OTICSCREAM: A Python module (and a cooking recipe) for the identification of penalizing configurations in computer experiments

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Introduction

Context and motivations

- Industrial motivations: risk analysis in nuclear safety
  - Deterministic analyses ("worst cases")
    - Historical
    - Supposed to be "conservative" enough
    - **But** sometimes, far from reality!
  - Probabilistic analyses ("Best Estimate Plus Uncertainty" or **BEPU**)
    - Supposed to produce more realistic physics!
    - Needs to take (explicitly) uncertainties into account!
    - **But** safety margins need to be identified clearly!

- Simulation of an Intermediate-Break Loss-Of-Coolant Accident[1]
  - Modeling of a primary circuit (cold leg) of a PWR[2]
  - Simulation of a thermal-hydraulic transient scenario
  - Best-estimate computer model: the CATHARE2 code

[1] IBLOCA

[2] Pressurized Water Reactor

Context and motivations

❑ Simulation of an IBLOCA using the CATHARE2 code

- ➤ Uncertainty sources in input:
  - Type #1: Initial/boundary conditions ➜ probabilistic ($\mathcal{U}$, trunc. $\mathcal{N}$)
  - Type #2: Physical parameters ➜ probabilistic ($\mathcal{U}$, $\mathcal{LU}$, trunc. $\mathcal{N}$, $\mathcal{LN}$)
  - **Type #3: Scenario parameters ➜ not proba. (lower/upper bounds)**
- ➤ Scalar output quantity of interest (QoI):
  - Second peak of cladding temperature (PCT)

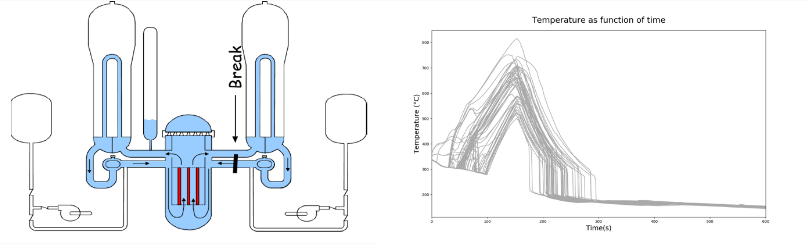


Figure 1: IBLOCA in a PWR (©CEA) / PCT trajectories from CATHARE2 (©EDF).

Context and motivations

- ❑ Main objectives
  - ➤ How to identify the most **penalizing configurations** for Type #3 inputs (scenario parameters) regardless the other sources of uncertainties (Type #1 and Type #2)?
  - ➤ **Penalizing configurations ➜ Leading to high PCT values**
- ❑ Main challenges/constraints
  - ➤ Large number of inputs ($\approx$ 100) ➜ Effective dimension might be lower!
  - ➤ Complex phenomena / strongly nonlinear response!
  - ➤ Computational cost ➜ Only $\approx 10^3$ simulations available!
  - ➤ Industrial/regulatory context ➜ crude Monte Carlo (i.i.d.)

Questions

- How to handle these challenges and constraints?
- Can we propose a generic methodology?

The ICSCREAM methodology

ICSCREAM: a four-step methodology

- Non-exhaustive list of available tools in the UQ literature
  - Global sensitivity analysis techniques to reduce the input dimension
  - Smart adaptive surrogate modeling strategies
  - Approximation tools based on low-rank or projection-based methods
  - Adaptive strategies for robust inversion [RB19]

    ➜ We probably need to combine all these things together, as in a cooking recipe!

- A possible answer: the ICSCREAM (ice-cream) methodology
  - Originally proposed as a **specific answer** in the nuclear safety context (see [MIC22])
  - **But** can still be seen as a **generic methodology** for a large panel of applications!
  - Based on state-of-the-art UQ techniques (and a few advanced tools) gathered in a **modular framework**!
  - Adapted to a **given-data** context (no access to the computer model)!

ICSCREAM: a four-step methodology

❏ The ICSCREAM methodology in a nutshell!

Step 1 — Learning sample generation (simulation-based / given-data)

Step 2 — Screening and ranking with HSIC-based indices

Step 3 — Surrogate model build-ing and validation

Step 4 — Identification of penalizing values

Step 1

Step 1: Monte Carlo sampling ("given-data" context)

❑ A few notations and preliminary hypotheses:

➤ Real-valued & deterministic black-box model:

$$\mathcal{M} : \left| \begin{array}{ccc} \mathcal{X} \subseteq \mathbb{R}^d & \longrightarrow & \mathcal{Y} \subseteq \mathbb{R} \\ \mathrm{X} & \longmapsto & Y = \mathcal{M}(\mathrm{X}) \end{array} \right. \tag{1}$$

➤ Probabilistic modeling of d **independent** input physical variables:

$$\mathrm{X} := (\underbrace{X_1, X_2, \ldots, X_p}_{\mathrm{X}_{\mathrm{pen}}}, \underbrace{X_{p+1}, \ldots, X_d}_{\mathrm{X}_{\mathrm{alea}}})^\top \sim P_{\mathrm{X}} \quad \text{over} \quad \mathcal{X} = \bigtimes_{i=1}^{d} \mathcal{X}_i \tag{2}$$

where:

- $\mathrm{X}_{\mathrm{pen}}$ ➜ candidate inputs to be **penalized** s.t. $\mathrm{X}_{\mathrm{pen}} \sim \prod_{i=1}^{p} \mathcal{U}\left([a_i, b_i]\right)$
- $\mathrm{X}_{\mathrm{alea}}$ ➜ aleatoric variables s.t. $\mathrm{X}_{\mathrm{alea}} \sim P_{\mathrm{X}_{\mathrm{alea}}}$

➤ **Learning sample** ➜ get a n-size **i.i.d.** sample of the couple (X, Y):

$$\left(\mathrm{X}^{(j)}, Y^{(j)}\right)_{(1 \leq j \leq n)} = \left(X_1^{(j)}, X_2^{(j)}, \ldots, X_d^{(j)}, Y^{(j)}\right)_{(1 \leq j \leq n)} \tag{3}$$

with $P_{\mathrm{X}^{(j)}} = P_{\mathrm{X}}$ and $Y^{(j)} = \mathcal{M}\left(X_1^{(j)}, X_2^{(j)}, \ldots, X_d^{(j)}\right), \forall j \in \{1, \ldots, n\}$

➤ **Risk analysis** ➜ a typical QoI is the α**-order quantile** estimated using the empirical estimator $\widehat{q}_\alpha(Y)$

Step 2

Step 2: Global and target sensitivity analyses

- Two usual settings in sensitivity analysis [DGIP21]
  - "Can we split the inputs into two classes $\{\text{noninfluential}, \text{influential}\}$?"
    ➜ Screening
  - "Is it possible to rank the inputs with respect to their influence?"
    ➜ Ranking
- Global (GSA) vs. target sensitivity analysis (TSA)
  - "Does an input X_i have an influence on the global variability of Y?"
    ➜ GSA study
  - "Does an input X_i have an influence on exceeding an output threshold (e.g., $\{Y > q_\alpha(Y)\}$) or not?"
    ➜ TSA study [RM18, SLRDV19, MC21]

Step 2: Global and target sensitivity analyses

- A brief overview of the literature
  - Sobol' indices [PT17, PD19]
  - Indices based on dissimilarity measures (e.g., Borgonovo indices, Csiszár f-divergences, etc.) [BP16, Rah16]
  - **Hilbert-Schmidt Independence Criterion** (**HSIC**) [GBSS05, DV15]
    - ➜ Allows to measure influence beyond the variance
    - ➜ Adapted to the "given-data" context
    - ➜ Allows to perform GSA and TSA without having much trouble
    - ➜ Indices come together with a rigorous statistical framework

Step 2: Global and target sensitivity analyses

- A brief overview about HSIC indices
  - Basic idea: to assess the dependency between the random variables X_i and Y by comparing an infinite collection of features of both $P_{X_i,Y}$ and $P_{X_i}P_Y$
  - We consider a dependence measure, the **maximum mean discrepancy** (**MMD**) between $P_{X_i,Y}$ and $P_{X_i}P_Y$, which is expressed as the distance between their mean embeddings in some RKHS[3].

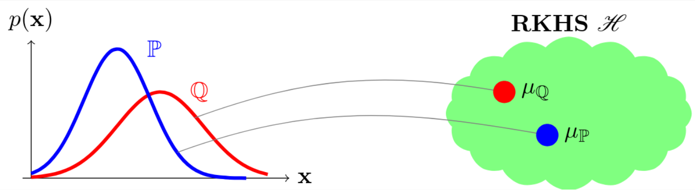


Figure 2: Embedding of marginal distributions (source: [MFSS17]).

[3] Reproducing Kernel Hilbert Space.

Step 2: Global and target sensitivity analyses

- A brief overview about HSIC indices
  - A first mathematical expression:

$$\begin{aligned} \mathrm{HSIC}_{\kappa_i\kappa}(X_i, Y) &= \mathrm{MMD}^2_{\kappa_i\kappa}(P_{(X_i,Y)}, P_{X_i}P_Y) && \text{(4a)} \\ &= \mathbb{E}[\kappa_i(X_i, X_i^{'})\kappa(Y, Y^{'})] + \mathbb{E}[\kappa_i(X_i, X_i^{'})]\mathbb{E}[\kappa(Y, Y^{'})] && \text{(4b)} \\ &- 2\mathbb{E}[\mathbb{E}[\kappa_i(X_i, X_i^{'})|X_i]\ \mathbb{E}[\kappa(Y, Y^{'})|Y]] \end{aligned}$$

  - A fundamental property ➜ if the kernels κ_i and κ are **characteristic**

$$\mathrm{HSIC}_{\kappa_i\kappa}(X_i, Y) = 0 \Leftrightarrow X_i \perp Y \qquad (5)$$

  - In practice ➜ one uses various types of **estimators** and a **statistical hypothesis testing** in order to decide whether an input is noninfluential or not

Step 3

Step 3: Gaussian process surrogate modeling

- **Gaussian process (GP) regression** [RW06]
  - Goal: build a predictor $\widetilde{\mathcal{M}}(\cdot)$ that mimics the behavior of $\mathcal{M}(\cdot)$ using a **dataset** $\mathcal{D} = \{(\mathrm{x}^{(i)}, y^{(i)}),\ i = 1, \ldots, n\}$ (supervised learning)
  - Probabilistic surrogate model ➜ assume

$$Y(\mathrm{x}) \sim GP(\mu(\mathrm{x}), \Sigma(\mathrm{x}', \mathrm{x})) \tag{6}$$

  - GP conditioning on data (universal kriging predictor):

$$\widehat{Y}(\mathrm{x}) = [Y(\mathrm{x})|\mathcal{D}, \sigma^2, \boldsymbol{\theta}] \sim \mathcal{N}_1(\mu_{\widehat{Y}}(\mathrm{x}), \sigma^2_{\widehat{Y}}(\mathrm{x})) \tag{7}$$

  - Estimation strategies for $(\sigma^2, \boldsymbol{\theta})$ ➜ MLE [MIVDV08]

Step 3: Gaussian process surrogate modeling

- GP building in practice
  - GP metamodel will be a function of several kind of inputs:
    - Explanatory inputs: $\mathsf{X}_{\text{exp}} = \{\mathsf{X}_{\text{PII}} \cup \mathsf{X}_{\text{pen}}\}$
    - Secondary influential inputs: X_{SII}
    - Neglected inputs: $\mathsf{X}_{\epsilon} = \{\mathsf{X} \setminus \{\mathsf{X}_{\text{exp}} \cup \mathsf{X}_{\text{SII}}\}\}$
  - GP mean: either constant or linear basis
  - X_{exp} ➜ tensorized anisotropic covariance function (Matérn ν)

$$R_{\boldsymbol{\theta}_{\text{exp}}}(\mathsf{x}_{\text{exp}}, \mathsf{x}'_{\text{exp}}) = \prod_{i=1}^{d_{\text{exp}}} R_{\theta_i}(x_{\text{exp}}^{(i)} - x_{\text{exp}}^{\prime (i)}) \tag{8}$$

  - X_{SII} ➜ isotropic covariance function (Matérn ν)

$$R_{\theta_{\text{SII}}}(\mathsf{x}_{\text{SII}}, \mathsf{x}'_{\text{SII}}) = R_{\theta_{\text{SII}}}(||\mathsf{x}_{\text{SII}} - \mathsf{x}'_{\text{SII}}||_2) \tag{9}$$

  - X_{ϵ} ➜ homoscedastic nugget effect
  - Resulting tensorized covariance:

$$\Sigma(\mathsf{x}, \mathsf{x}') = \sigma^2 \left(R_{\boldsymbol{\theta}_{\text{exp}}}(\mathsf{x}_{\text{exp}}, \mathsf{x}'_{\text{exp}}) R_{\theta_{\text{SII}}}(\mathsf{x}_{\text{SII}}, \mathsf{x}'_{\text{SII}}) + \gamma \delta_{(\mathsf{x}, \mathsf{x}')}\right) \tag{10}$$

  - GP metamodel either built directly or **sequentially**
  - Optimization of hyperparameters ➜ multi-start + LHS + optim. algo.

Step 3: Gaussian process surrogate modeling

- Cross-validation metrics
  - Validation of the GP predictor:
    - Analysis of the standardized residuals
    - Computation of the **predictivity coefficient** Q^2

$$Q^2 = 1 - \frac{\sum_{j=1}^{n_{\mathrm{val}}} \left(y^{\mathrm{val},(j)} - \hat{y}^{\mathrm{val},(-j)} \right)^2}{\sum_{j=1}^{n_{\mathrm{val}}} \left(y^{\mathrm{val},(j)} - \bar{y}^{\mathrm{val}} \right)^2} \tag{11}$$

    - QQ-plot, rate of good classification, ...
  - Validation of the GP predictive variance:
    - Computation of the **Predictive Variance Adequacy** (PVA) [Bac13]

$$\mathrm{PVA} = \left| \log \left(\frac{1}{n_{\mathrm{val}}} \sum_{j=1}^{n_{\mathrm{val}}} \frac{\left(y^{\mathrm{val},(j)} - \hat{y}^{\mathrm{val},(-j)} \right)^2}{\widehat{\sigma^2}_{(-j)}} \right) \right| \tag{12}$$

    - Comparison of theoretical levels of GP-based confidence intervals and observed levels
    - Many other metrics can be considered for validation [DILGM22]
- Validation based on subsampling techniques
  - Computation of Q^2 using **kernel herding** [FIM+22]

Step 4

Step 4: Identification of penalizing configurations

- Identification of the penalizing values wrt. the QoI
  - Goal: perform an uncertainty propagation with the GP surrogate model in order to compute

$$\widehat{P}(\mathsf{X}_{\mathrm{pen}}) = \mathcal{P}(Y_{\mathrm{GP}}(\mathsf{X}_{\mathrm{exp}}, \mathsf{X}_{\mathrm{SII}}) > \widehat{q}_\alpha(Y) \mid \mathsf{X}_{\mathrm{pen}} = \mathsf{x}_{\mathrm{pen}}) \tag{13a}$$

$$= \ldots \text{(more details in [MIC22])} \tag{13b}$$

$$= 1 - \int_{\widetilde{\mathcal{X}}_{\mathrm{exp}}} \Phi\left(\frac{\widehat{q}_\alpha - \mu_{\widehat{Y}}(\mathsf{x})}{\sigma_{\widehat{Y}}(\mathsf{x})}\right) \mathrm{d}P_{\widetilde{\mathsf{X}}_{\mathrm{exp}}}(\widetilde{\mathsf{x}}_{\mathrm{exp}}) \tag{13c}$$

  where $\widetilde{\mathsf{X}}_{\mathrm{exp}} = \{\mathsf{X}_{\mathrm{exp}} \cup \mathsf{X}_{\mathrm{SII}}\} \setminus \mathsf{X}_{\mathrm{pen}}$
  - Assumption: $\widetilde{\mathsf{X}}_{\mathrm{exp}}$ and $\mathsf{X}_{\mathrm{pen}}$ are **independent**
  - In practice ➜ intensive Monte Carlo sampling to estimate this multidimensional integral

oticscream

Numerical illustration with 'oticscream'

- oticscream: a Python module based on OpenTURNS
  - A full Python package that uses/relies on OpenTURNS
  - Implements the full methodology proposed in [MIC22] but with a few more extensions!
  - Available ➜ https://github.com/vchabri/oticscream

Numerical illustration with ‘oticscream’

- **Let’s imagine a role-playing game!**
  - You’re an R&D engineer. Your colleague physicist gives you:
    - A Monte Carlo (i.i.d.) sample of size $n = 250$
    - A list of input variables (15 random ones vs. 5 scenario parameters)
    - A target risk measure for its studies: $q_{0.90}(Y)$

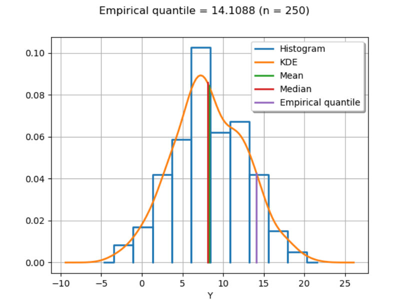
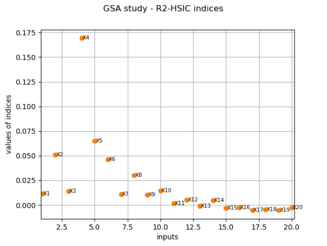


Figure 3: Empirical distribution of the output.

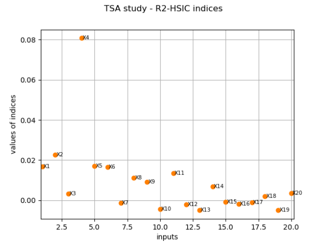
- **Step 1:**
  - Estimate the QoI: $\widehat{q}_{0.90}(Y) \approx 14.11$

Numerical illustration with ‘oticscream’

❑ Step 2: perform GSA and TSA using HSIC-based indices



(a)



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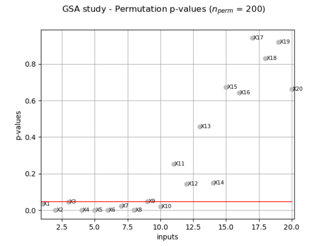

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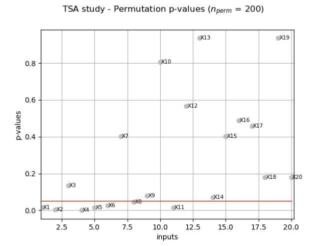
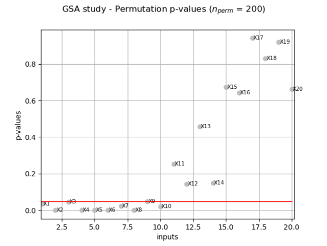


(d)

Numerical illustration with ‘oticscream’

- Step 2: perform GSA and TSA using HSIC-based indices



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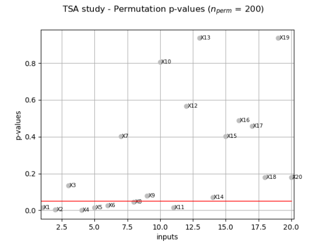

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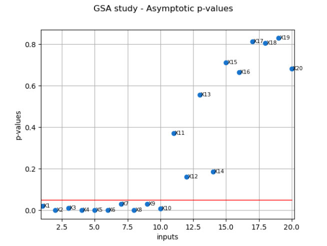

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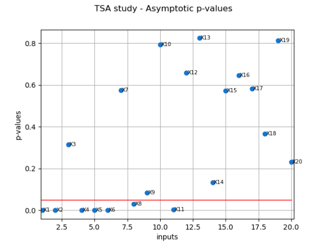
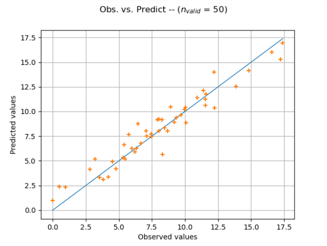


(h)

- Step 3: you build the GP metamodel and validate it



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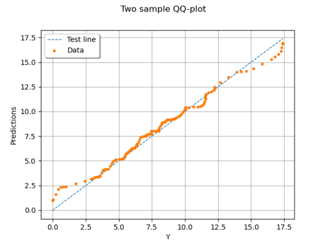

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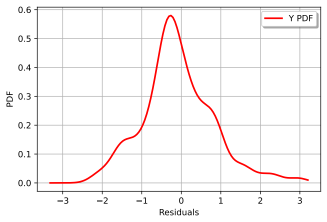
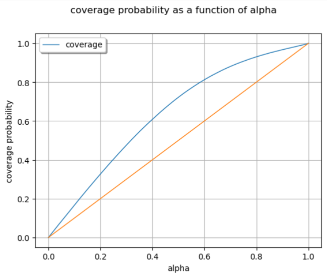
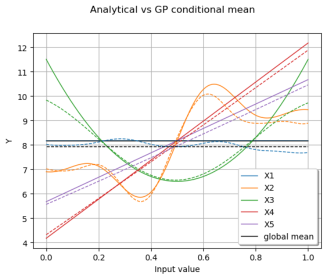




- Step 4: use the conditional GP metamodel



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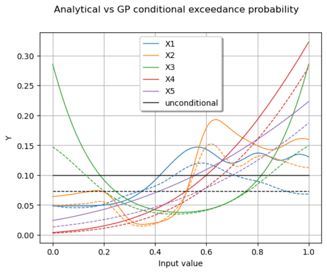

(n)

Conclusion

Conclusion

- Summary
  - Main goal: find penalizing configurations for some scenario parameters
  - ICSCREAM: a four-step methodology
  - Uses both state-of-the-art UQ techniques and more refined tools

    ➜ Talk by M. Keller and F. Delcoigne (JU-OT 2025)

Conclusion

❑ Limitations and perspectives

- ➤ This is a first attempt to “automate” a recipe for finding penalizing values in a **given-data** context!
- ➤ **However**, in practice, it is difficult to provide global guarantees
  ➜ every step needs to be carefully controlled in practice
- ➤ About GSA / TSA using HSIC:
  - Use advanced multiple-testing strategies for robust selection
  - Add and use HSIC-ANOVA indices more adapted to ranking purposes!
- ➤ About metamodel training and validation:
  - Gu’s robust approaches for parameter estimation in GP regression [GWB18]
  - Take benefit from the large panel of validation metrics [DILGM22]
  - Work on kernel-herding-based validation metrics
- ➤ Enhance the testing and documentation of the Python module!
- ➤ Publish it on PyPI!

Thank your for your attention!

Any question?

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