

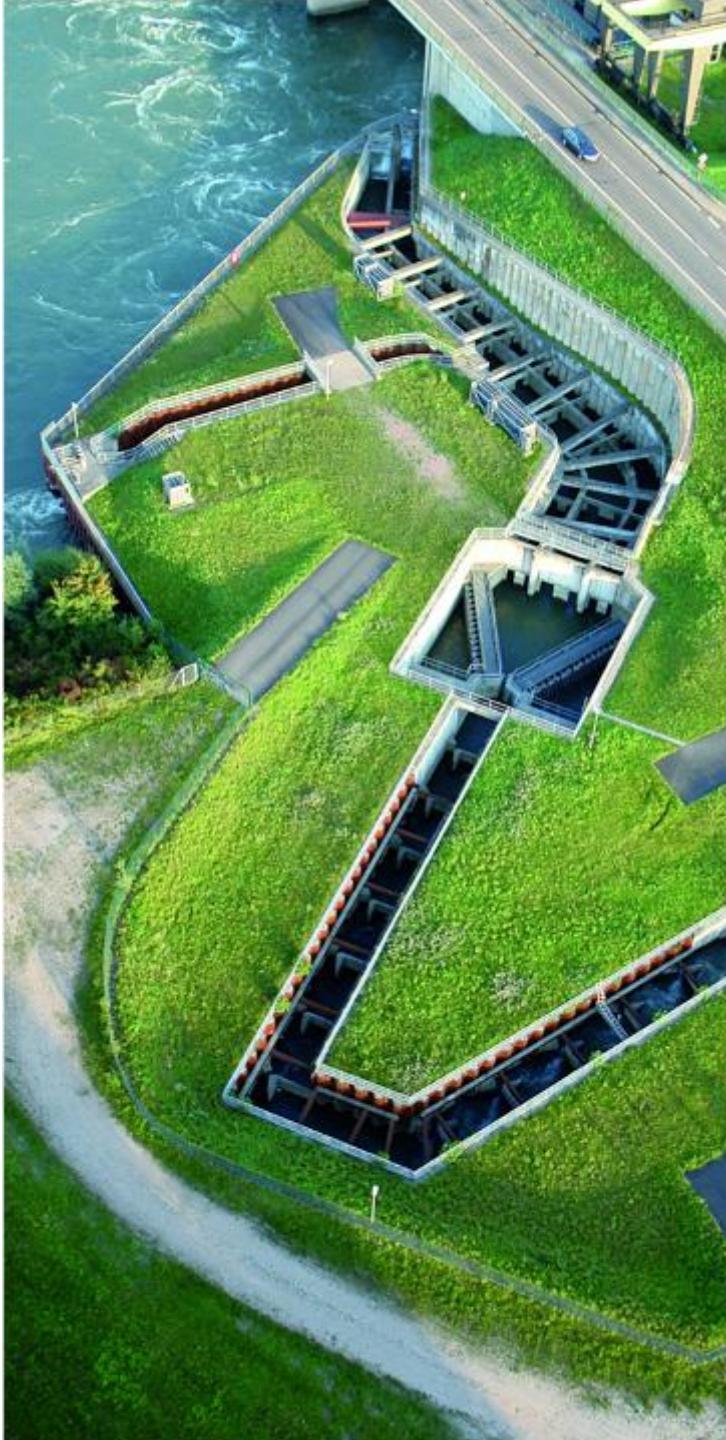
Quelques problématiques d'incertitudes en sûreté nucléaire

Bertrand IOOSS

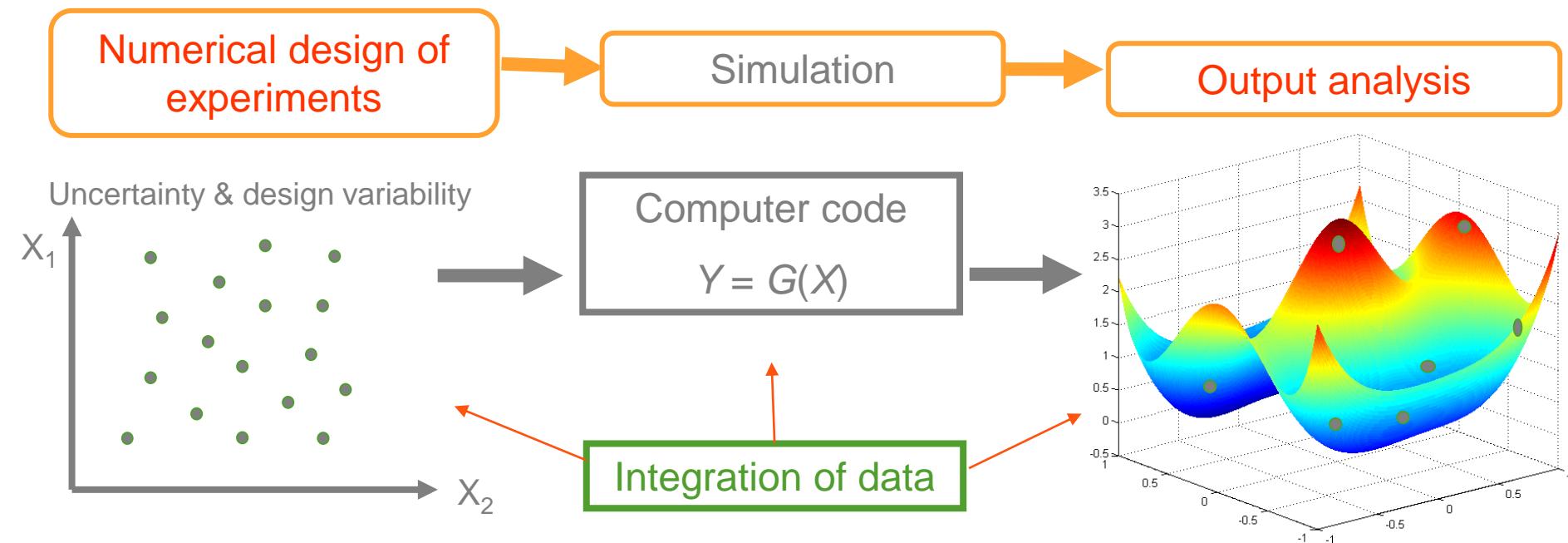
Électricité de France (EDF) - R&D, Chatou, France

with Roman Sueur, Thibaut Delage & Vincent Chabridon
(EDF R&D) and Amandine Marrel (CEA/DES)

GdR MaNu 2021, Le Croisic, October, 27th



Non-intrusive supervision of computer experiments



- ▶ Methods from engineering, numerical maths, proba/stats, machine learning, scientific computing, data assimilation, geostatistics, structural reliability, ...
- ▶ Keywords:
 - VVUQ (Validation, Verification and Uncertainty Quantification)**
 - DACE (Design & Analysis of Computer Experiments)**
 - GSA (Global Sensitivity Analysis)**
 - BEPU (Best-estimate Plus Uncertainties)**

Example: Simulation of IBLOCA accident

Pressurized Water Reactor scenario:

Loss of primary coolant accident due to
a break in cold leg

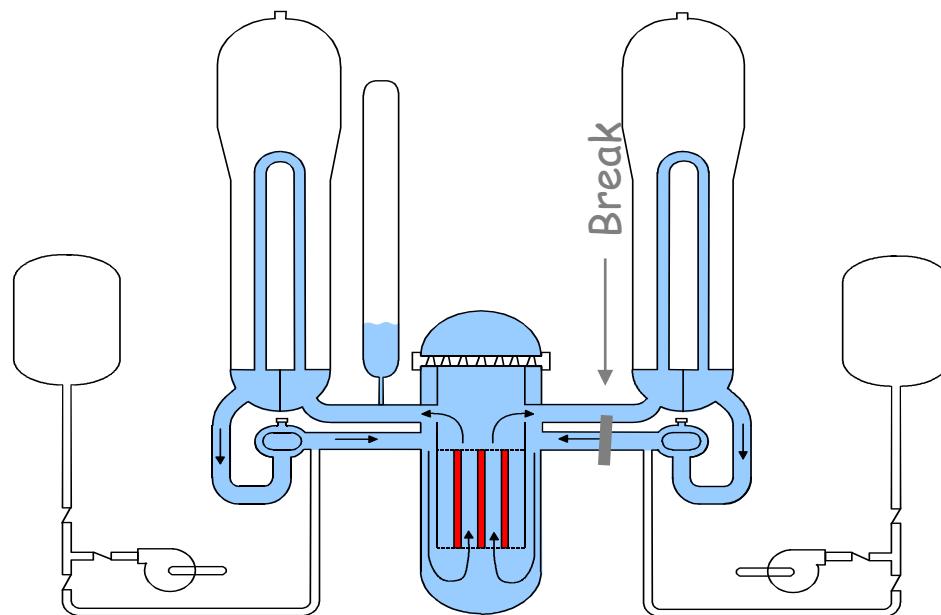
Variable of Interest :

Peak of cladding temperature (PCT)

d (~ 100) uncertain input variables X :

Critical flowrates, initial/boundary
conditions, phys. eq. coef., ...

Probabilistic modeling: f_X



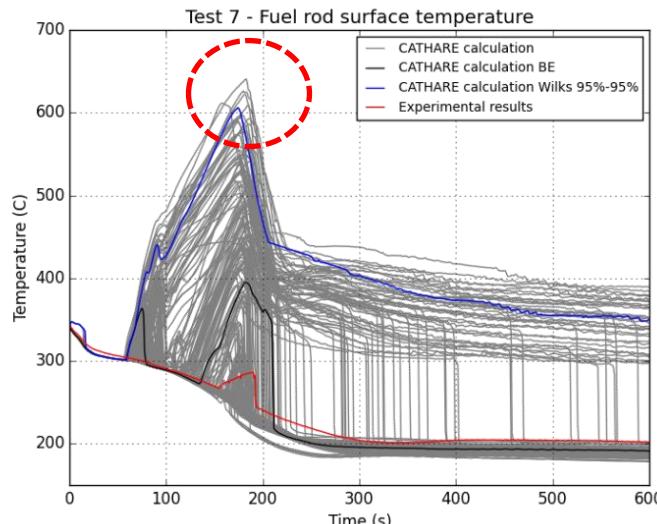
Modelled using CATHARE2 code:

(thermal-hydraulic phenomena)

CPU cost for one code run > 1 hour

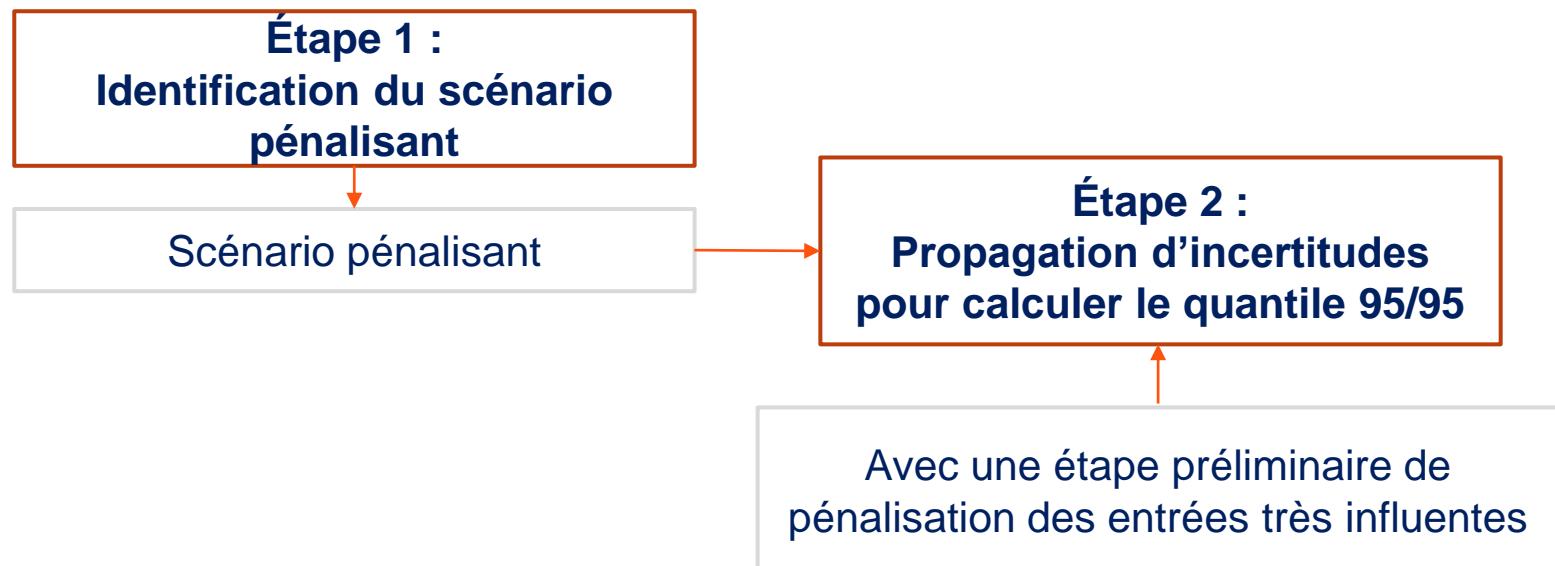
In industrial studies: $N \sim O(1000)$ runs

**Statistical quantity of interest (QoI):
High quantile (e.g. 95%) of the PCT**



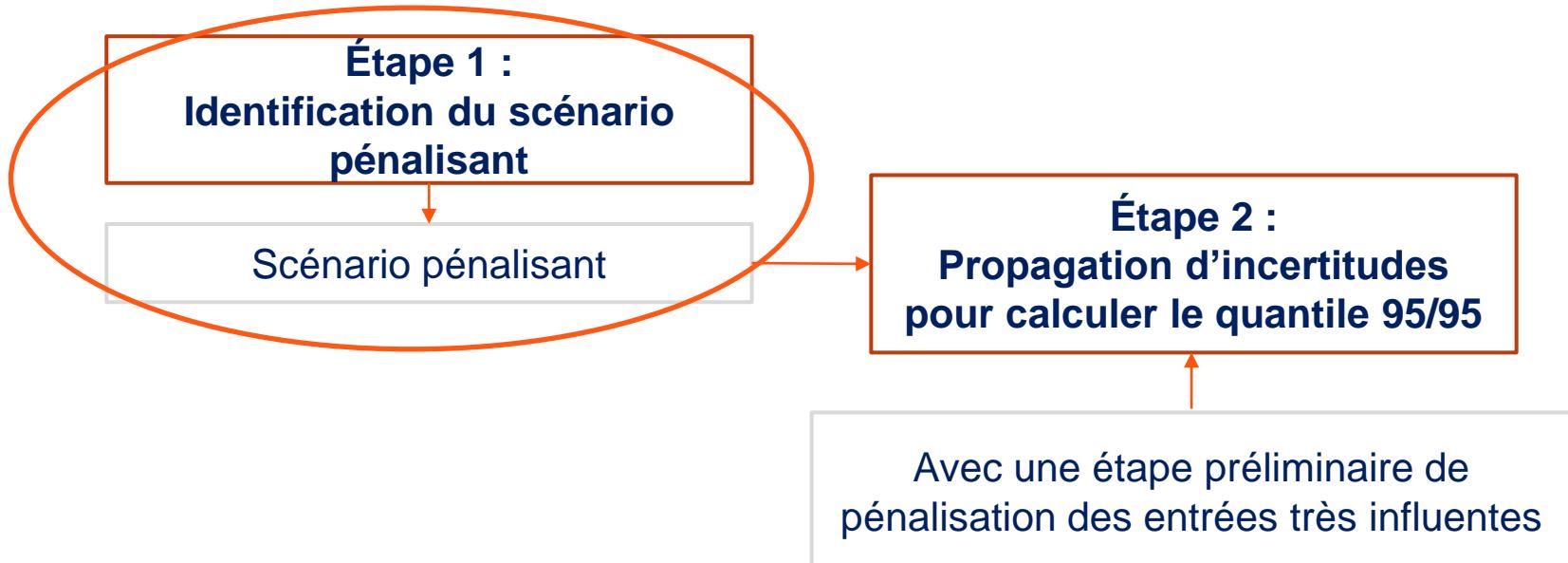
2 PROBLÉMATIQUES ISSUS D'UN DOSSIER D'INGÉNIERIE

- Environ 100 paramètres d'entrée du code sont considérés aléatoires, de 3 types :
 - Type 1 : Conditions initiales et aux limites ;
 - Type 2 : incertitudes modèles
 - Type 3 : paramètres scénario
- La méthode (nommée Cathsbi) se décline en 2 étapes :



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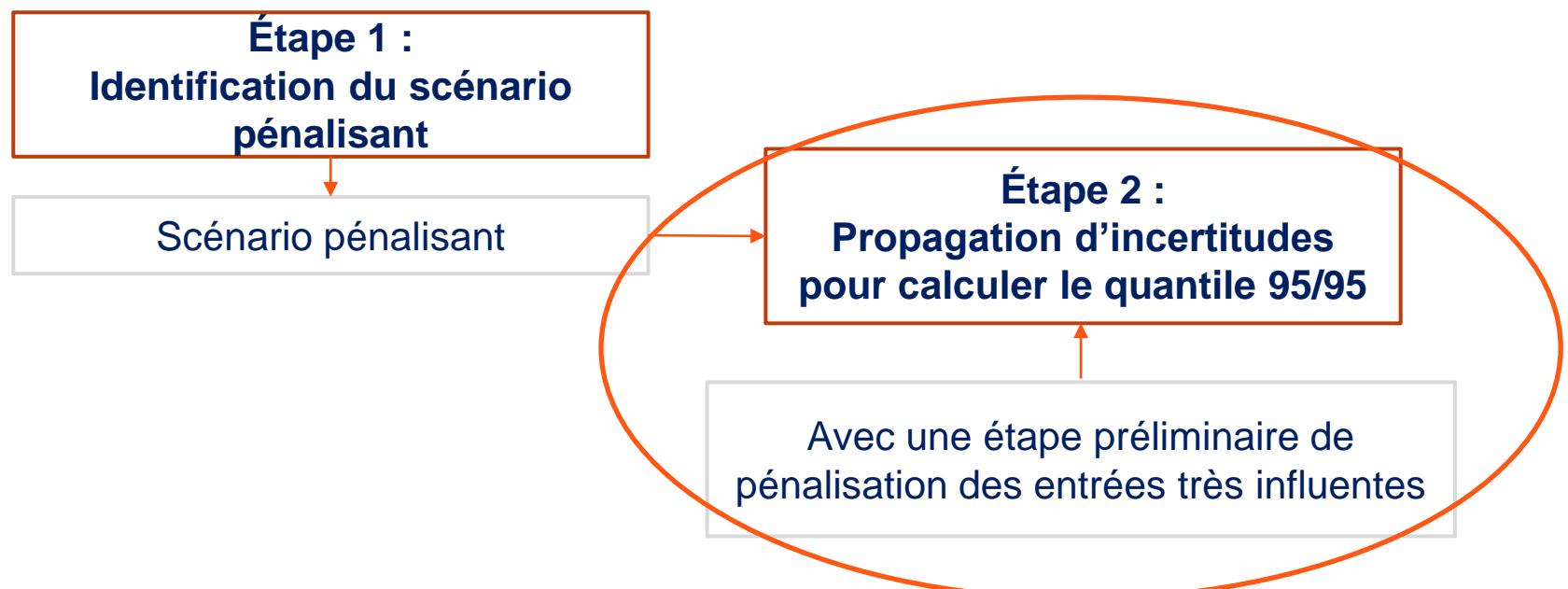
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Point saillant: la méthode actuelle est basée sur l'analyse manuelle de plusieurs séries de calculs => développement d'une méthode automatique basée sur un seul batch

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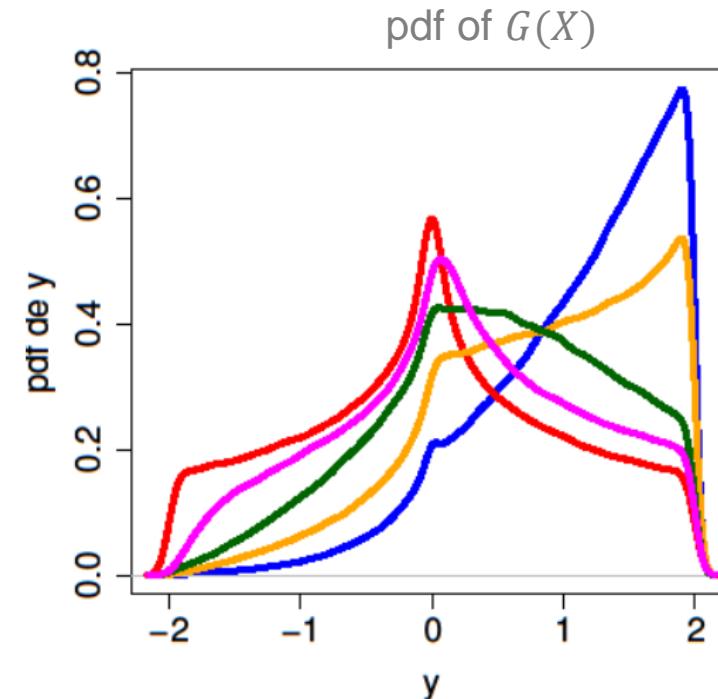
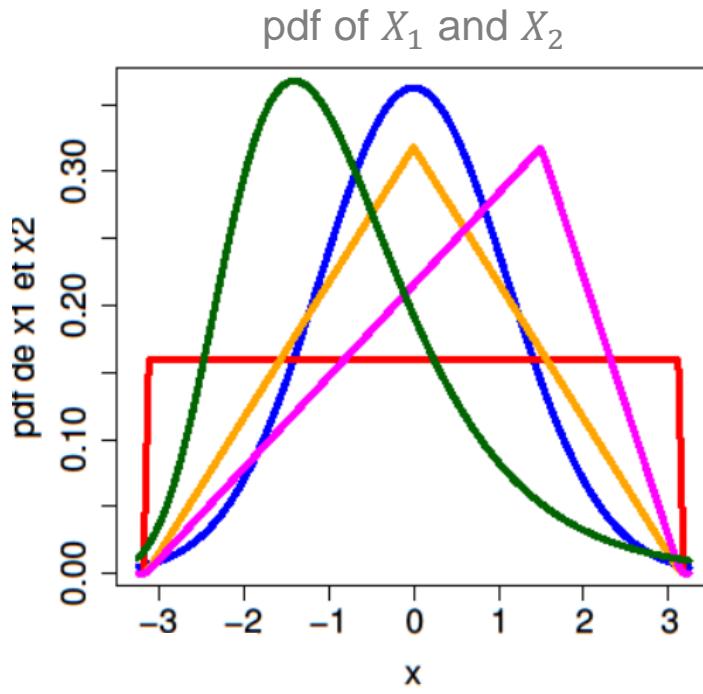


Point saillant: nécessité de justifier les modélisations probabilistes faites sur les entrées
=> Robustesse de la quantité d'intérêt (quantile) aux lois des entrées

IMPORTANCE OF INPUT PROBABILITY DISTRIBUTIONS IN UNCERTAINTY QUANTIFICATION

$G(X) = G(X_1, X_2) = \cos(X_1) + \cos(X_2)$; X_1 and X_2 are independent with same pdf

Strong impact of the choice of the input pdf on the output distribution, and particularly on some quantities of interest: probability of exceedance, quantile, ...



=> Needs of sensitivity analysis wrt pdf of the inputs

NOTATIONS

We want to study a deterministic computer code G which :

- is « costly » (CPU time, memory,...).
- has d input variables
- allows calculating the value $G(X)$ for a given set of input values $X = (X_1, \dots, X_d)$

Constraints: we will have only access to one batch of N computations

The input variables are uncertain, hence we denote

- $\mathbb{X} \subset \mathbb{R}^d$ the domain of variation of the random vector X
- $f = \prod_{i=1}^d f_i$ the probability density function of X
 - ▶ each f_i is the density of X_i , the i -th marginal of X
 - ▶ the uncertain input variables X_1, \dots, X_d are considered independent

The QoI can be: 1) a failure probability $\text{Proba}(Y > t)$, 2) α -order quantile $q^\alpha = \inf\{t \in \mathbb{R}, F_Y(t) \geq \alpha\}$, 3) α -order superquantile $Q^\alpha = \mathbb{E}[G(X)|G(X) \geq q^\alpha]$, ...

=> Robustness of these QoI wrt uncertainty in some f_i ,

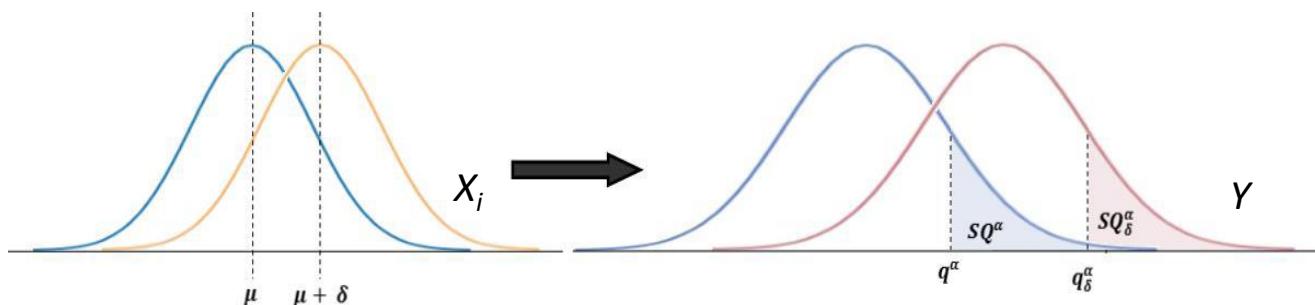
PLI (PERTURBED LAW-BASED INDICES)

We aim at quantifying the impact of a perturbation on the pdf of X_i

For example, what happens if we replace $E(X_i) = \mu_i$ by $E(X_i) = \mu_i + \delta$?

We define the **PLI-quantiles** as : $S_{i\delta} = \left(\frac{q_{i\delta}^\alpha}{q^\alpha} - 1 \right)$ (same way for any QoI)

- It gives results in terms of percentage of perturbations
- $S_{i\delta} = 0$ when $q_{i\delta}^\alpha = q^\alpha$ i.e. when f_i has no impact on the quantile
- The sign of $S_{i\delta}$ indicates how the perturbation modifies the quantile



ESTIMATION: REVERSE IMPORTANCE SAMPLING

- We have N obs. (the model calculations) : $(x^{(1)}, \dots, x^{(N)}) \rightarrow (y^{(1)}, \dots, y^{(N)})$
- We start from classical Monte-Carlo estimators:
 - if QoI = failure probability ($\text{Proba}(Y \leq t)$): $\hat{p} = 1/N \sum_{n=1}^N \mathbb{I}_{\{y^{(n)} \leq t\}}$
 - if QoI = quantile: $\hat{q}^{\alpha N} = \inf\{t \in \mathbb{R}, \hat{F}_Y^N(t) \geq \alpha\}$ where $\hat{F}_Y^N(t) = 1/N \sum_{n=1}^N \mathbb{I}_{\{y^{(n)} \leq t\}}$
- Let us note $f_{i\delta}$ the perturbed density of f_i by δ , we can estimate $p_{i\delta}$, $F_{i\delta}(t)$, $q_{i\delta}^\alpha$ with the same sample than for p , $F_Y(t)$, q^α by « reverse importance sampling »:

[Lemaître et al., 2015; Sueur et al., 2017]

$$\hat{p}_{i\delta}^N = \frac{1}{N} \sum_{n=1}^N \mathbb{I}_{\{y^{(n)} \leq t\}} L_i^{(n)} \text{ with } L_i^{(n)} = \frac{f_{i\delta}(x_i^{(n)})}{f_i(x_i^{(n)})}$$
$$\hat{F}_{i\delta}^N(t) = \sum_{n=1}^N \mathbb{I}_{\{y^{(n)} \leq t\}} L_i^{(n)} / \sum_{n=1}^N L_i^{(n)} ; \hat{q}_{i\delta}^{\alpha N} = \inf\{t \in \mathbb{R}, \hat{F}_{i\delta}^N(t) \geq \alpha\}$$

No need of new runs of G model

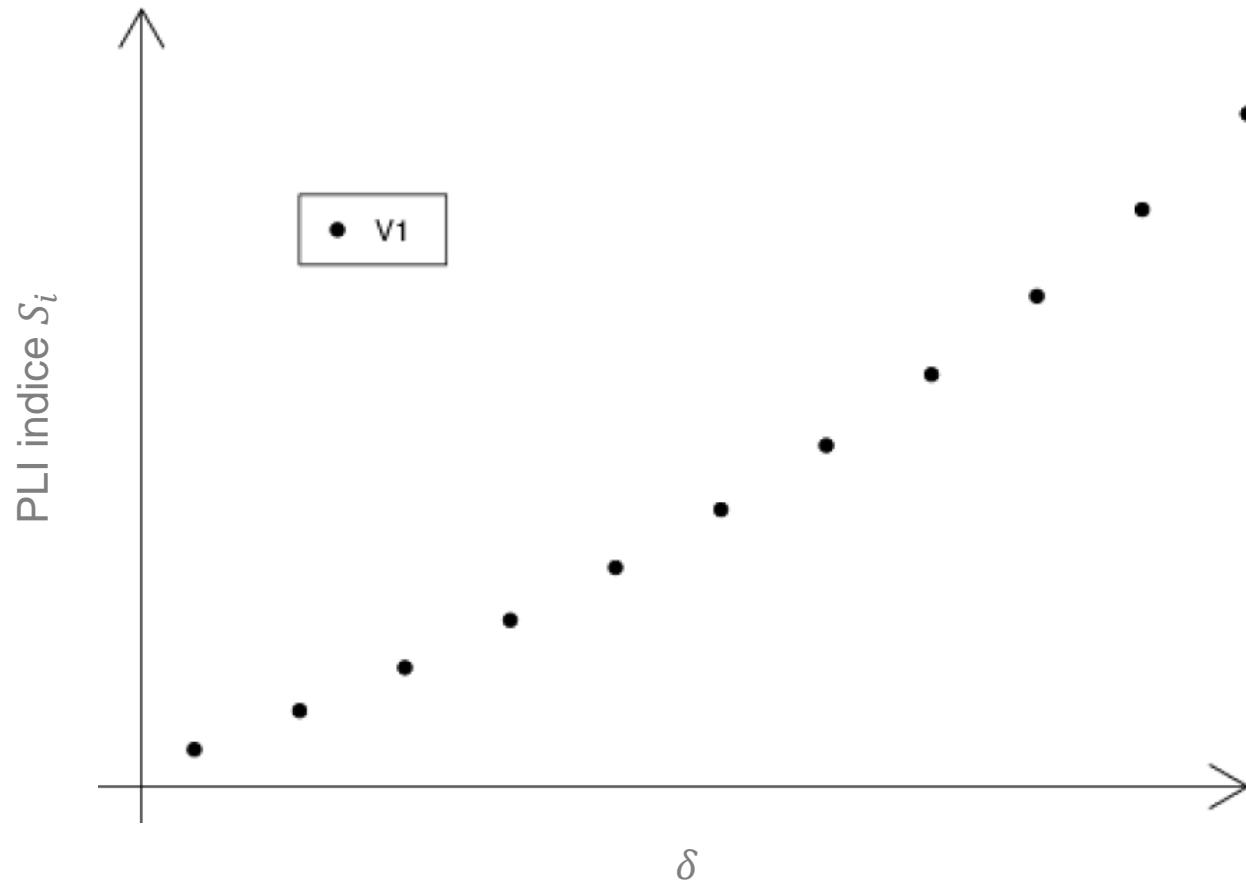
PLI INDICES ESTIMATION

We then estimate the PLI with the so-called plug-in estimator, for the PLI-quantile:

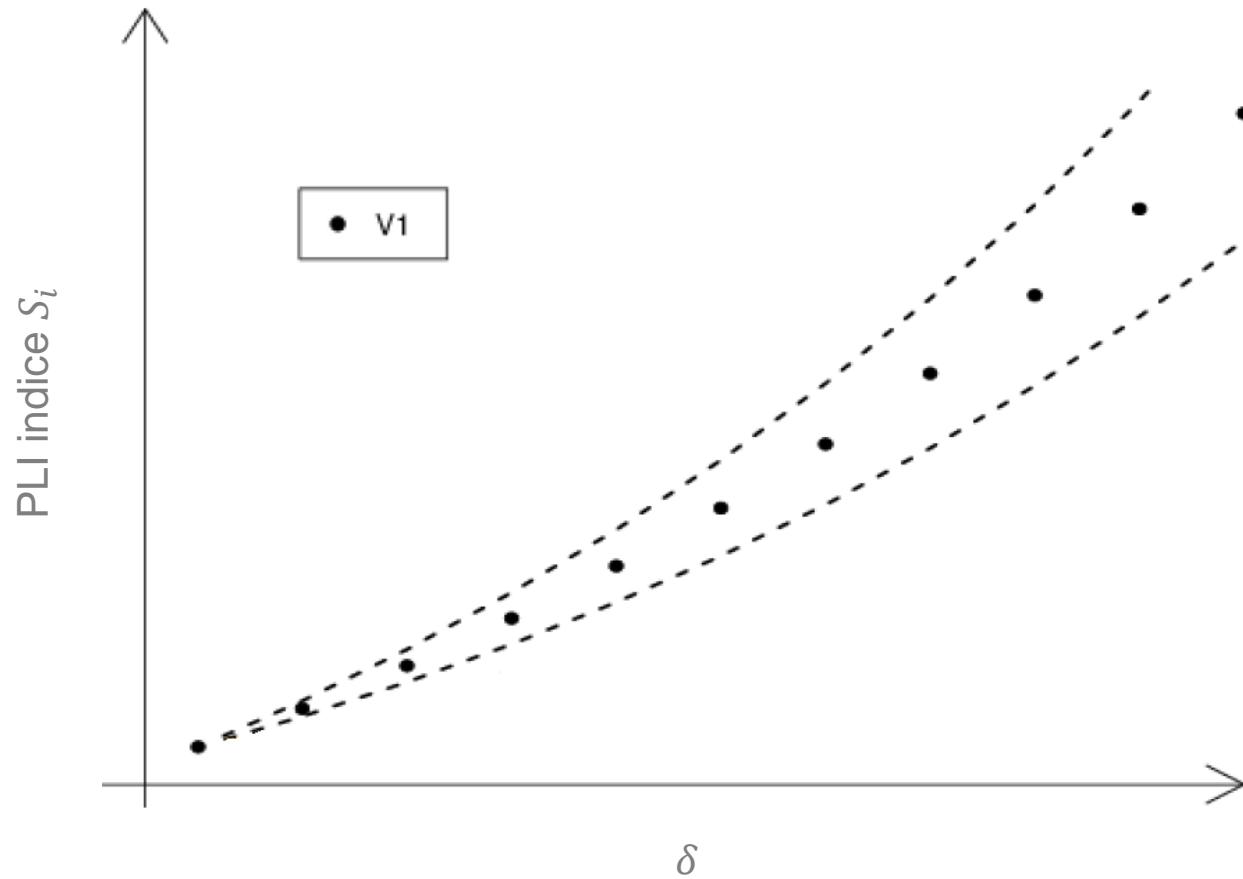
$$\hat{S}_{i\delta}^N = \left(\frac{\hat{q}_{i\delta}^{\alpha N}}{\hat{q}^{\alpha N}} - 1 \right)$$

- Convergence and central limit theorems of this estimator have been obtained ([Lemaître et al., 2015 for failure probability; Gauchy et al., 2020 for quantile]), with natural assumption $\text{Supp}(f_{i\delta}) \subseteq \text{Supp}(f_i)$, and others more complex:
 - For example, for PLI-quantile: $\int_{\text{Supp}(f_i)} \left(\frac{f_{i\delta}(x)}{f_i(x)} \right)^3 dx < +\infty$
- For PLI-quantile, **confidence intervals are easier to compute by bootstrap**

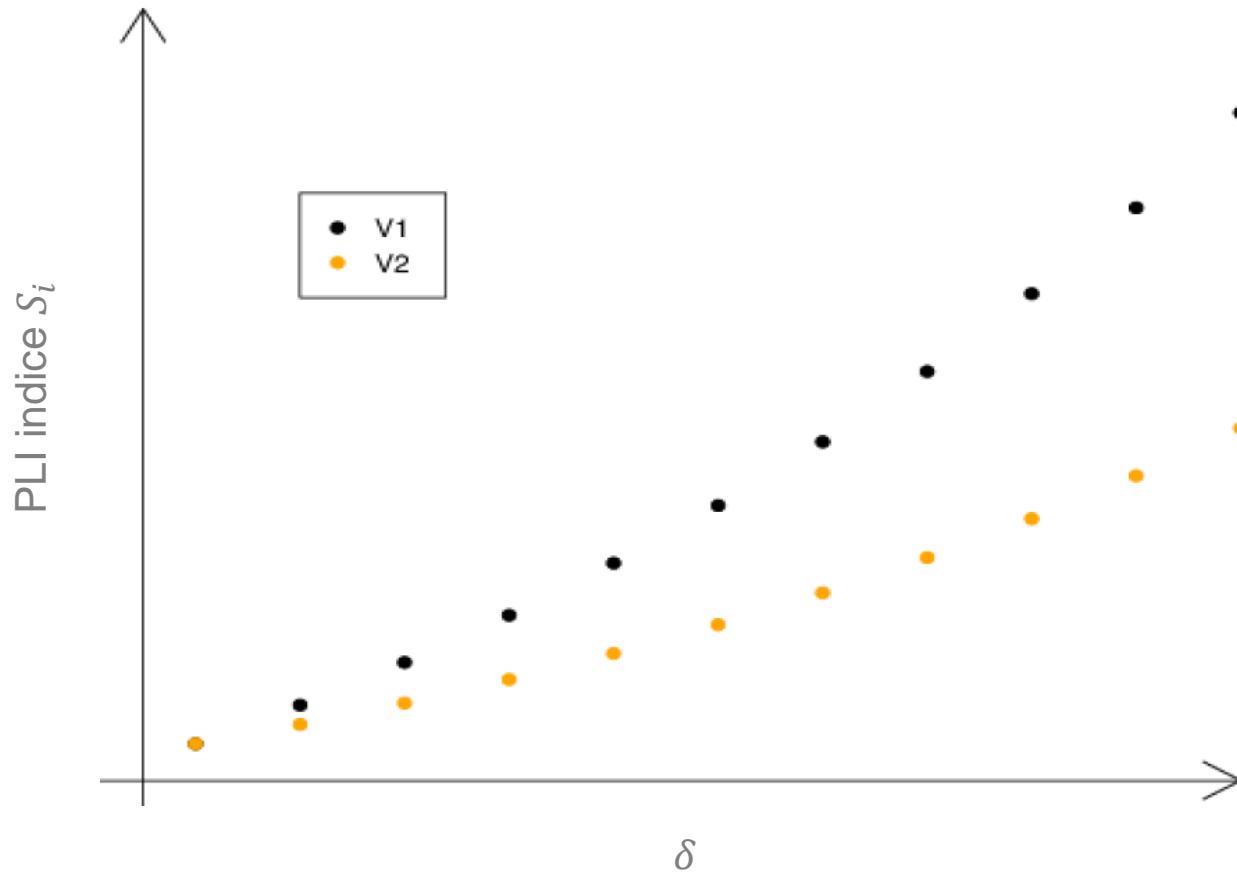
ILLUSTRATION



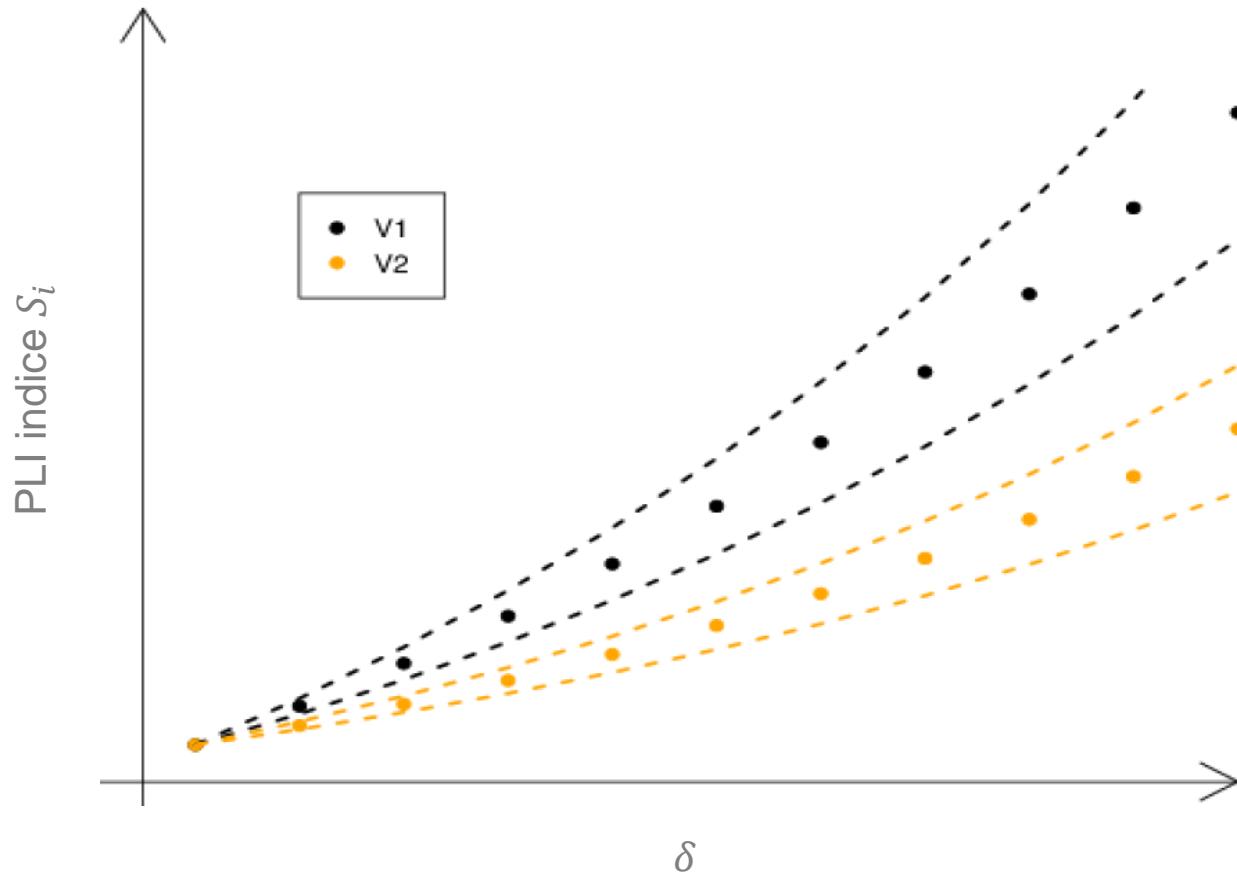
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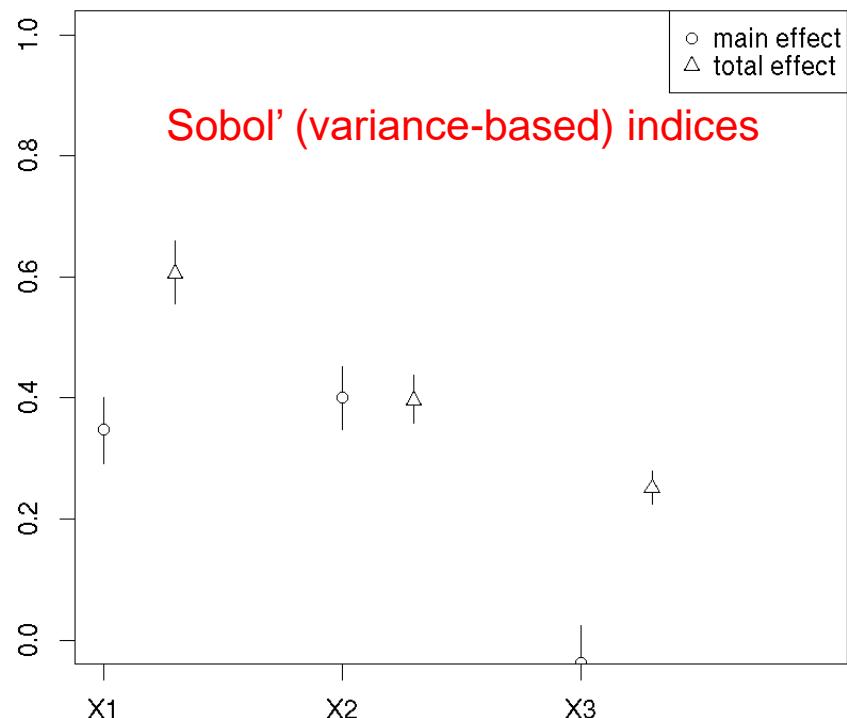
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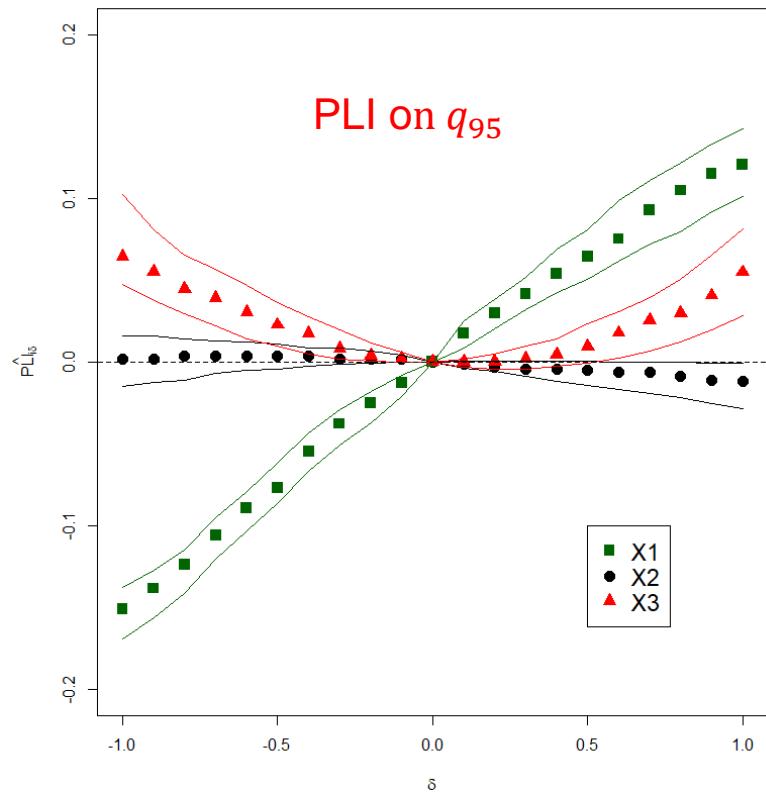
ANALYTICAL EXAMPLE

$$G(X) = \sin(X_1) + 7 * \sin^2(X_2) + 0,1 * X_3^4 * \sin(X_1); \quad X_i \sim U(-\pi, \pi) \text{ independent}$$

Standard global sensitivity analysis



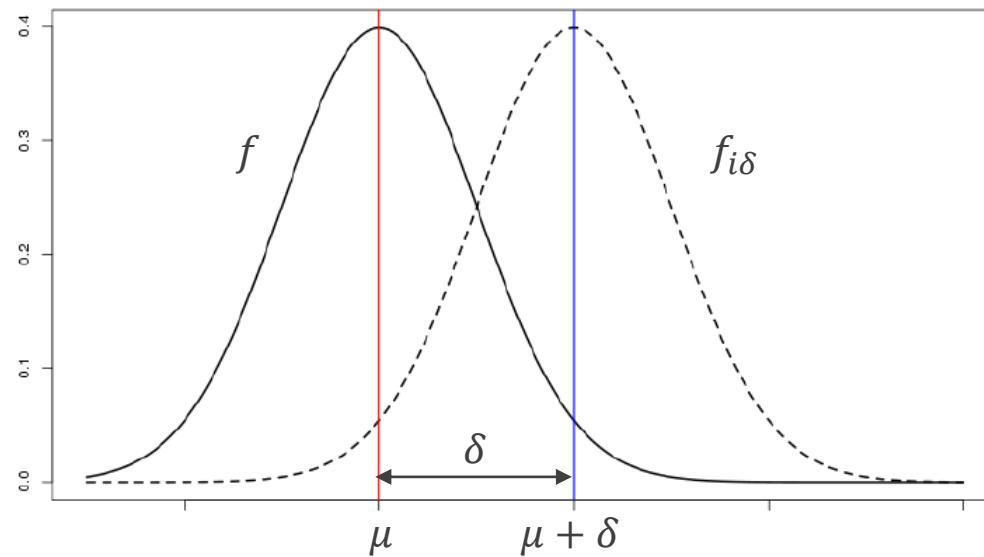
PLI-based sensitivity analysis



The provided information are different

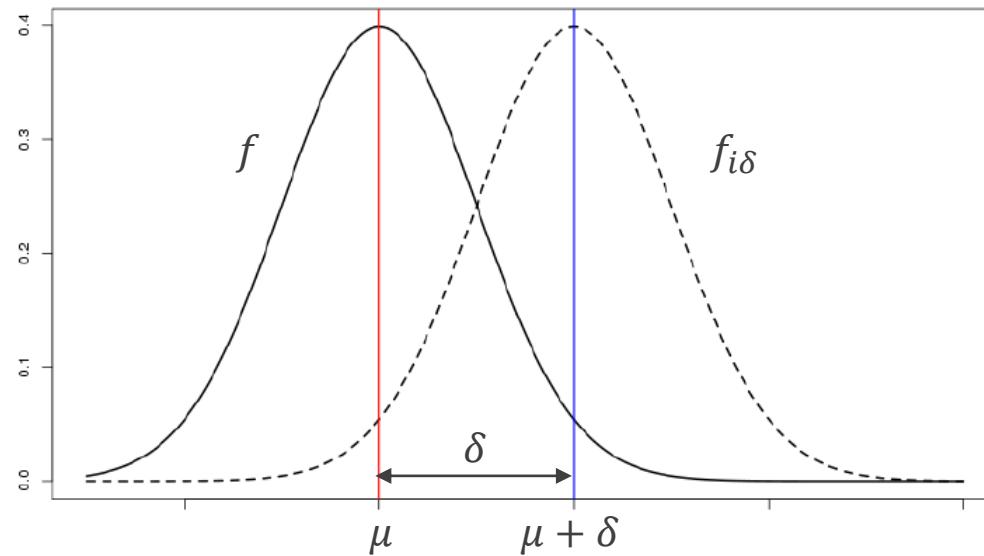
HOW TO DEFINE A DENSITY PERTURBATION ?

- Let's assume that the X_i input variable has a normal distribution $X_i \sim \mathcal{N}(\mu, \sigma^2)$
- What if the mean of X_i was not μ but $\mu + \delta$?



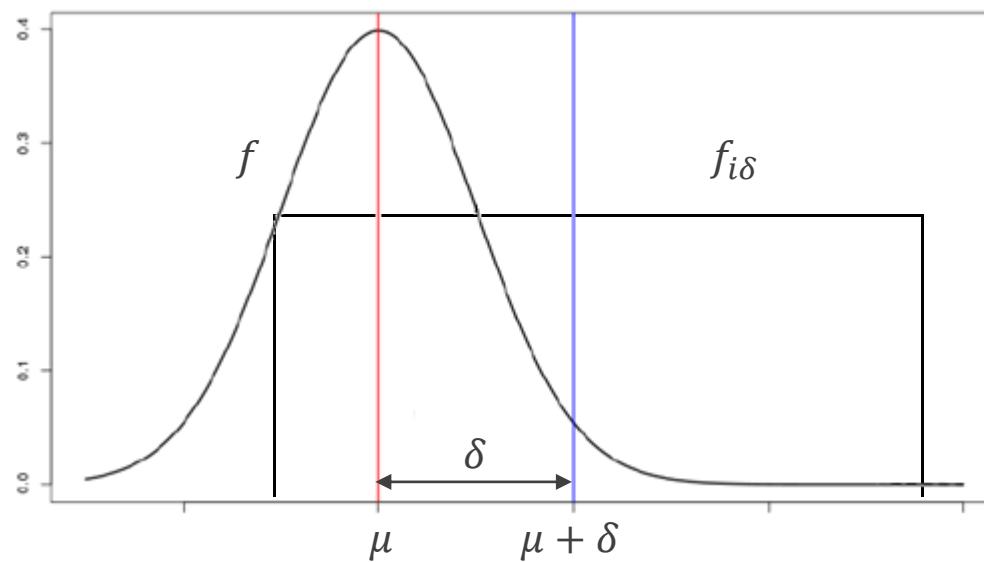
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- Let's assume that the X_i input variable has a normal distribution $X_i \sim \mathcal{N}(\mu, \sigma^2)$
- How to define $f_{i\delta}$ with the constraint $\int_{\mathbb{X}_i} x_i f_{i\delta}(x_i) dx_i = \mu + \delta$?



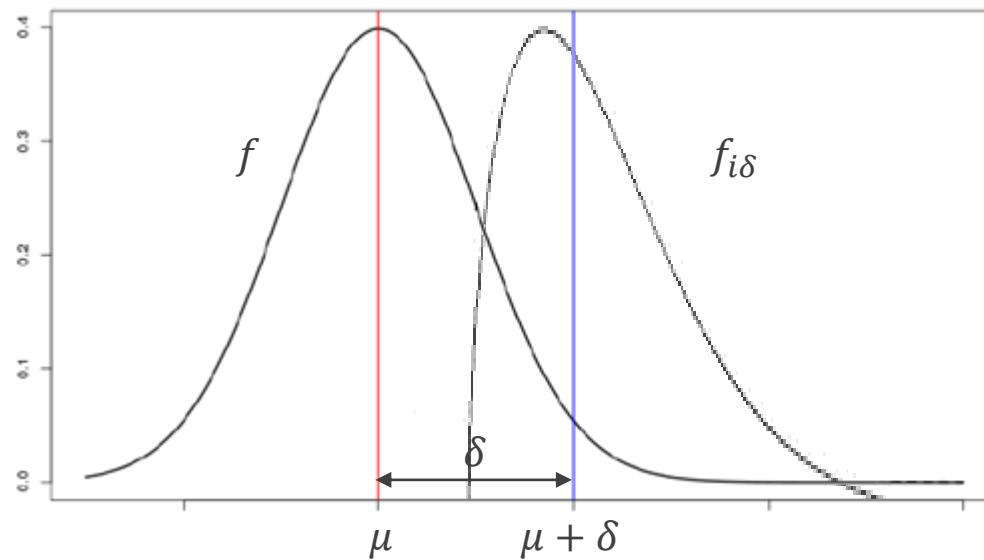
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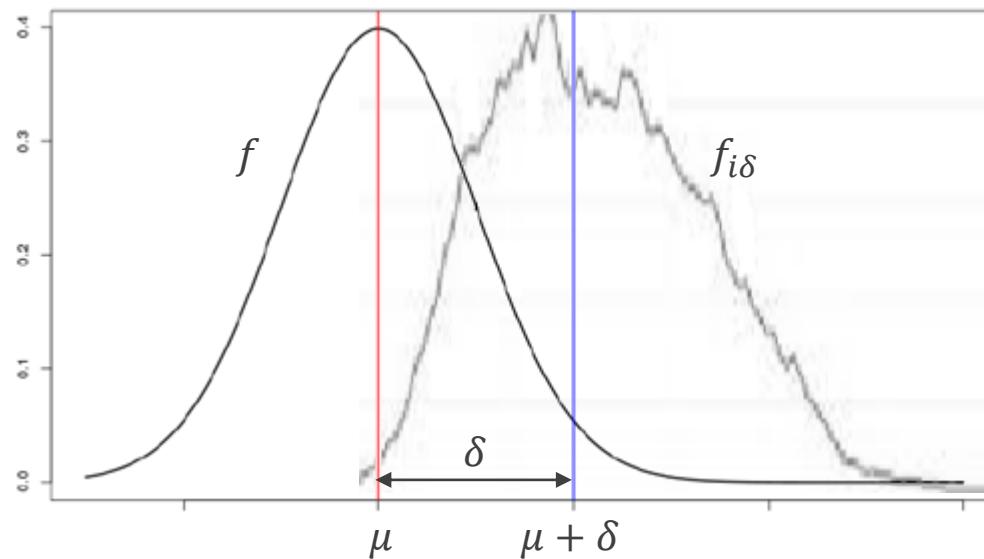
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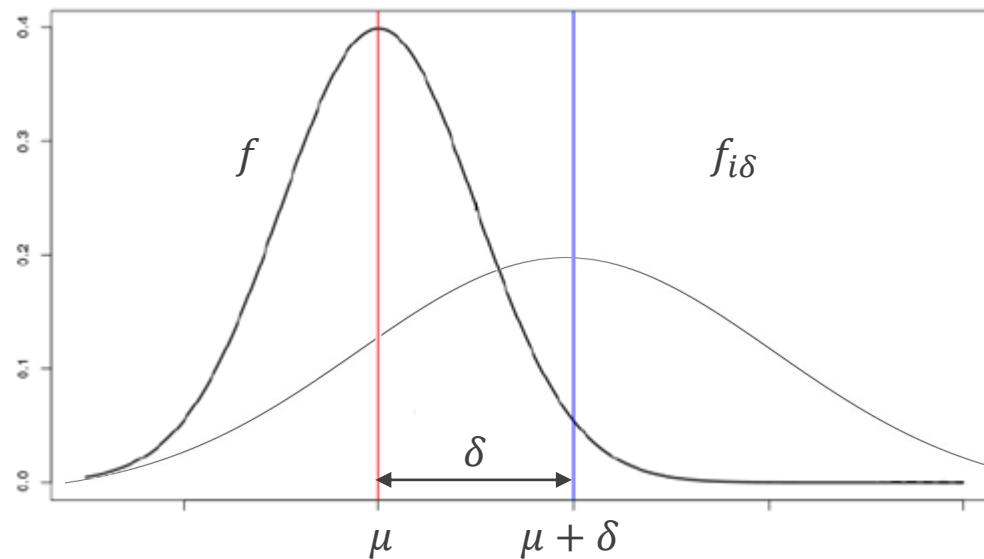
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HOW TO DEFINE A DENSITY PERTURBATION ?

- We suggest to define the perturbed density $f_{i\delta}$ as the closest one from the initial f_i in the sense of the entropy, under the constraint of perturbation
- i.e. in the sense of Kullback-Leibler divergence : [Lemaître et al., 2015]

$$KL(\pi_1, \pi_2) = \int_{-\infty}^{+\infty} \pi_1(x) \log \left(\frac{\pi_1(x)}{\pi_2(x)} \right) dx$$

- So we can give a general formal definition for $f_{i\delta}$ in the following way :

$$f_{i\delta} = \underset{\pi}{\operatorname{argmin}} \quad KL(\pi, f_i) \\ \text{s.t. } \mathbb{E}_{\pi}[g_k] = \delta_k \\ k=1, \dots, K$$

where : - g_1, \dots, g_K are K linear constraints on the modified density

- and $\delta_1, \dots, \delta_K$ are the values for the perturbed parameters

In this framework, a Gaussian distrib. which is perturbed remains Gaussian

This perturbation approach can be criticized [Gauchy et al., 2020]

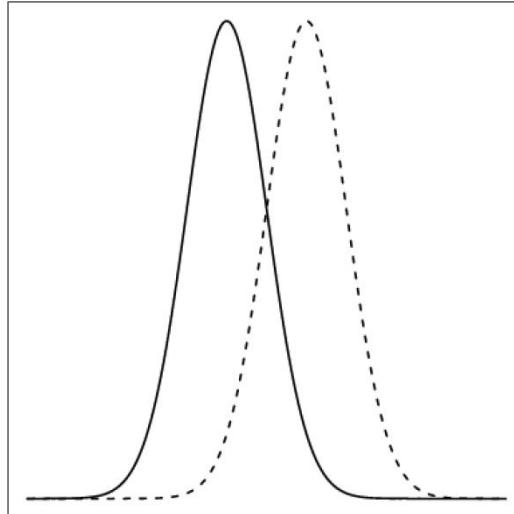
EXAMPLES OF PERTURBED PDF

Mean μ ; Variance σ^2

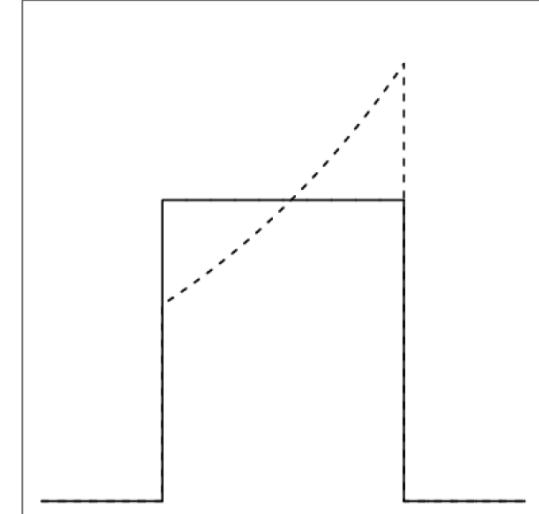
Mean perturbation

$$\mathbb{E}[X_i] = \mu + \delta$$

Gaussian



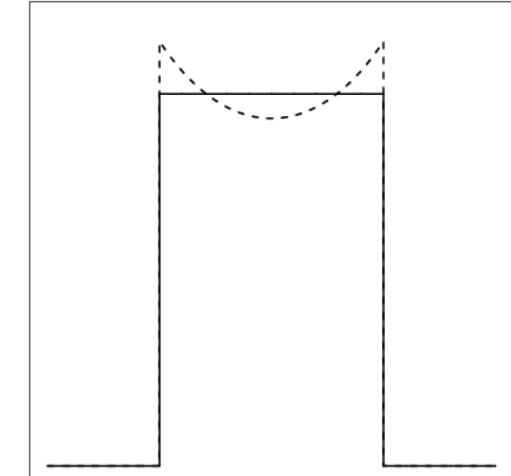
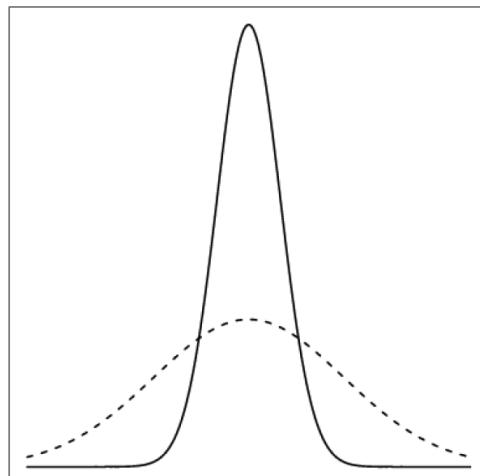
Uniform



Variance perturbation

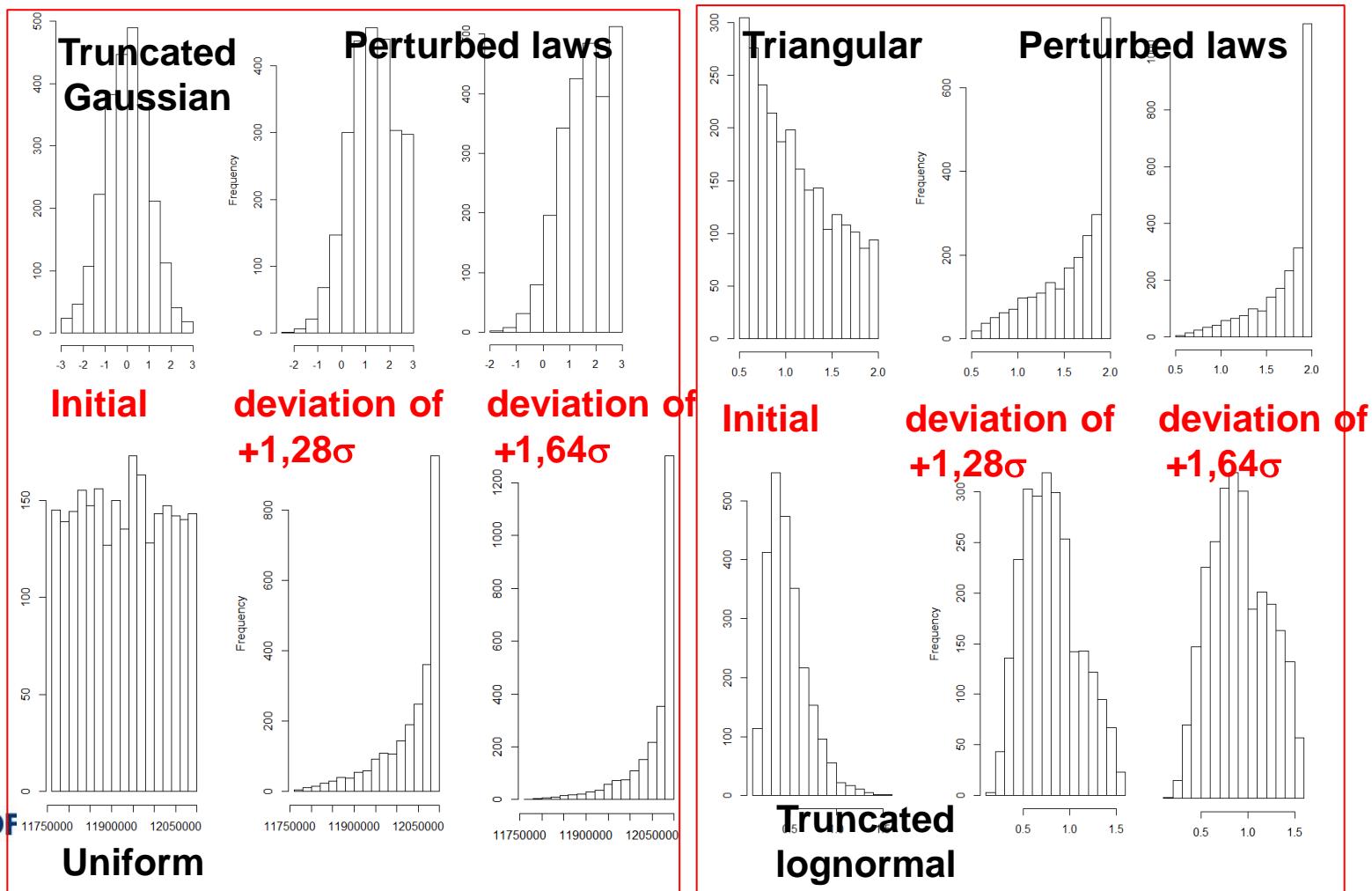
$$\mathbb{E}[X_i] = \mu$$

$$\text{Var}[X_i] = \sigma^2 + \delta$$



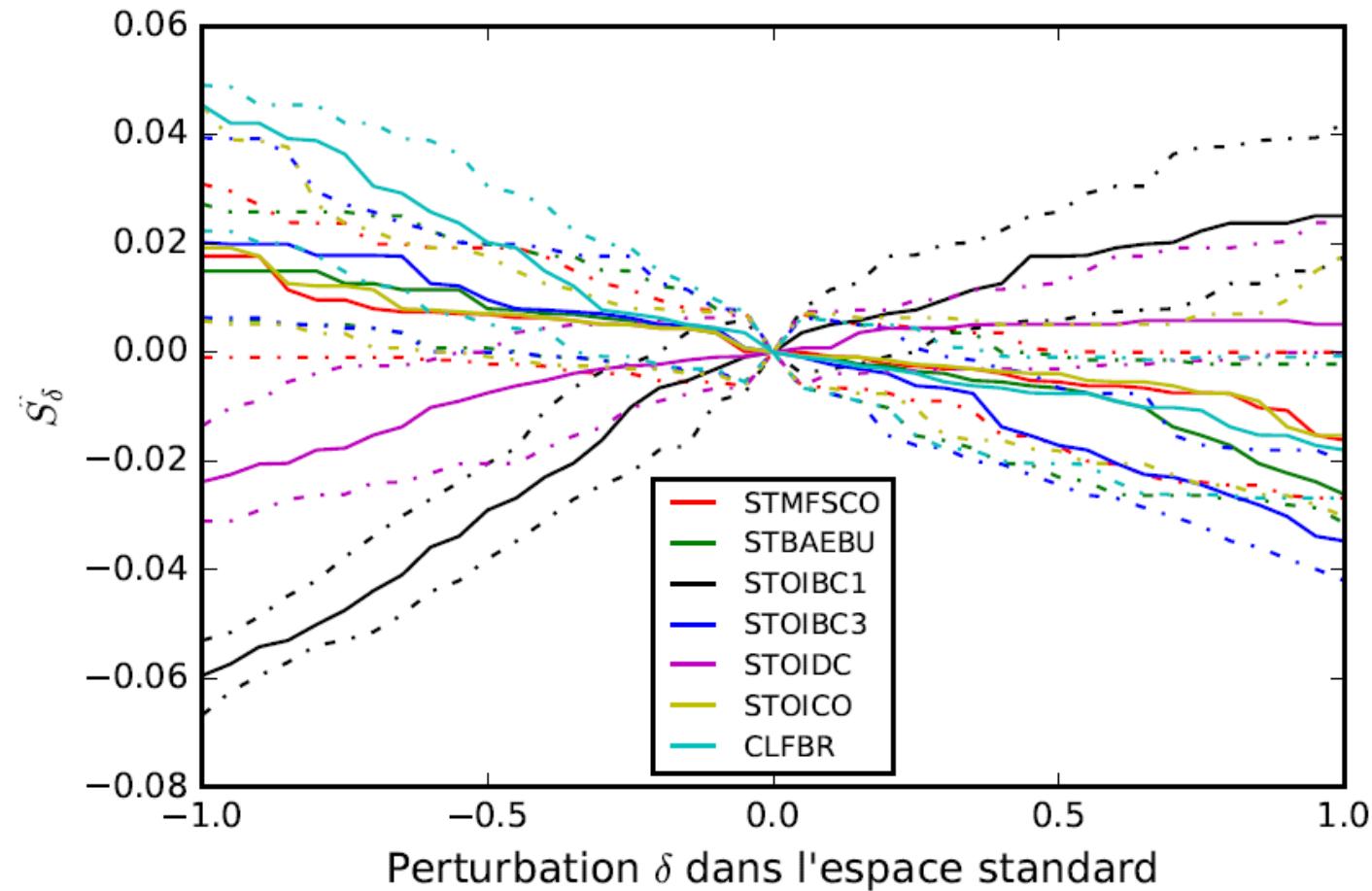
THERMAL-HYDRAULIC MODEL OF A MOCKUP

- 27 inputs with truncated Gaussian, log-normal, uniform, log-uniform, triangular pdf
- Monte-Carlo sampling of 1000 runs
- Perturbation on the mean between [-1;1] in the standard space (each input $\sim \mathcal{N}(0,1)$)



RESULTS

- Graphs show the PLI of the 7 most influential variables
- 90%-confidence intervals are obtained by bootstrap

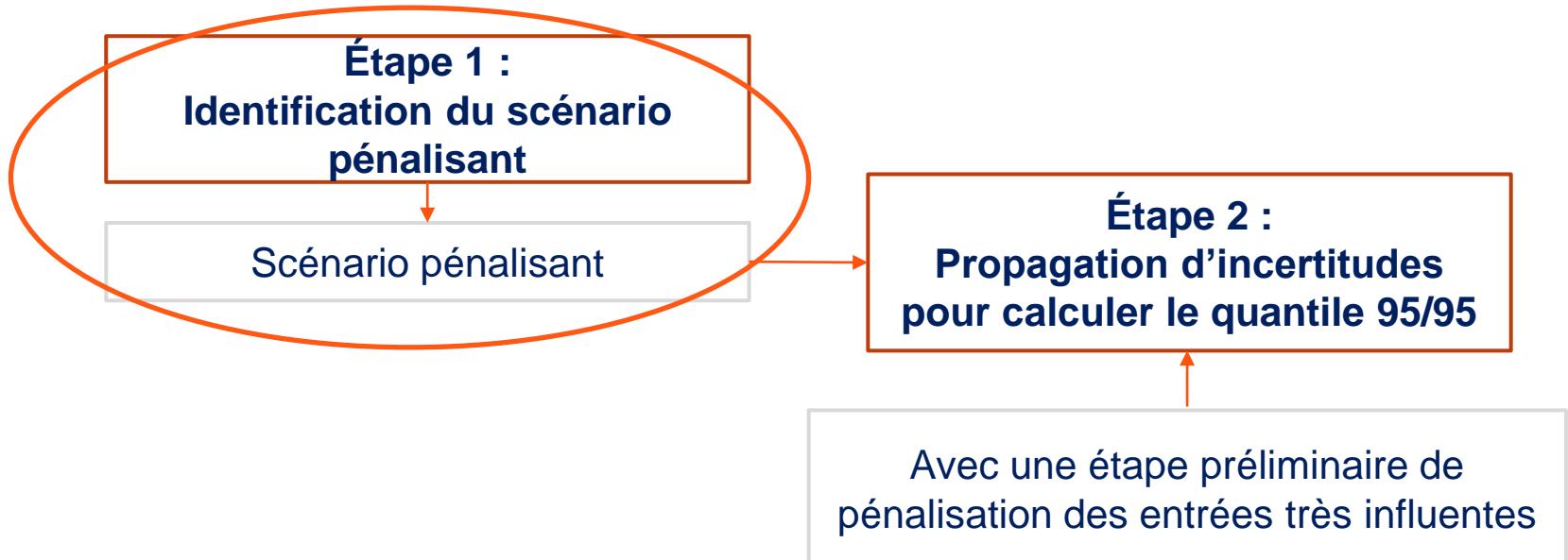


Observations: quantile seems to be robust towards the pdf (less than 5% variation), sign of the PLI allows to know which value allows us to be conservative

Utilisation des PLI dans un dossier industriel (Cathsbi) : hiérarchisation finale des entrées influentes et détection de leur « côté » pénalisant (augmente le quantile)

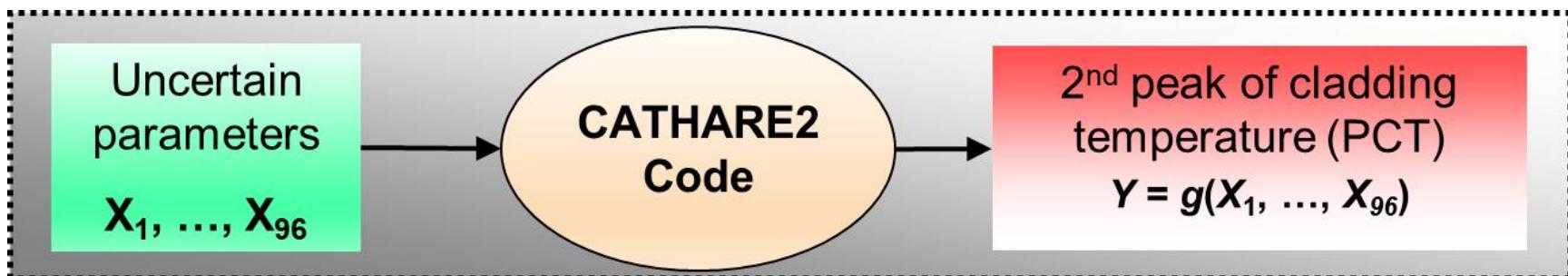
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ICSCREAM: IDENTIFICATION OF PENALIZING CONFIGURATIONS USING SCREENING AND METAMODEL



- In IB-LOCA modeling framework, uncertain input parameters are:
 - ▶ (Type 1) initial/boundary conditions ⇒ probabilistic (\mathcal{U}, \mathcal{N})
 - ▶ (Type 2) Parameters of physical models ⇒ probabilistic ($\mathcal{U}, \mathcal{LU}, \mathcal{N}, \mathcal{LN}$)
 - ▶ (Type 3) **Scenario parameters (min / max bounds)** ⇒ no probabilistic

ICSCREAM final objective

Identify the most penalizing configurations for Type 3 inputs,
regardless to the uncertainties of Types 1 & 2 inputs.

Penalizing configurations \Leftrightarrow leading to high PCT values

INDUSTRIAL CONSTRAINTS

Very large number of inputs (~100), but effective dimension might be lower

- Each CATHARE simulation ~ 1 hour ⇒ **one batch of around 1000 simulations**
 - Phenomena involved in the model are complex **with strong non-linearities**
 - Black-box model ⇒ intrusive methods not possible
- ⇒ **Efficient methodology combining Screening, sensitivity analysis, metamodel and inversion under uncertainty**
- ⇒ **Adapted to VERY HIGH DIMENSIONAL test case**

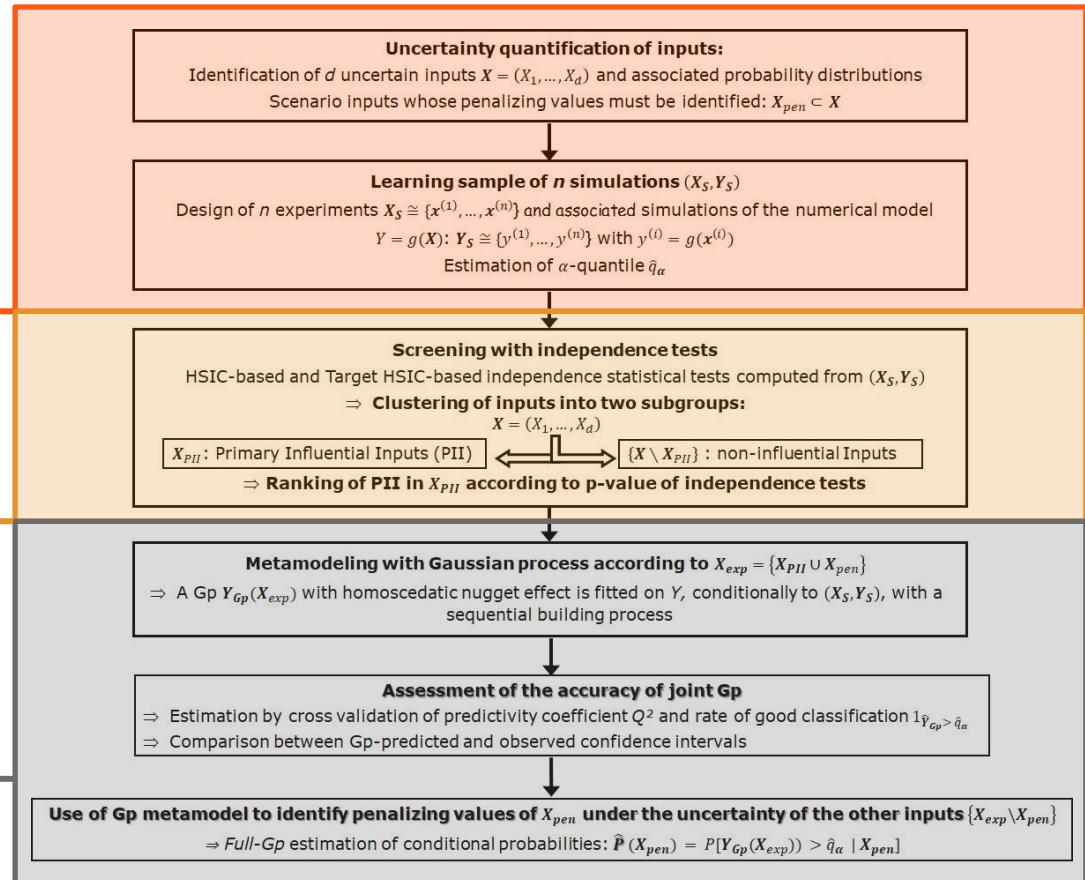
ICSCREAM: A FOUR-STEPS METHODOLOGY

Step 1 – Quantification & propagation of uncertainties

Step 2 – Global sensitivity analysis (screening with HSIC)

Step 3 – Construction & validation of a metamodel

Step 4 – Inversion

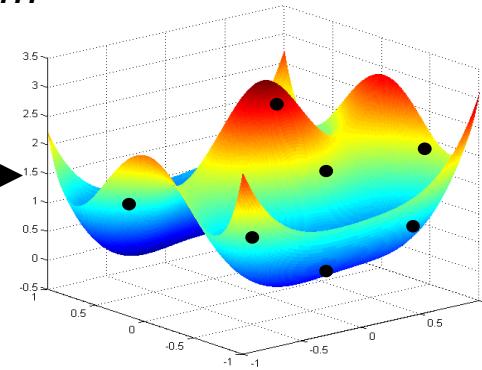
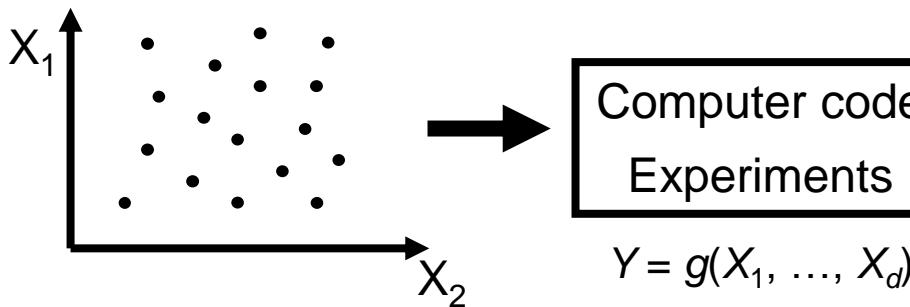


STEP 3: Approximation with a metamodel

Goal: replace code by a statistical function called metamodel

- ✓ With good approximation and prediction capabilities \Rightarrow to be controlled
- ✓ With a negligible cpu cost for prediction
- ✓ Built from a Monte Carlo sample of n experiments ($n \sim 10^d$)

Ex : Polynomials, splines, neural networks, regression trees...



Choice: Gaussian process (GP) metamodel

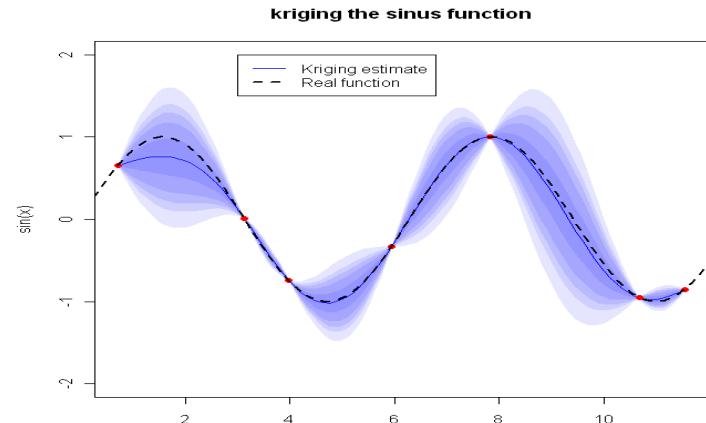
see Rasmussen & Williams [2005]

Part of *Supervised Machine Learning*

Advantage: gives a prediction with an associated error bound (Gaussian distribution at each point)



How to build the GP in large dimension?



STEP 3: Approximation with GP Metamodel

Brief reminds on GP

see Rasmussen & Williams [2005]

- ✓ Kernel-based method of supervised learning from (X_s, Y_s) . Response is considered as a realization of a random GP field:

$$Y(\mathbf{x}) \sim GP(\mu(\mathbf{x}), k(\mathbf{x}', \mathbf{x}))$$

With $\mu(\mathbf{x})$ the mean and $k(\mathbf{x}', \mathbf{x})$ the covariance function.

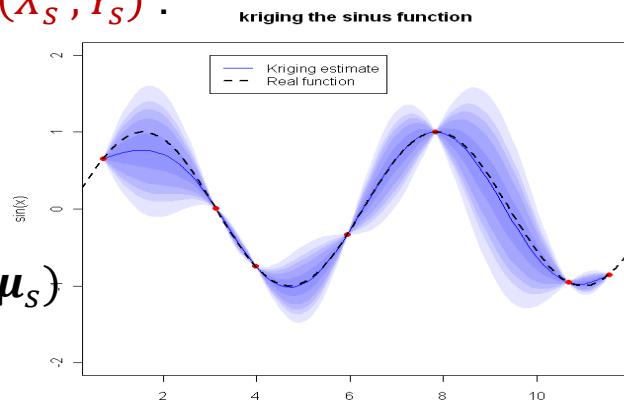
⇒ Predictive GP is the GP conditioned by the observations (X_s, Y_s) :

$$Y(\mathbf{x}^*)|_{Y(X_s)=Y_s} \sim GP(\hat{\mu}(\mathbf{x}^*), \hat{s}(\mathbf{x}', \mathbf{x}^*))$$

With

- $\hat{\mu}(\mathbf{x}^*) = E[Y(\mathbf{x}^*)|Y(X_s) = Y_s] = \mu(\mathbf{x}^*) + k_{X_s, \mathbf{x}^*}^T K_{X_s, X_s}^{-1} (Y_s - \mu_s)$
- $\hat{s}(\mathbf{x}', \mathbf{x}^*) = \text{Cov}[Y(\mathbf{x}^*)|Y(X_s) = Y_s] = k_{X_s, \mathbf{x}^*}^T K_{X_s, X_s}^{-1} k_{X_s, \mathbf{x}^*}$

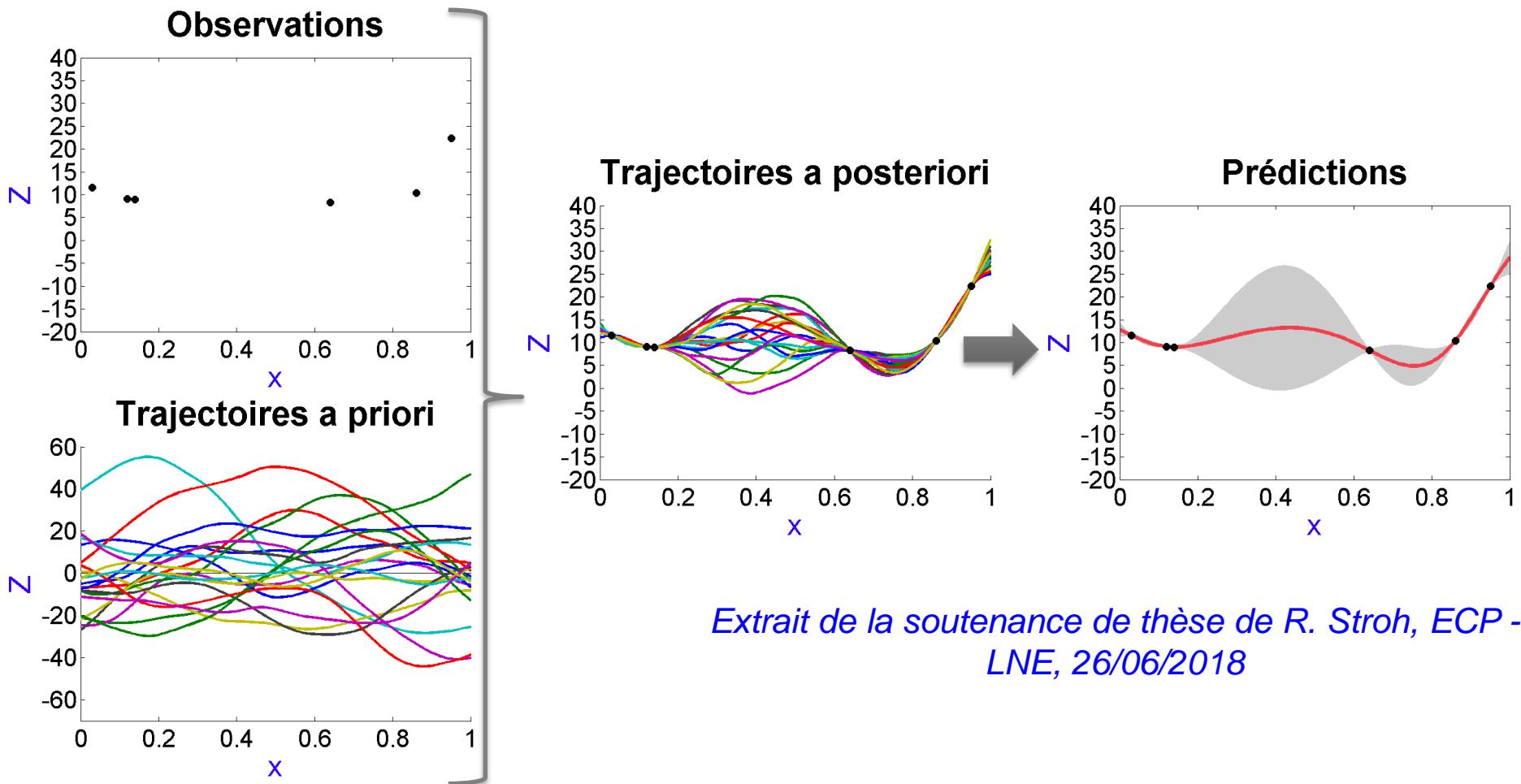
where μ_s corresponds to μ evaluated at X_s , k_{X_s, \mathbf{x}^*} the covariance between X_s and \mathbf{x}^* and K_{X_s, X_s} the covariance matrix for X_s



⇒ Conditional mean $\hat{\mu}(\mathbf{x}^*)$ serves as the predictor at location \mathbf{x}^*

⇒ Prediction variance (i.e. mean squared error) given by conditional covariance $\hat{s}(\mathbf{x}^*, \mathbf{x}^*)$

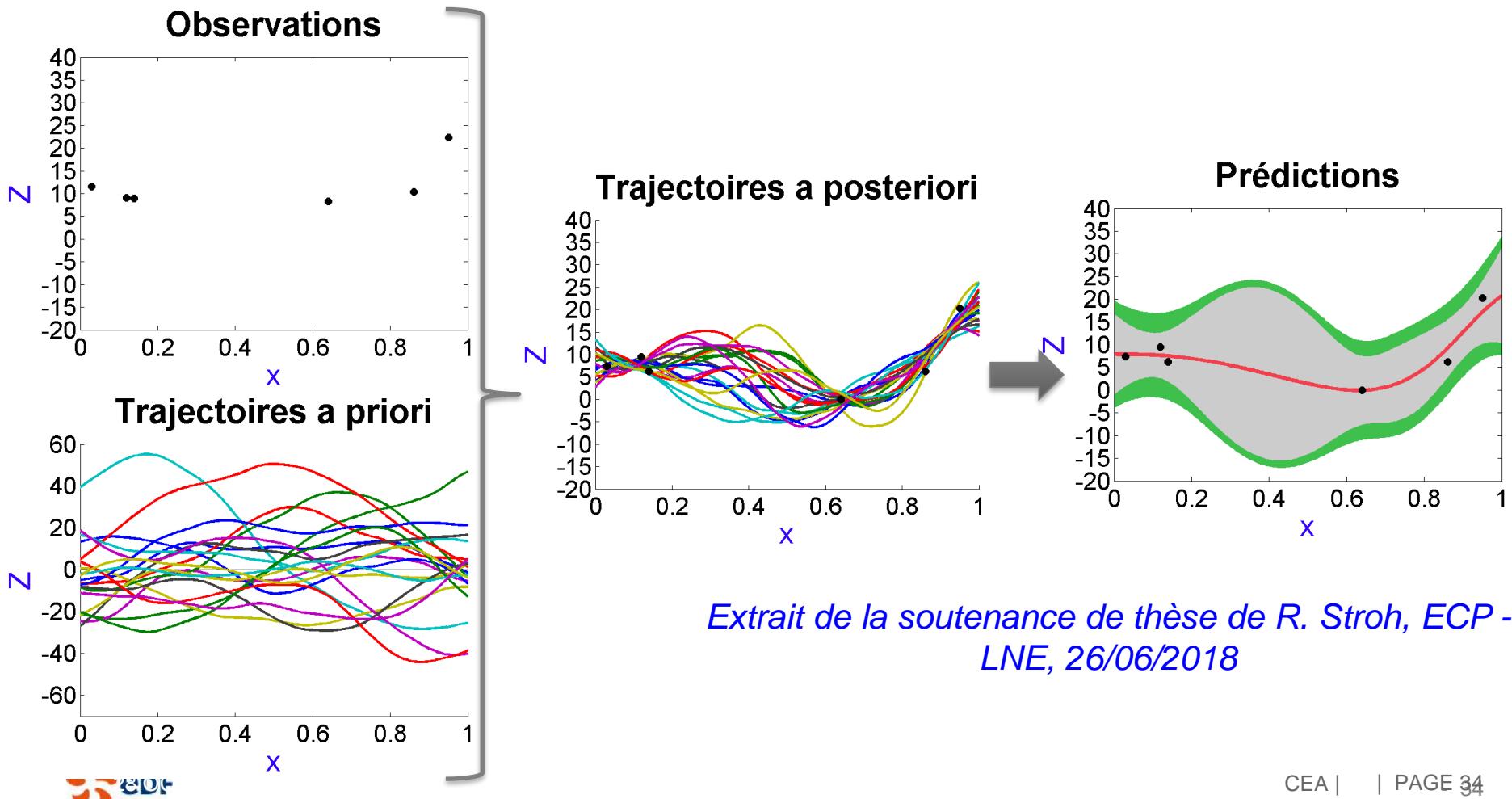
STEP 3: Approximation with GP Metamodel



Extrait de la soutenance de thèse de R. Stroh, ECP - LNE, 26/06/2018

STEP 3: Approximation with GP Metamodel

With homoscedastic nugget effect



STEP 3: Approximation with GP Metamodel

➤ Validation of GP predictor:

- ✓ Study of residuals computed on a test sample or by Cross Validation (CV)
- ✓ Predictivity coefficient Q^2 (formula given for test sample $(x^{test,(i)}, y^{test,(i)})_{1 \leq i \leq n_{test}}$)

$$Q^2 = 1 - \frac{\sum_{i=1}^{n_{\text{test}}} (y^{test,(i)} - \hat{y}^{test,(i)})^2}{\sum_{i=1}^{n_{\text{test}}} (y^{test,(i)} - \bar{y}^{test})^2}$$

where $\hat{y}^{test,(i)}$ is the metamodel predictor and \bar{y}^{test} the empirical test sample mean.

The closer to one the Q^2 , the better the accuracy of the metamodel predictor.

- ✓ QQ-plot, rate of good classification $Y > q_{90}$ and correlation coefficient $1_{[Y > q_{90}]}$

➤ Validation of GP predictive variance:

- ✓ Predictive Variance adequacy (PVA): Prediction errors of the same order as the prediction variances? \Rightarrow « Summary » of standardized residuals (by CV)

$$PVA = \log \left(\frac{1}{n_{\text{test}}} \sum_{i=1}^{n_{\text{test}}} \frac{(Y^{(i)} - \hat{y}^{(i)})^2}{MSE(\mathbf{x}^{(i)})} \right)$$

- ✓ Comparison of **theoretical levels** of GP-confidence intervals and **observed levels**:



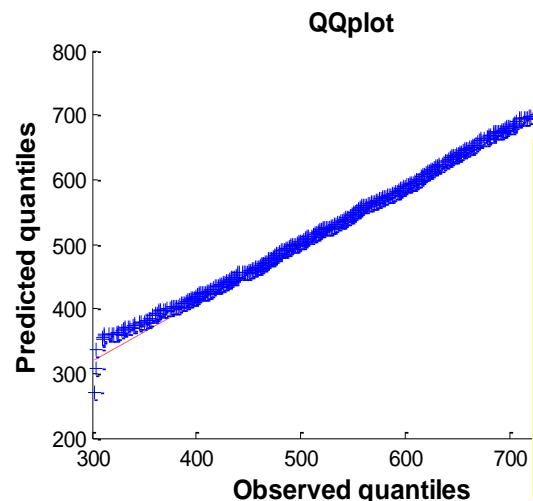
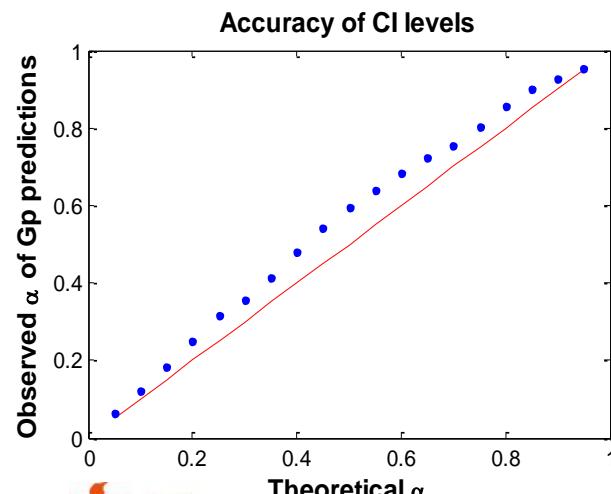
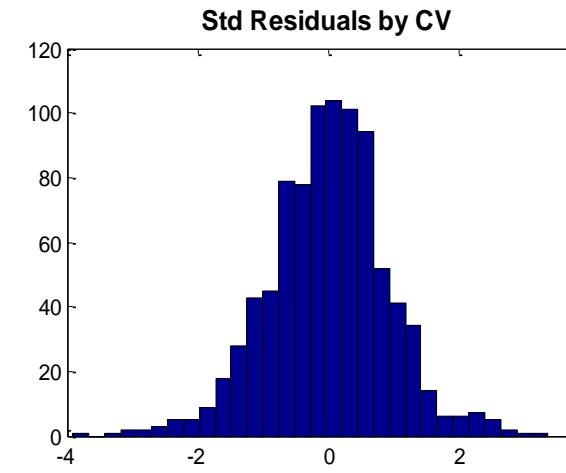
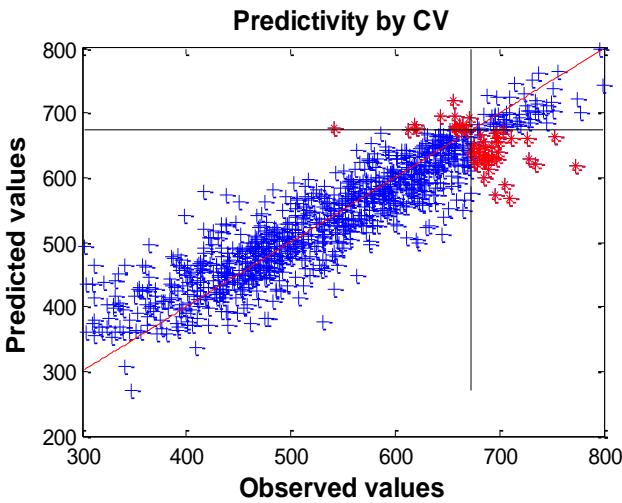
\Rightarrow For GP-predictions intervals of level α_{theo} : rate of observed data lying in the intervals (by CV)

see Demay et al. [2021]

STEP 3: Approximation with GP Metamodel

Application on IBLOCA test case

Assessment of accuracy and predictivity of final GP metamodel built on $N = 889$ simulations



⇒ 82 % of PCT variance explained by the GP built with the 20 selected 96 inputs

⇒ 18% of variance unexplained: inaccuracy of the GP + total effect of the 76 neglected inputs

STEP 4: Uncertainty propagation with GP

Step 4: Uncertainty propagation with GP metamodel to identify the penalizing values of X_{pen} under the uncertainty of the other inputs $\{X \setminus X_{pen}\}$

⇒ Precisely capture critical configurations of $X_{pen} = \{X_{127}, X_{143}\}$ which lead to the highest probability of $PCT > \hat{q}_{0.9}(Y)$ (under randomness of the other variables)

$$\begin{aligned}
 \hat{P}(X_{pen}) &= P[Y_{Gp}(X_{exp}) > \hat{q}_{0.9} | X_{pen}] \\
 &= 1 - \mathbb{E}(1_{Y_{Gp}(X_{exp}) \leq \hat{q}_{0.9}} | X_{pen}) \\
 &= 1 - \mathbb{E}(1_{Y_{Gp}(\tilde{X}_{exp}, X_{pen}) \leq \hat{q}_{0.9}} | X_{pen}) \\
 &= 1 - \mathbb{E}(\mathbb{E}(1_{Y_{Gp}(\tilde{X}_{exp}, X_{pen}) \leq \hat{q}_{0.9}} | \tilde{X}_{exp}) | X_{pen}) \\
 &= 1 - \int_{\tilde{X}_{exp}} \Phi\left(\frac{\hat{q}_{0.9} - \hat{Y}_{Gp}(\tilde{X}_{exp}, X_{pen})}{\sqrt{MSE[\hat{Y}_{Gp}(\tilde{X}_{exp}, X_{pen})]}}\right) d\mathbb{P}_{\tilde{X}_{exp}}(\tilde{X}_{exp})
 \end{aligned}$$

\tilde{X}_{exp} and X_{pen} are independent

Variation domain of \tilde{X}_{exp} Joint distribution of \tilde{X}_{exp}

- In practice, for each value of $X_{pen} = \{X_{127}, X_{143}\}$, computation of $\hat{P}(X_{pen})$ by intensive Monte-Carlo computation (integral in dimension 18)

STEP 4: Uncertainty propagation with GP

Application on IBLOCA test case

Use of final GP metamodel built on $N = 889$ simulations and with only 20 explanatory inputs

Results:

- Considered critical threshold (90% - empirical quantile) $\hat{q}_{0.9} = 673.2^\circ\text{C}$
- Estimated probability of overpass $\hat{q}_{0.9}$ with GP: $\mathbf{P}[Y_{GP} > \hat{q}_{0.9}] = 0.1005$

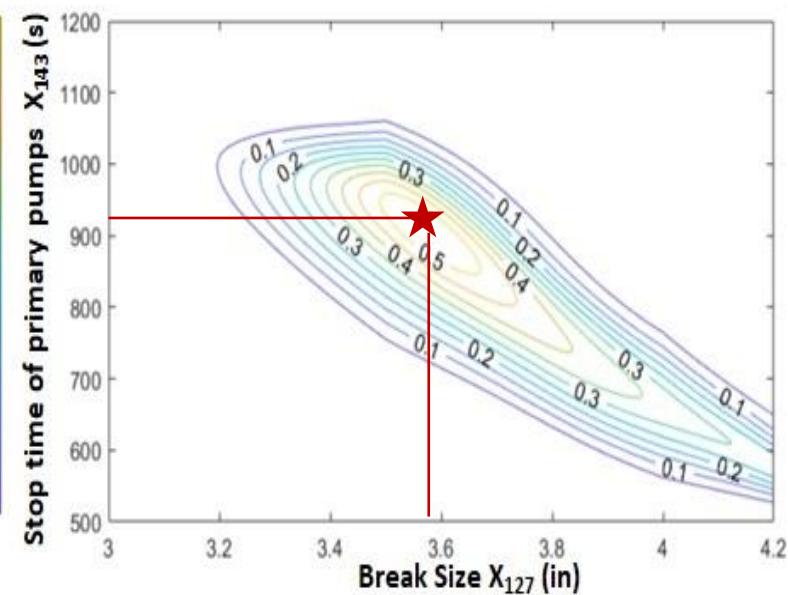
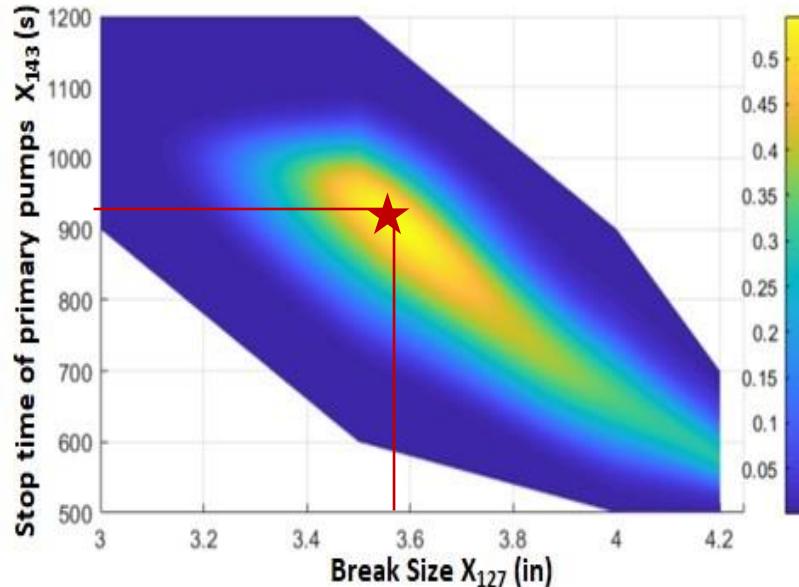
⇒ Coherence of results

STEP 4: Uncertainty propagation with GP

Application on IBLOCA test case

Computation of $\hat{P}(X_{pen})$

Probability of exceeding $\hat{q}_{0,9} = 673.18^\circ C$, according to X_{127} and X_{143}



- ▶ Strong interaction between the two scenario parameters
- ▶ Worst case: (3.57 inches, 907.8 seconds) $\Rightarrow \hat{P} \approx 0.55$
- ▶ Physical explanation: these two parameters drive the degradation of the water inventory
 - The smaller X_{127} , the longer the pump will have to run for the same inventory degradation
 - If $X_{127} < 3.3 \Rightarrow$ the water inventory does not degrade too much (whatever GMPP)
-  $X_{127} > 3.9 \Rightarrow$ break tends to be prevailing and reduces the impact of stop time of GMPP

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