AN INFORMATION GEOMETRY APPROACH OF ROBUSTNESS ANALYSIS IN UNCERTAINTY QUANTIFICATION OF COMPUTER CODES

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EDF R&D PRISME

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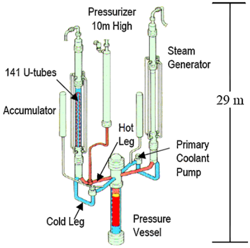
Introduction



Variables	Description
X1	Minimal film temperature
X2	Interfacial friction
X3	Interfacial friction
X4	Interfacial friction
X5	Interfacial friction
X6	Interfacial friction
X7	Critical flowrate

CATHARE code simulates a thermohydraulic transient during a specific accident.

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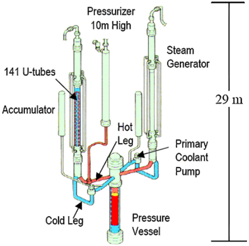
Hypothesis: Suppose X_i mutually independent.

CATHARE



Input variables	Probability distribution
X1	Uniform $\mathcal{U}([-44.9, 63.5])$
X2	Truncated Log Normal $\mathcal{LN}(0, 0.76)$ on $[0.1, 10]$
X3	Truncated Log Normal $\mathcal{LN}(0, 0.76)$ on $[0.1, 10]$
X4	Truncated Log Normal $\mathcal{LN}(0, 0.76)$ on $[0.1, 10]$
X5	Truncated Log Normal $\mathcal{LN}(0, 0.76)$ on $[0.1, 10]$
X6	Truncated Log Normal $\mathcal{LN}(-0.1, 0.45)$ on $[0.23, 3.45]$
X7	Truncated Normal $\mathcal{N}(6.4, 4.27)$ on $[0, 12.8]$

Experimental data and expert judgement help choosing probability distributions.

- Input parameters probability distribution is a strong prior in risk assessment studies.

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Internship objectives

- Input parameters probability distribution is a strong prior in risk assessment studies.
- The impact on the quantity of interest Y (here, the peak cladding temperature) by a **probability density perturbation** has to be assessed
- The initial density f_i of variable X_i is **perturbed** into $f_{i\delta}$
- Main issue: How to define such a perturbation ?

State of the art of density perturbations for robustness analysis in UQ

Recall the Kullback-Leibler divergence between two probability density functions p and q.

$$KL(p||q) = \int_{\mathbb{R}} p(x) \log \frac{p(x)}{q(x)} dx$$

- Pertubed density $f_{i\delta}$ is defined by minimizing the functional $q \to KL(q||f_i)$ with moments constraints. [1]

- Example: $\int x f_{i\delta}(x)dx = \delta_i, \int x^2 f_{i\delta}(x)dx = \delta_i$

[1] Paul Lemaitre's PhD thesis, *Analyse de sensibilité en fiabilité des structures*, Université de Bordeaux, 2014

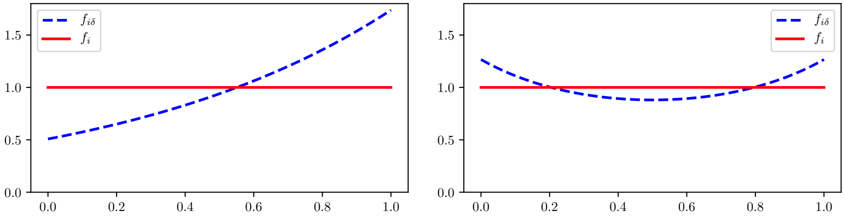


Figure 1: Mean (left figure) and variance (right figure) perturbation of $\mathcal{U}(0,1)$ density.

- **Idea**: Applying variational perturbation approach only to the standard Gaussian density (easier in terms of computation.)

- Be X a random variable with cdf F. We define:

$$S = \Phi^{-1}(F(X)) \ ,$$

  with Φ the cdf of the standard Gaussian density $\mathcal{N}(0, 1)$.

- Perturb the so called standard space variable S and then go back to the physical space using F^{-1}:

$$F_\delta = F^{-1}(\Phi(S + \delta))$$

- For random vector: use the more general Rosenblatt transform.

Graphical illustration - standard space approach

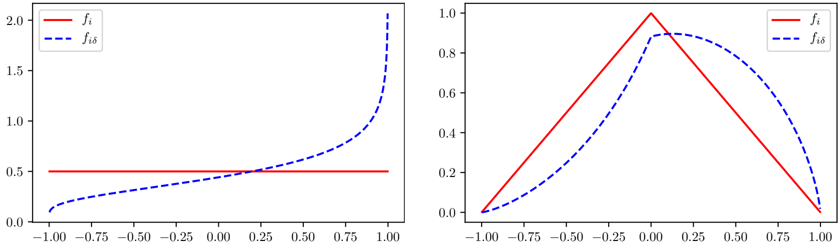


Figure 2: Standard space transformation of the $\mathcal{U}(-1, 1)$ and $\mathcal{T}(-1, 0, 1)$ probability densities with a mean shift of $\delta = 0.5$.

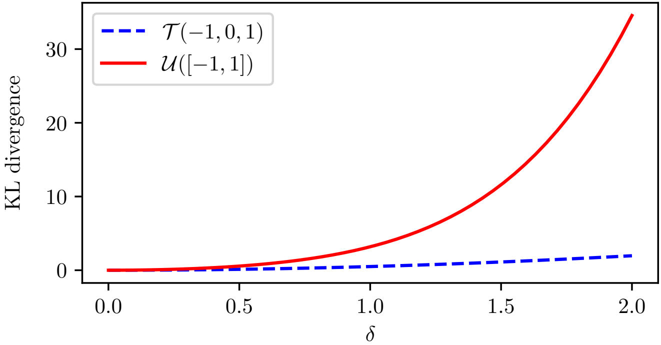


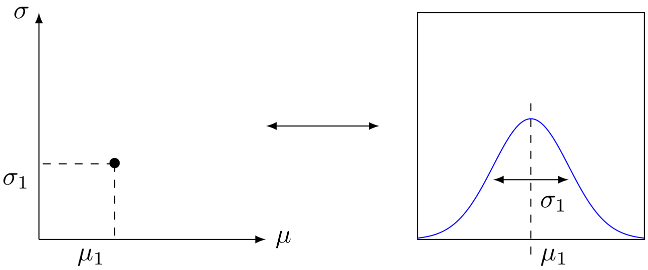
Figure 3: KL divergence between initial density $\mathcal{T}(-1,0,1)$ and $\mathcal{U}(-1,1)$ and their associated perturbed density

Standard space - drawbacks

- Unpredictable behaviour in the physical space
- Impossible to compare perturbations for the same δ values with different initial densities f_i.

Parametric framework

- Only parametric models are considered $\mathcal{S} = \{f_\theta, \theta \in \Theta \subset \mathbb{R}^d\}$
- Example: Gaussian distributions $\{\mathcal{N}(\mu, \sigma^2), (\mu, \sigma) \in \mathbb{R} \times \mathbb{R}^{+*}\}$



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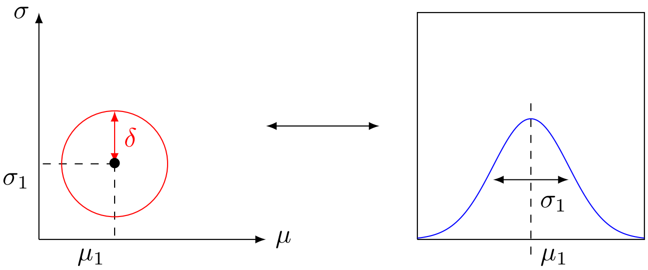

Information geometry: definition and interpretation

- Fisher information endows statistical models with a remarkable geometric structure.

- Let $\mathcal{S} = \{f_\theta, \theta \in \Theta \subset \mathbb{R}^d\}$ a parametric statistical model

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- A Riemannian manifold is defined on $\mathcal{S}$
- To each point θ is associated a tangent space $T_\theta\mathcal{S} \simeq \mathbb{R}^d$
- The latter scalar product is defined in $T_\theta\mathcal{S}$:

$$\forall u, v \in T_\theta\mathcal{S},\ \langle u, v\rangle_\theta = u^T I(\theta) v \ ,$$

where $I(\theta)$ is the Fisher information matrix evaluated in θ.

$$I(\theta) = \mathbb{E}\Big[(\nabla_\theta \log f_\theta(X))(\nabla_\theta \log f_\theta(X))^T\Big]$$

Fisher information is a key feature in asymptotic statistics.

Cramer Rao lower bound:

Let $\hat{\theta}$ be an unbiaised estimator of θ, then

$$V(\hat{\theta}) \geq I(\theta)^{-1} \,, \tag{1}$$

where $V(\hat{\theta})$ is the covariance matrix of the estimator.

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- Let $t \to q(t)$ be a $\mathcal{C}^1$ path in Θ, its length is defined by:

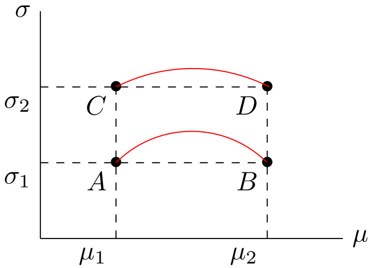
$$l(q) := \int_0^1 \sqrt{\langle \dot{q}(t), \dot{q}(t) \rangle_{q(t)}} dt \ ,$$

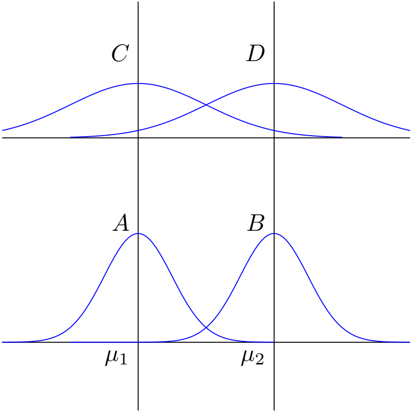
- the Fisher distance f_{θ_1} and f_{θ_2} is defined by:

$$d_F(f_{\theta_1}, f_{\theta_2}) = \inf_{q \in \mathcal{C}(\theta_1, \theta_2)} l(q) \ ,$$

where $\mathcal{C}(\theta_1, \theta_2)$ is the set of $\mathcal{C}^1$ path between θ_1 and θ_2.

Consider the space $\{\mathcal{N}(\mu, \sigma^2), (\mu, \sigma) \in \mathbb{R} \times \mathbb{R}^{+*}\}$





- Let $X_1, ..., X_n$ a n sized sample from the probability density f_θ.
- We denote by $\widehat{\theta}_n$ the maximum likelihood estimator

Central limit theorem:

$$\sqrt{n}(\widehat{\theta}_n - \theta) \xrightarrow{\mathcal{L}} \mathcal{N}(0, I(\theta)^{-1}) \ , \tag{2}$$

- The probability density of $\widehat{\theta}_n$ is:

$$p(\widehat{\theta}_n, \theta) \propto e^{-\frac{n}{2}\delta\theta^T I(\theta)\delta\theta}$$

- All distributions on the Fisher sphere are equivalent perturbed densities from f_{θ_0}.

Geodesics computation

- All distributions on the Fisher sphere are equivalent perturbed densities from f_{θ_0}.
- We need to compute all geodesics such that $q(0) = \theta_0$ and $d_F(q(0), q(1)) = \delta$ for $\delta \in \mathbb{R}^+$ fixed.

GEODESICS COMPUTATION

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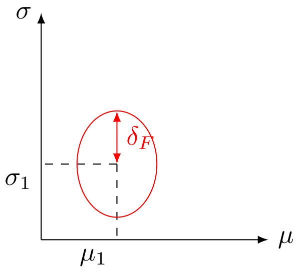

Let $t \to q(t)$ a path, with $p = I(q)\dot{q}$, the hamiltonian is written:

$$H(p,q) = \frac{1}{2} p^T I^{-1}(q) p \; .$$

If $t \to q(t)$ is a geodesic, then the function $t \to H(p(t), q(t))$ is constant.

A geodesic statisfies the following system of ordinary differential equations:

$$\begin{cases} \dot{q} = \frac{\partial H}{\partial p} \\ \dot{p} = -\frac{\partial H}{\partial q} \end{cases} \tag{3}$$

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- With $(q(0), p(0))$ defined, the ODE system (3) has an unique solution thanks to Cauchy's theorem
- Geodesics are computed using numerical methods.

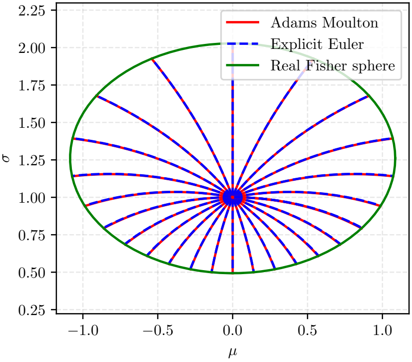

Figure 4: Fisher sphere $\delta = 1$ - Coordinate space

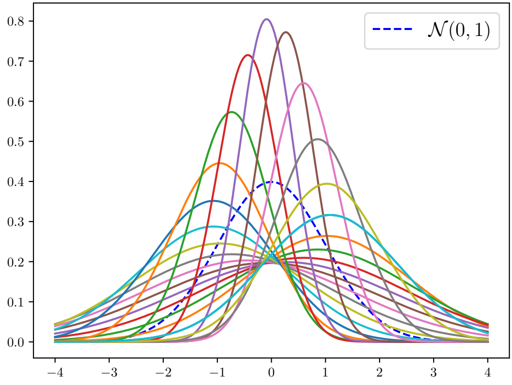

Figure 5: Fisher sphere $\delta = 1$ - densities space

Applications in sensitivity analysis: PLI indices

Application to sensitivity analysis

- We aim to measure the impact of density perturbation of input X_i to Y

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- We obtain the **minimum** and the **maximum** of $S_{i\delta}$ for $f_{i\delta}$ in the Fisher sphere of radius δ centered in f_i.

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- We obtain the **minimum** and the **maximum** of $S_{i\delta}$ for $f_{i\delta}$ in the Fisher sphere of radius δ centered in f_i.
- This new methodology is called OF-PLI (*Optimal Fisher based PLI*).

PLI ESTIMATION

- Industrial simulation code are often time-expensive.

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- We want to estimate the PLI without resampling X_i from the perturbed density.
- We consider a sample $(\mathbf{X}^{(1)}, ..., \mathbf{X}^{(N)})$ with X_i sampled from f_i and a simulation code G:

$$\hat{F}_{i\delta}(t) = \frac{\sum_{n=1}^{N} \frac{f_{i\delta}(X_i^{(n)})}{f_i(X_i^{(n)})} \mathbb{1}_{(G(\mathbf{X}^{(n)})<t)}}{\sum_{n=1}^{N} \frac{f_{i\delta}(X_i^{(n)})}{f_i(X_i^{(n)})}}$$

This is the reverse importance sampling (RIS) estimator of the cdf of $G(\mathbf{X})$

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  This is the reverse importance sampling (RIS) estimator of the cdf of $G(\mathbf{X})$
- the perturbed quantile $q_{i\delta}^{\alpha}$ is estimated with the empirical quantile of $\hat{F}_{i\delta}$.

- Self normalized cdf estimator $\hat{F}_{i\delta}(t)$ is used because it is bounded. Moreover, it possess better asymptotic properties.
- The estimator $\hat{S}_{i\delta} = \frac{\hat{q}^{\alpha}_{i\delta} - \hat{q}^{\alpha}}{\hat{q}^{\alpha}}$ built verify a CLT.

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- The estimator $\hat{S}_{i\delta} = \frac{\hat{q}^{\alpha}_{i\delta} - \hat{q}^{\alpha}}{\hat{q}^{\alpha}}$ built verify a CLT.
- Main hypothesis for the CLT: $\mathbb{E}\left[\left(\frac{f_{i\delta}(X)}{f_i(X)}\right)^2\right] < +\infty$

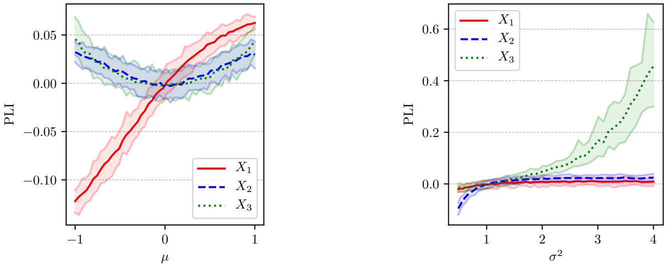
Practical implementation of the OF-PLI

- Empirical criterion for choice of δ_{max}: Minimal number of $G(\mathbf{X}^{(i)})$'s values greater or lesser than the perturbed quantile.

- We take 3 independent random variables (X_1, X_2, X_3) with a standard Gaussian distribution $\mathcal{N}(0, 1)$.
- The output variable is the analytical function

$$G(x_1, x_2, x_3) = \sin(x_1) + 7\sin(x_2)^2 + 0.1x_3^4 \sin(x_1)\ . \tag{4}$$

Numerical results: PLI with Kullback-Leibler minimization



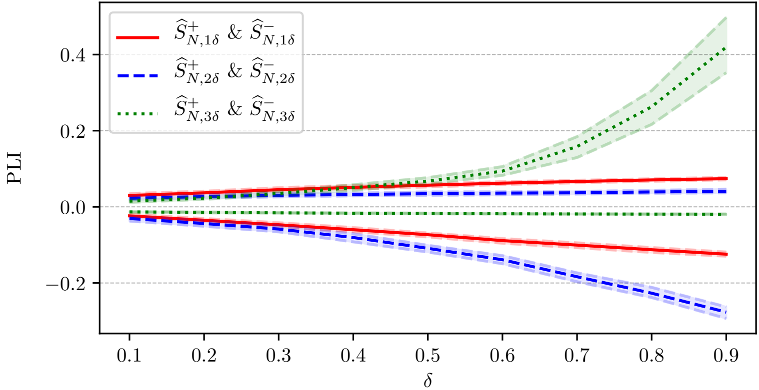


Figure 7: OF-PLI for the Ishigami function with a 100 points grid on the Fisher sphere.

Flood model

- OF-PLI computation for the flood model, quantifying the flooding risk of industrial facilities.

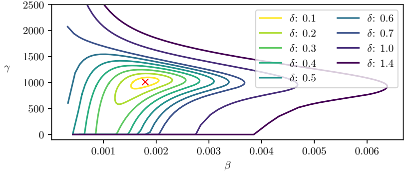
Flood model

Variable n°	Name	Description	Probability distribution	Admissible values
1	Q	Maximal annual flowrate	Gumbel $\mathcal{G}(1013, 558)$	$[500, 3000]$
2	K_s	Strickler coefficient	Normal $\mathcal{N}(30, 7.5)$	$[15, +\infty]$
3	Z_v	Upstream level of the river	Triangular $\mathcal{T}(50)$	$[49, 51]$
4	Z_m	Downstream level of the river	Triangular $\mathcal{T}(55)$	$[54, 56]$

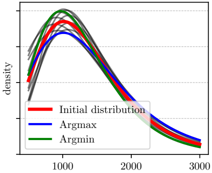
Input parameters of the flood model with their associated probability distribution

- We denote H the maximal annual water level.

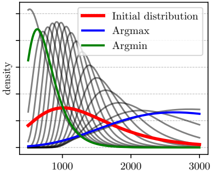
$$H = \left(\frac{Q}{300 K_s \sqrt{2.10^{-4}(Z_m - Z_v)}} \right)^{0.6}.$$



(a) Fisher sphere for an increasing δ.



(b) Densities on the Fisher sphere ($\delta = 0.1$).



(c) Densities on the Fisher sphere ($\delta = 1.4$).

Figure 8: Analysis of the density perturbation of the variable Q.

Numerical results for the flood model

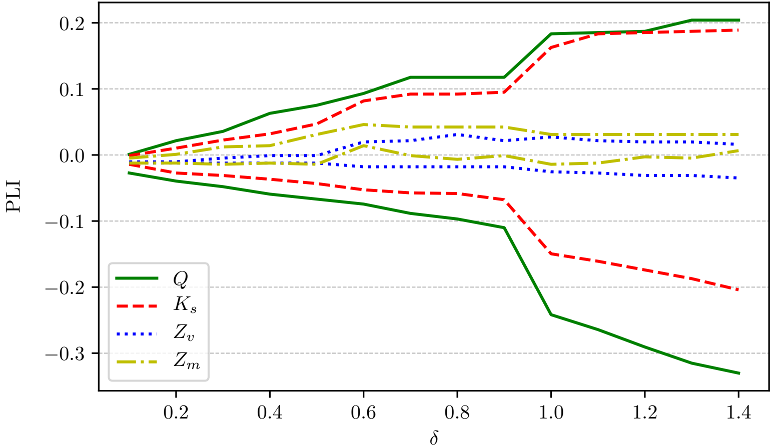


Figure 9: OF-PLI for the flood model on 100 points on the Fisher sphere.

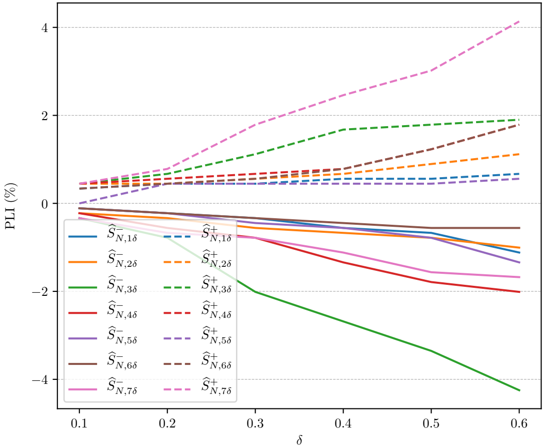


Figure 10: OF-PLI for CATHARE code

- Definition of a new framework of density perturbation, development of a numerical solver in Python (OpenTurns inside).

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- Theoretical results.

Conclusion

- Definition of a new framework of density perturbation, development of a numerical solver in Python (OpenTurns inside).
- Theoretical results.
- Accepted paper in Technometrics (link on the UQsay website.)
- Perspectives: simultaneous pertubation of several density of input parameters, dependent input parameters.

References

Questions ?

Supposons que F_i soit différentiable en q^α avec $F_i'(q^\alpha) > 0$ et $F_{i\delta}$ soit différentiable en $q_{i\delta}^\alpha$ avec $F_{i\delta}'(q_{i\delta}^\alpha) > 0$. On note $\Sigma = \begin{pmatrix} \sigma_i^2 & \tilde{\theta}_i \\ \tilde{\theta}_i & \tilde{\sigma}_{i\delta}^2 \end{pmatrix}$ tel que:

$$\sigma_i^2 = \frac{\alpha(1-\alpha)}{f_i(q^\alpha)^2} \ .$$

$$\tilde{\sigma}_{i\delta}^2 = \frac{\mathbb{E}\left[\left(\frac{f_{i\delta}(X_i)}{f_i(X_i)}\right)^2 \left(\mathbb{1}_{(G(\mathbf{X}) \leq q_{i\delta}^\alpha)} - \alpha\right)^2\right]}{f_{i\delta}(q_{i\delta}^\alpha)^2} \ .$$

$$\tilde{\theta}_i = \frac{\mathbb{E}\left[\frac{f_{i\delta}(X_i)}{f_i(X_i)} \mathbb{1}_{(G(\mathbf{X}) \leq q^\alpha)} \mathbb{1}_{(G(\mathbf{X}) \leq q_{i\delta}^\alpha)}\right] - \alpha \mathbb{E}[\mathbb{1}_{(G(\mathbf{X}) \leq q_{i\delta}^\alpha)}]}{f_i(q^\alpha) f_{i\delta}(q_{i\delta}^\alpha)} \ .$$

Alors en supposant Σ inversible et $\mathbb{E}\left[\left(\frac{f_{i\delta}(X_i)}{f_i(X_i)}\right)^2\right] < +\infty$. On obtient:

$$\sqrt{N}\left(\hat{\theta}_N - \begin{pmatrix} q^\alpha \\ q^\alpha_{i\delta} \end{pmatrix}\right) \xrightarrow{\mathcal{L}} \mathcal{N}(0, \Sigma) \ .$$

La densité perturbée f_δ est défini par:

$$f_\delta = \underset{\pi \in \mathcal{P},\ s.t\ \mathbb{E}_\pi[X] = \mathbb{E}_f[X] + \delta}{\arg\min} KL(\pi || f) \ ,$$

où $KL(.||.)$ est la divergence de Kullback-Leibler.

Soit $X \sim f$ la transformation de Rosenblatt est défini par:

$$U = \Phi^{-1}(F(X)) \ ,$$

où Φ est la fonction de répartition de la loi $\mathcal{N}(0,1)$ et F la fonction de répartition de X. Ainsi, $U \sim \mathcal{N}(0,1)$