Statistical approaches in nuclear safety problems: recent advances around sensitivity analysis and metamodelling

FROM RESEARCH TO INDUSTRY

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Workshop "Statistical methods for safety and decommissioning"

University of Avignon
Numerical Simulation – Experimental results – Database

Assessment of a accidental scenario on PWR: Break Loss Of Coolant Accident (B-LOCA)

1/ Experimental results

BETHSY experimental facility: 3-loop reduced scale model (1/100 in vol., real size in height) of a 900 MWe Framatome pressurized water reactor (PWR)

2/ Data

Thermal-hydraulics variables, physical properties and coefficients, ...

3/ Numerical simulation

CATHARE simulator

Thermal-hydraulic simulation of multiphase flow dynamics developed by the CEA with EDF, FRAMATOME and IRSN
Risk assessment in nuclear accident analysis

- **Safety studies**: compute a failure risk (margins, rare events) and prioritize the risk indicators, with validated computer/numerical models.

- **Numerical simulators**: fundamental tools to understand, model & predict physical phenomena.

- **Large number of input parameters**, characterizing the studied phenomenon or related to its physical and numerical modelling.

- **Uncertainty on some input parameters** → impacts the uncertainty on the output, the evaluation of safety margins.

- **BEPU (Best Estimate Plus Uncertainties)**: realistic models & uncertain inputs → Better assessment of the real margins.

\[
Y = \mathcal{M}(X_1, \ldots, X_d)
\]
Risk assessment in nuclear accident analysis

- **How to deal with uncertainties in numerical simulation?**
  - Probabilistic framework and statistical methods
  - Monte Carlo-based approaches and data analysis ⇒ Data Sciences
  - Essential use of machine learning

- **Data-driven methods** in support of physical modeling, analysis and forecasting
  - To propagate the uncertainties of the inputs
  - Assess their impact on the simulator predictions
  - Estimate probabilities of failure, quantiles, safety margins
  - Identify the most influential uncertain inputs: sensitivity analysis
  - Calibrate modeling parameters & input uncertainty w.r.t. experimental results
  - Validate the numerical simulator accuracy w.r.t. experimental results
  - Identify optimal configurations
General uncertainty quantification methodology

Step B: Quantification of uncertainty sources

Probabilistic modeling ⇒ Distributions

Uncertain inputs
\[ X = [X_1, \ldots, X_d] \]

Numerical model or simulator
\[ g : \mathbb{R}^d \rightarrow \mathbb{R} \]

Variable of interest
\[ Y = g(X) \]

Metamodelling
\[ \hat{Y} = \hat{g}(X) \approx g(X) \]

Step D: Sensitivity analysis

Decision Criterion
Ex: probability < 10^{-b}

Extracted and modified from De Rocquigny et al. (2008)
Step B: Quantification of uncertainty sources

Probabilistic modeling \( \Rightarrow \) Distributions

\( P_{X_1}, P_{X_2}, P_{X_d} \)

Step A: Specification of the problem

Uncertain inputs \( X = [X_1, \ldots, X_d] \)

Numerical model or simulator \( g: \mathbb{R}^d \rightarrow \mathbb{R} \)

Variable of interest \( Y = g(X) \)

Metamodelling \( \hat{Y} = \hat{g}(X) \approx g(X) \)

Step D: Sensitivity analysis

Quantity of interest
Ex: variance, probability...
Recent advances in Sensitivity Analysis
⇒ Focus on HSIC measures
Quantitative SA and ranking purpose:
- Quantify the impact of each uncertain input and interaction → Ranking
- Identify the variables to be fixed or further characterized in order to obtain the largest reduction of the output uncertainty

Screening purpose. Separate the inputs into two groups: influential and non-influential
- Non-influential variables fixed without consequences on the output uncertainty
- In support of model reduction
- To build a simplified model, a metamodel ⇒ ICSCREAM methodology

Global SA within a probabilistic framework

→ Valuable information to understand $G$ and underlying phenomenon
Global Sensitivity Analysis (GSA) of numerical simulators

Non exhaustive-list of available methods...

\( p = \text{number of inputs} \)

- Easily interpretable
- Expensive in practice
- Only nullity of total indices \( \Leftrightarrow \) independence

\[ p\text{-independent} \quad (N \sim 100) \]

Density and kernel-based Smoothing

Modified from Iooss et Lemaître [2015]

HSIC

\[ N \sim 100 \]

\[ N \sim 1000p \]

\( N \) Number of model evaluations

Modified from Iooss et Lemaître [2015]
A few notations

- **Black-box model**

  \[ Y = \mathcal{M}(X_1, \ldots, X_d) \]

  - \( X_1, \ldots, X_d \) are \( d \) independent inputs, evolving in domain \( X_1, \ldots, X_d \)
  - \( Y \) evolves in domain \( \mathcal{Y} \)
  - \( P_X \) denotes the probability distribution of \( X \)
  - \( P_{X,Y} \): the joint probability measure and \( P_Y \otimes P_X \) the product of marginal distributions

- **Only a \( n \)-sample of simulations is available**

  \( \mathcal{M} \) unknown, only Monte-Carlo sample \( (X^{(j)}, Y^{(j)})_{1 \leq j \leq n} \) where \( Y^{(j)} = \mathcal{M}(X^{(j)}) \)
How to evaluate the sensitivity in a probabilistic way? ⇔ Independence

By comparing $P_{X_iY}$ with $P_{X_i} \otimes P_Y$

$$S_i = d(P_{X_iY}, P_{X_i} \otimes P_Y)$$

where $d$ a dissimilarity measure between two probability distributions

$d$ can be based on Maximum Mean Discrepancy:

$$\text{MMD}(\mathbb{P}, \mathbb{Q}) = \sup_{f \in \mathcal{H}} \left[ \mathbb{E}_\mathbb{P} f(Y) - \mathbb{E}_\mathbb{Q} f(Y) \right]$$

With $\mathcal{H} =$ unit ball in a (characteristic) RKHS (Reproducing Kernel Hilbert Space)

$$\Rightarrow S_i = \text{MMD}^2(P_{X_iY}, P_{X_i} \otimes P_Y) = \text{HSIC}(X_i, Y)$$

Hilbert-Schmidt Independence Criterion
**HSIC review: a kernel-based GSA method**

MMD² applied between $P_{X_i Y}$ and $P_{X_i} \otimes P_Y \Rightarrow HSIC(X_i, Y)\mathcal{H}_{X_i},\mathcal{H}_Y$

$\mathcal{H}_{X_i}$ and $\mathcal{H}_Y$ RKHS associated to $X_i$ and $Y$, resp:

Kernel $k_{X_i}: X_i \times X_i \rightarrow \mathbb{R}$ with feature space $\mathcal{H}_{X_i}$ and feature map $\varphi_{X_i}$ (not unique)

Kernel $k_Y: Y \times Y \rightarrow \mathbb{R}$ with feature space $\mathcal{H}_Y$ and feature map $\varphi_Y$

$K_{X_i}(x, x') = \langle \varphi_{X_i}(x), \varphi_{X_i}(x') \rangle_{\mathcal{H}_{X_i}}$ and $K_Y(y, y') = \langle \varphi_Y(y), \varphi_Y(y') \rangle_{\mathcal{H}_Y}$

**Kernel embedding** of a distribution $\mathbb{P}_Z$ into RKHS with kernel $K_Z$

$\mu_{\mathbb{P}_Z}(z) = \mathbb{E}_{Z \sim \mathbb{P}_Z}[K_Z(Z, z)] = \langle \mu_{\mathbb{P}_Z}, K_Z(\cdot, z) \rangle_{\mathcal{H}_Z}$

Muandet et al. [2017]

**Picture extracted from G. Sarazin’s (CEA) slides**

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**Caption:**

- **Text:** Picture extracted from G. Sarazin’s (CEA) slides

**Diagram Description:**

- **Text:** Space of all probability distributions for the input-output pair

- **Text:** Tensorized RKHS
HSIC review: a kernel-based GSA method

**MMD^2** applied between $P_{X_i \mid Y}$ and $P_{X_i} \otimes P_Y \Rightarrow HSIC(X_i, Y)_{\mathcal{H}_{X_i}, \mathcal{H}_Y}$

$\mathcal{H}_{X_i}$ and $\mathcal{H}_Y$ RKHS associated to $X_i$ and $Y$, resp:

- Kernel $k_{X_i}: X_i \times X_i \rightarrow \mathbb{R}$ with feature space $\mathcal{H}_{X_i}$ and feature map $\varphi_{X_i}$
- Kernel $k_Y: Y \times Y \rightarrow \mathbb{R}$ with feature space $\mathcal{H}_Y$ and feature map $\varphi_Y$

$K_{X_i}(x, x') = \langle \varphi_{X_i}(x), \varphi_{X_i}(x') \rangle_{\mathcal{H}_{X_i}}$ and $K_Y(y, y') = \langle \varphi_Y(y), \varphi_Y(y') \rangle_{\mathcal{H}_Y}$

$\textbf{HSIC} = \text{distance in the RKHS between the images of the two distributions of interest}$

\[
\Rightarrow HSIC(X_i, Y)_{\mathcal{H}_{X_i}, \mathcal{H}_Y} = \text{MMD}^2_{\mathcal{H}_{X_i}, \mathcal{H}_Y}(P_{X_i \mid Y}, P_{X_i} \otimes P_Y) = \left\| \mu_{P_{X_i \mid Y}} - \mu_{P_{X_i} \otimes P_Y} \right\|_{\mathcal{H}_{X_i}, \mathcal{H}_Y}^2
\]

- Space of all probability distributions for the input-output pair
- Tensorized RKHS

*Extracted from G. Sarazin’s (CEA) slides*
**HSIC review: a kernel-based GSA method**

**MMD² applied between** $P_{X_i,Y}$ and $P_{X_i} \otimes P_Y \Rightarrow HSIC(X_i, Y)_{\mathcal{H}_{X_i}, \mathcal{H}_Y}$  

$\mathcal{H}_{X_i}$ and $\mathcal{H}_Y$ RKHS associated to $X_i$ and $Y$, resp :  
Kernel $k_{X_i}: \mathcal{X}_i \times \mathcal{X}_i \to \mathbb{R}$ with feature space $\mathcal{H}_{X_i}$ and feature map $\varphi_{X_i}$  
Kernel $k_Y: \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$ with feature space $\mathcal{H}_Y$ and feature map $\varphi_Y$  

\[ K_{X_i}(x, x') = \langle \varphi_{X_i}(x), \varphi_{X_i}(x') \rangle_{\mathcal{H}_{X_i}} \quad \text{and} \quad K_Y(y, y') = \langle \varphi_Y(y), \varphi_Y(y') \rangle_{\mathcal{H}_Y} \]

**HSIC** = distance in the RKHS between the images of the two distributions of interest  
\[ \Rightarrow HSIC(X_i, Y)_{\mathcal{H}_{X_i}, \mathcal{H}_Y} = \text{MMD}^2_{\mathcal{H}_{X_i}, \mathcal{H}_Y}(P_{X_i,Y}, P_{X_i} \otimes P_Y) = \| C_{X,Y} \|^2_{HS} \]

With $C_{X,Y}$ the covariance operator between features maps:  
\[ C_{X,Y} = \mathbb{E}_{X,Y} [\varphi_X(X) \otimes \varphi_Y(Y)] - \mathbb{E}_X[\varphi_X(X)] \otimes \mathbb{E}_Y[\varphi_Y(Y)] \]

**HSIC** "summarizes" the cross-cov between feature maps  
\[ \Rightarrow \text{Large panel of input-output dependency can be captured.} \]

Gretton et al. [2005]
**Characteristic kernels and RKHS** \(\Rightarrow\) *Injective canonical feature map*

\(\Rightarrow\) **Equivalence to independence:** \(\text{HSIC}(X, Y) = 0 \Leftrightarrow X \perp Y\)

**Ex:** Gaussian Kernel

\[
k(x_i, x_i') = \exp\left(-\frac{(x_i-x_i')^2}{2\lambda^2}\right)
\]

**Estimation: Kernel Trick** \(\Rightarrow\) Feature map linked to kernel function

Very simple M-C estimator from a \(n\)-sample of simulations \((X_i^{(j)}, Y^{(j)})\) \(1 \leq j \leq n\)

\[
\overline{\text{HSIC}}(X, Y) = \frac{1}{n-1} \text{Tr}(K_iHLH)
\]

where \(H = I_n - \frac{1}{n}\), \(K_i = \left(k_i \left(X_i^{(j)}, X_i^{(j')}\right)\right)_{1 \leq j, j' \leq n}\) and \(L = \left(k(Y^{(j)}, Y^{(j')})\right)_{1 \leq j, j' \leq n}\)

**Statistical Properties:**

- Asymptotically unbiased, variance of order \(O(1/n)\)
- If \(X \perp Y\), \(n\overline{\text{HSIC}}(X, Y)\) converges asymptotically to a Gamma distribution
Normalization for sensitivity analysis:

$$R^2_{HSIC} = \frac{HSIC(X,Y)}{\sqrt{HSIC(X,X)HSIC(Y,Y)}}$$

$\Rightarrow R^2_{HSIC} \in [0,1]$ for easier interpretation

Influence($X_{[1]}$) > Influence($X_{[2]}$) > … > Influence($X_{[d]}$)

Where order $[\cdot]$ is such that $\hat{R}^2_{H,X_{[1]}} > \hat{R}^2_{H,X_{[2]}} > \cdots > \hat{R}^2_{H,X_{[d]}}$

$\Rightarrow$ Use for ranking of inputs

Independence tests: $HSIC(X, Y) = 0 \iff X \perp Y$ (with characteristic kernels!)

- Null hypothesis: $\mathcal{H}_0 : X \perp Y$ against $\mathcal{H}_1 : X \not\perp Y$
- Test statistics: $n\widehat{HSIC}(X, Y)$
- Decision rule: $\mathcal{H}_0$ rejected iff $n\widehat{HSIC}(X, Y) > q_{1-\alpha}$

where $q_{1-\alpha}$ is the $(1 - \alpha)$ quantile of $n\widehat{HSIC}(X, Y)$ under $\mathcal{H}_0$

$\Rightarrow$ Use for screening of inputs
Use of HSIC for GSA of numerical simulators

HSIC-based independence tests for screening

How to have the distribution $n\text{HSIC}(X_i, Y)$ under $\mathcal{H}_0$ to compute \textit{p-value}?

- If $n$ large: asymptotic test based on approximation with Gamma distribution (Gretton et al. (2008))
- If $n$ small: Permutation-based approximation (De Lozzo & Marrel (2016a), Meynaoui [2019], El Amri & Marrel [2021a])

Gamma distribution

\[
P\text{-value} = Pr \left[ \text{HSIC}(X_i, Y) > \text{hsic}_{obs} \right]
\]

Interpretation of \textit{p-value} for a level $\alpha$ ($\alpha = 5\%$ or $10\%$) for screening:

$\checkmark$ \textit{pval} < $\alpha$ $\Rightarrow$ $H_0$ (Independence) rejected $\Rightarrow$ $X_i$ is significantly influential
Use of HSIC for GSA of numerical simulators

- **HSIC as indices of Sensitivity Analysis**
  - Focus the SA analysis on the difference between $P_{X,Y}$ with $P_X \otimes P_Y$
  - Power of RKHS $\rightarrow$ HSIC=one of the most successful non-parametric dependence measure
  - Capture a large spectrum of relationships
  - Able to deal with many types of variables and purposes:
    - **Goal-oriented SA for safety studies** (Marrel & Chabridon [2021], Iooss & Marrel[2019]) : To measure the input influence in a restricted output domain: $Y \in C$
      $\Rightarrow$ Numerous applications for safety and risk assessment ($C$: critical safety domain, e.g. $C = \{Y|Y > \text{critical value}\}$)
    - **SA of multivariate or functional output (or inputs)** $\Rightarrow$ definition of specific kernels
      Atmospheric dispersion model with spatio-temporal output (De Lozzo & Marrel [2016b]), Dynamic compartmental epidemiologic model on COVID-19 (El Amri & Marrel [2021b])
    - Efficiency demonstrated in numerous industrial applications, especially with small sample size $n$ and large dimension $d$
  - Use in support of metamodeling in large dimension $\rightarrow$ ICSCREAM Methodology
Recent advances in Metamodeling ⇒ Focus on Gaussian Process (GP) Regression
Step B: Quantification of uncertainty sources

Probabilistic modeling ⇒ Distributions

Step A: Specification of the problem

Uncertain inputs

\[ X = [X_1, ..., X_d] \]

Numerical model or simulator

\[ g : \mathbb{R}^d \rightarrow \mathbb{R} \]

Variable of interest

\[ Y = g(X) \]

Metamodelling

\[ \hat{Y} = \hat{g}(X) \approx g(X) \]

Quantity of interest

Ex: variance, probability...

\[ P_Y \]
Crucial use of metamodel (machine learning)

In case of costly $G$:
Model reduction or Approximation with Machine learning (ML)

**metamodel** $Z_{app} \approx g(X)$

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

*Ex*: Polynomials, splines, neural networks, regression trees…
**Crucial use of metamodel (machine learning)**

**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?
- How to build the GP for chaotic code?
- How to build the GP for functional or other type of data?
- Integration of physical constraints? *cf. Bachoc’s talk*
Crucial use of metamodel (*machine learning*)

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

\[
Y(x) \sim GP(\mu(x), k(x', x))
\]

With \(\mu(x)\) the mean and \(k(x', x)\) the covariance function.

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

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

With

- \(\hat{\mu}(x^*) = E[Y(x^*)|Y(X_s) = Y_s] = \mu(x^*) + k_{X_s,x^*}K_{X_s,X_s}^{-1}(Y_s - \mu_s)\)

- \(\hat{s}(x', x^*) = \text{Cov}[Y(x^*)|Y(X_s) = Y_s] = k_{X_s,x^*}K_{X_s,X_s}^{-1}k_{X_s,x^*}\)

where \(\mu_s\) corresponds to \(\mu\) evaluated at \(X_s\), \(k_{X_s,x^*}\) the covariance between \(X_s\) and \(x^*\) and \(K_{X_s,X_s}\) the covariance matrix for \(X_s\)

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

⇒ **Prediction variance** (*i.e. mean squared error*) given by **conditional covariance** \(\hat{s}(x^*, x^*)\)
Illustration: the **ICSCREAM** methodology for the IB-LOCA nuclear accident
Simulation of IB-LOCA nuclear accident

Accidental scenario on pressurized water reactor: IB-LOCA
LOss of primary Coolant Accident due to a Intermediate Break in cold leg

$d (~ 100)$ input random variables:
Critical flowrates, initial/boundary conditions, phys. eq. coef., ...

Modelled with CATHARE2 code:
- Models complex thermal-hydraulic phenomena
- Large CPU cost for one code run ( > 1 hour )

Variable of Interest:
2$^{nd}$ peak of cladding temperature (PCT) = scalar output
Objective in IB-LOCA safety study

- In IB-LOCA modeling framework, uncertain input parameters are:
  - (Type 1) Initial conditions, physical model parameters \( \Rightarrow \) Probabilistic \( (\mathcal{U}, \mathcal{LU}, \mathcal{N}, \mathcal{LN}) \)
  - (Type 2) Scenario parameters (min / max bounds) \( \Rightarrow \) No probabilistic

Objective in support of safety studies
Identify the most **penalizing configurations** for Type 2 inputs, under the uncertainties of Type 1 inputs.

Penalizing configurations \( \Leftrightarrow \) leading to high PCT values

**IB-LOCA**: Intermediate Break LOss of Coolant Accident
Problems & constraints

- Very large number of inputs (~100), but effective dimension might be lower
- Each CATHARE simulation ~ 1 hour ⇒ around 1000 simulations available
- Phenomena involved are complex with strong non-linearities
- Black-box model: intrusive methods not possible

⇒ Monte Carlo sampling + advanced statistical tools for data analysis
  - Screening and sensitivity analysis
  - Approximation with metamodel
  - Uncertainty propagation

⇒ Adapted to VERY HIGH DIMENSIONAL test case (~100 uncertain inputs)

⇒ ICSCREAM* methodology in 4 Main Steps
  *Identification of penalizing Configurations using SCREening And Metamodel
STEP 1: Monte Carlo Sampling design

**Uncertainty quantification of uncertain inputs + scenario inputs to be penalized** $X_{pen}$

Uncertain inputs $X = (X_1, \ldots, X_{d'})$ with probability distributions + scenario inputs $X_{pen}$

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**Step 1: Learning sample of $n$ simulations** $(X_S, Y_S)$

Monte-Carlo design of $n$ experiments $X_S = \{x^{(1)}, \ldots, x^{(n)}\}$ and associated CATHARE2 PCT outputs $Y_S$
**STEP 1: Monte Carlo Sampling design**

*Illustration on the IB-LOCA test case*

- **$d = 96$ uncertain variables** with probability distributions $\mathbb{P}_X$ (almost indep.)
- **$n = 889$ CATHARE2 simulations**: Monte-Carlo sample ($X \sim \mathbb{P}_X$)

Empirical quantile 90%: $q_{0.9} \approx 673.18 ^\circ C$

**Critical configurations** are defined as: $PCT > q_{0.9}$

**Scatter plots with 1-D local polynomials for trends**

**Complex relationships** of PCT w.r.t. $X$

**Metamodelling of PCT** with such a large number of inputs is a hard task!!
Among 96 inputs, 2 scenario inputs to be penalized (here dependent):

- \( X_{127} \) (break size): uniform distribution on [3, 4.2] inches
- \( X_{142} \) (factor for GMPP stop time): uniform random variable whose range of variation depends on the value of \( X_{127} \)

**Objective:**
Precisely capture critical configurations of \((X_{127}, X_{142})\) which lead to the highest probability of PCT exceeding \(q_{0.9} \) (\(\approx 673.18 \, ^\circ C\))

\[ X_{pen} = \{X_{127}, X_{142}\} \subset X \]
STEP 2: Screening & ranking of inputs

Uncertainty quantification of uncertain inputs + scenario inputs to be penalized $X_{pen}$

Step 1: Learning sample of $n$ simulations $(X_S, Y_S)$

Step 2: Screening and ranking with HSIC-based independence tests from $(X_S, Y_S)$
Identify and rank the inputs of primary influence with HSIC-based tests

**Global** Sensitivity Analysis

- **Global (G-) HSIC**

**Goal-oriented** Sensitivity Analysis:
- focus on exceeding the 90%-quantile

- **Target (T-) HSIC**
Global-HSIC tests

~ 18 influential inputs in GSA
Influence ++ : X142 (GMPP time)  
Influence + : X127 (break size)  
Influence : X113, X110, X11 
Lower influence : X50, X42, X112, X83, X64, X125, X55, X103, X36, X27, X54, X102, X52 

~ 19 influential inputs in TSA  
Influence ++ : X142 (GMPP time)  
Influence + : X113, X110, X127, X125, X83 
Lower influence : X42, X103, X76, X50, X55, X54, X2, X27, X28, X21, X84, X64, X11 

T-HSIC ⇒ Impact on exceeding the 90%-quantile $\hat{q}_{0.9}(Y)$
**STEP 2: Screening & ranking of inputs**

*Illustration on the IB-LOCA test case*

**Global-HSIC tests**

~ 18 influential inputs in GSA
- Influence ++ : X142
- Influence + : X127
- Influence : X113, X110, X11

Lower influence : X50, X42, X112, X83, X64, X125, X55, X103, X36, X27, X54, X102, X52

~ 19 influential inputs in TSA
- Influence ++ : X142
- Influence + : X113, X110, X127, X125, X83

Lower influence : X42, X103, X76, X50, X55, X54, X2, X27, X28, X21, X84, X64, X11

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**From aggregation, selection of around 20 inputs**

**Inputs ordered by influence \( d^* \), using \( P\)-values**
STEP 3: Approximation with a GP Metamodel

Uncertainty quantification of uncertain inputs + scenario inputs to be penalized $X_{pen}$

Step 1: Learning sample of $n$ simulations $(X_S, Y_S)$

Step 2: Screening and ranking with HSIC and T-HSIC independence tests from $(X_S, Y_S)$

Step 3: Sequential Metamodelling $\rightarrow$ Gaussian process (GP) regression from $(X_S, Y_S)$

Challenge to be addressed here: how to build the GP in large dimension (d~100) ?

Use the information of screening and ranking from HSIC $\Rightarrow$ Sequential estimation of GP hyperparameters
Assessment of accuracy and predictivity of final GP metamodel built on $N = 889$ simulations

- $Q^2: 82\%$ 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
- Low PVA and good $\alpha$-CI plot: accurate confidence intervals in prediction
STEP 4: Uncertainty propagation with the GP

Uncertainty quantification of uncertain inputs + scenario inputs to be penalized $X_{pen}$

Step 1: Learning sample of $n$ simulations $(X_S, Y_S)$

Step 2: Screening and ranking with HSIC and T-HSIC independence tests from $(X_S, Y_S)$

Step 3: Sequential Metamodelling with Gaussian process (GP) from $(X_S, Y_S)$

Step 4: Uncertainty propagation with GP metamodel

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

$\Rightarrow$ 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)

Notations:
- $X_{exp}$ are explanatory inputs of the GP
- $\bar{X}_{exp} = X_{exp} \setminus X_{pen}$

$\hat{P}(X_{pen}) = P[Y_{GP}(X_{exp}) > \hat{q}_{0.9} | X_{pen}]$

$$= 1 - \int_{\bar{X}_{exp}} \Phi \left( \frac{\hat{q}_{0.9} - \hat{Y}_{GP}(\bar{X}_{exp}, X_{pen})}{\sqrt{MSE[\hat{Y}_{GP}(\bar{X}_{exp}, X_{pen})]}} \right) dP_{\bar{X}_{exp}}(\bar{X}_{exp})$$

Variation domain of $\bar{X}_{exp}$
Joint distribution of $\bar{X}_{exp}$

- $\bar{X}_{exp}$ and $X_{pen}$ are independent (necessary condition)
- $\Phi$ : CDF of standard Gaussian distribution

- In practice, for each value of $X_{pen} = \{X_{127}, X_{143}\}$, $\hat{P}(X_{pen})$ is estimated by intensive Monte-Carlo computation (here integral in dimension 18 in the use-case)
STEP 4: Uncertainty propagation with the GP

Illustration on the IB-LOCA 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)
  - If \( X_{127} > 3.9 \) \( \Rightarrow \) break tends to be prevailing and reduces the impact of stop time of GMPP
Some axes of research for uncertainty treatment

- **Model exploration : numerical Designs of Experiments (DoE)**
  - Space-filling designs for large number of uncertain inputs
  - How to tackle the curse of dimensionality?
  - Extension to functional (temporal/spatial) inputs?
  - Adaptive/sequential DoE (tractability in large dimension)

- **Sensitivity analysis techniques**
  - Advanced and robust screening (dimension reduction) and ranking techniques
  - Extension to functional (temporal/spatial) outputs?
  - Extension to correlated inputs?

- **Metamodeling for large number of uncertain inputs**
  - How to build accurate and reliable GP metamodel in very large dimension $d$?
  - Scalability with large sample size $n$?

- **Validation/Calibration of model (real experiments vs. calculations)**
  - Bayesian approaches
  - Definition of relevant metrics for validation
Some axes of research for uncertainty treatment

- Some are notably addressed within the ANR SAMOURAI project

  - **Advanced and robust screening and ranking**
    - Decomposition into main effects & interactions must be investigated
    - ⇒ Assess the use of **HSIC with ANOVA-like kernels** ([Da Veiga [2021]])
    - ⇒ Build associated independence tests
    - ⇒ Relevancy in support of metamodel building

  - **BuildGP in large dimension: improve reliability**
    - ⇒ More reliable estimation of hyperparameters
    - ⇒ Bayesian approach and sparse GP

  - **Adaptive/sequential DoE**
Some References