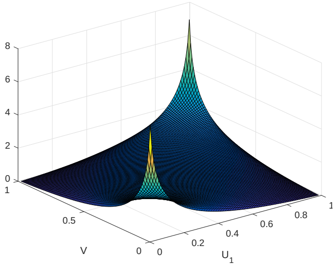
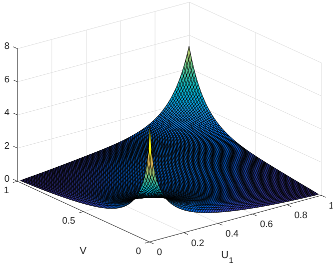
Example: $m = 3$; $(\alpha_1, \alpha_2, \alpha_3) = (\frac{2}{3}, \frac{4}{3}, 2)$; $N = 5,000$.



(e) True density copula c_1



(f) ME density copula

Estimation of δ_i

Step 4. $\Rightarrow \hat{c}_i$.

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Step 5. Approximate δ_i by

$$\delta_i \approx \frac{1}{2} \int_{[0,1]^2} |\hat{c}_i(u,v) - 1| \, dudv \ .$$

$$\delta_i \approx \hat{\delta}_i^{\mathrm{ME}} := \frac{1}{2N'} \sum_{k=1}^{N'} \left| \hat{c}_i(U_1^k, U_2^k) - 1 \right| , \ \{(U_1^k, U_2^k)\}_{k=1}^{N'} \overset{\text{i.i.d}}{\sim} U([0,1]^2) \, .$$

Estimation of δ_i

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Example: $m = 3$; $(\alpha_1, \alpha_2, \alpha_3) = (\frac{2}{3}, \frac{4}{3}, 2)$; $N = 5,000$; $N' = 10^6$.

$$\delta_1 = 0.1846 \ .$$

$$\hat{\delta}_1^{\text{ME}} = 0.1896$$

Budget: $N =$**5,000.**

A linear Gaussian model

Model output: $Y = \mathbf{AX}$ where $\mathbf{A} = [1.7\ 1.8\ 1.9\ 2]$ and where $\mathbf{X} \sim N(0, \Sigma)$ with

$$\Sigma = \begin{pmatrix} 1 & 1/2 & 1/3 & 1/4 \\ 1/2 & 1 & 1/2 & 1/3 \\ 1/3 & 1/2 & 1 & 1/2 \\ 1/4 & 1/3 & 1/2 & 1 \end{pmatrix} .$$

Set of parameters: $N = 5,000$ and $\{\alpha_k\} = \{\frac{2}{3}, \frac{4}{3}, 2\}$.

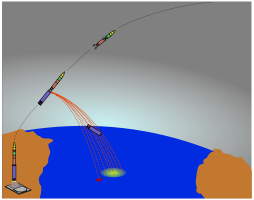
Input	Theoretical value δ_i	$\hat{\delta}_1^{ME}$ ($M = 100$ runs)		
		Mean	CV	RD
X_1	0.2857	0.2840	0.0174	-0.0058
X_2	0.3620	0.3538	0.0138	-0.0225
X_3	0.3792	0.3688	0.0121	-0.0274
X_4	0.3176	0.3141	0.0180	-0.0110

Ranking: $X_3 > X_2 > X_4 > X_1$.

Estimation of launch vehicle booster fallout zone

Computer code $\mathcal{M} : \mathbb{R}^{d=6} \to \mathbb{R}$: a simplified trajectory simulation code of the dynamic fallout phase of a generic launcher first stage.

- X_1: stage altitude perturbation
- X_2: velocity perturbation
- X_3: flight path angle perturbation
- X_4: azimuth angle perturbation
- X_5: propellant mass residual perturbation
- X_6: drag force error perturbation



Input[1]	Distribution	Mean	Std
X_1 (m)	Normal	0	1650
X_2 ($\mathrm{m.s^{-1}}$)	Normal	0	3.7
X_3 (rad)	Normal	0	0.001
X_4 (rad)	Normal	0	0.0018
X_5 (kg)	Normal	0	70
X_6 (dimensionless)	Normal	0	0.1

[1] The input variables are independent.

Estimation of launch vehicle booster fallout zone

Set of parameter: $N = 5,000$ and $\{\alpha_k\} = \{\frac{2}{3}, \frac{4}{3}, 2\}$.

Input:	X_1	X_2	X_3	X_4	X_5	X_6
Mean $\hat{\delta}_i^{ME}$	0.0154	0.1548	0.0692	0.1819	0.0155	0.0400
cv($\hat{\delta}_i^{ME}$)	0.2471	0.0400	0.0842	0.0235	0.2440	0.1140

$$S_i = \frac{\mathbb{V}\mathrm{ar}\left(\mathbb{E}\left[Y|X_i\right]\right)}{\mathbb{V}\mathrm{ar}\left(Y\right)} \quad , \quad S_{Ti} = \frac{\mathbb{E}\left[\mathbb{V}\mathrm{ar}\left(Y|\mathbf{X}_{\sim\ i}\right)\right]}{\mathbb{V}\mathrm{ar}\left(Y\right)} \ .$$

Input:	X_1	X_2	X_3	X_4	X_5	X_6
Mean $\hat{S}_i$	0.0047	0.2642	0.0712	0.1915	0.0040	0.0223
cv($\hat{S}_i$)	3.4040	0.0590	0.2414	0.0783	4.1093	0.8090
Mean $\hat{S}_{Ti}$	0.0151	0.6577	0.3826	0.2104	0.0169	0.2191
cv($\hat{S}_{Ti}$)	0.0266	0.0211	0.0238	0.0270	0.0248	0.0231

Results from [Derennes et al., 2019].

Conclusion and perspectives

Contributions

- A new estimation scheme of δ-sensitivity measures combining copula and maximum entropy framework with low budget simulation.
- The proposed method can handle models with correlated input or with heavy tailed distribution.

Future works

Estimation of higher order Borgonovo's indices.

$$\delta_{i,j} = \frac{1}{2}\int_{[0,1]^3}\left| c_{ij}(u,v,w) - \frac{f_{X_i,X_j}\left(F_{X_i}^{-1}(u), F_{X_j}^{-1}(v)\right)}{f_{X_i}(F_{X_i}^{-1}(u)) \times f_{X_j}(F_{X_j}^{-1}(v))}\right| dudvdw \ ,$$

c_{ij}: copula density of (X_i, X_j, Y).

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Thanks for your attention !