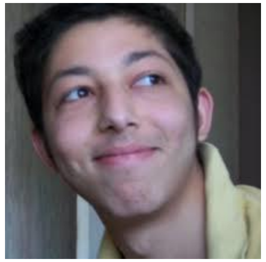
2 APPLICATIONS OF THE STEPWISE UNCERTAINTY REDUCTION STRATEGY FOR EXCURSION SET ESTIMATION

Delphine Sinoquet[1]

Reda El Amri[1], Celine Helbert[2], Morgane Menz[1], Miguel Munoz Zuniga[1], Clémentine Prieur[3]





[1] IFP Énergies Nouvelles
[2] École Centrale de Lyon
[3] Université Grenoble Alpes, INRIA

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CONTEXT : ROBUST/RELIABLE CONCEPTION

Uncertain variables
u

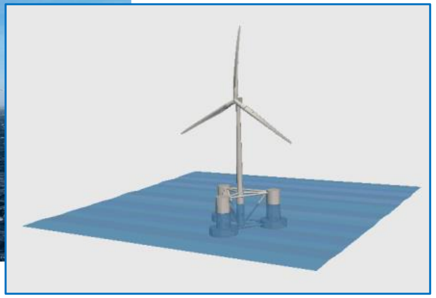
« Controlable » variables
= design variables x → **Black-box simulator** →

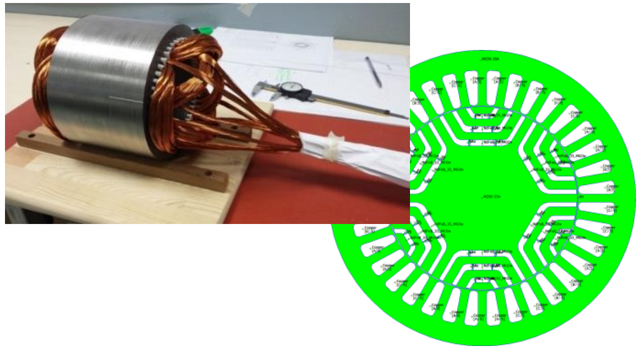
$f(x,u)$ Quantities
$g(x,u)$ of interest

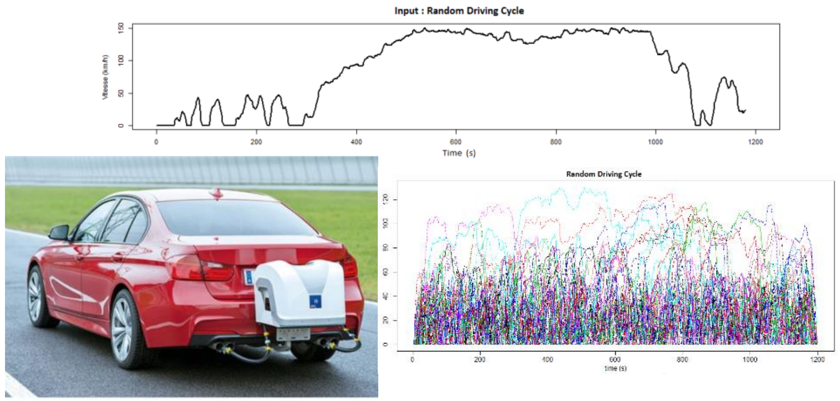
minimize/maximize
constraints

Applications for optimized design

- Reliability w.r.t environmental conditions (*e.g.* wind, wave)
- Robustness to dispersions of design variables (manufacturing), to component characteristics (*e.g.* magnetic properties of magnets), …







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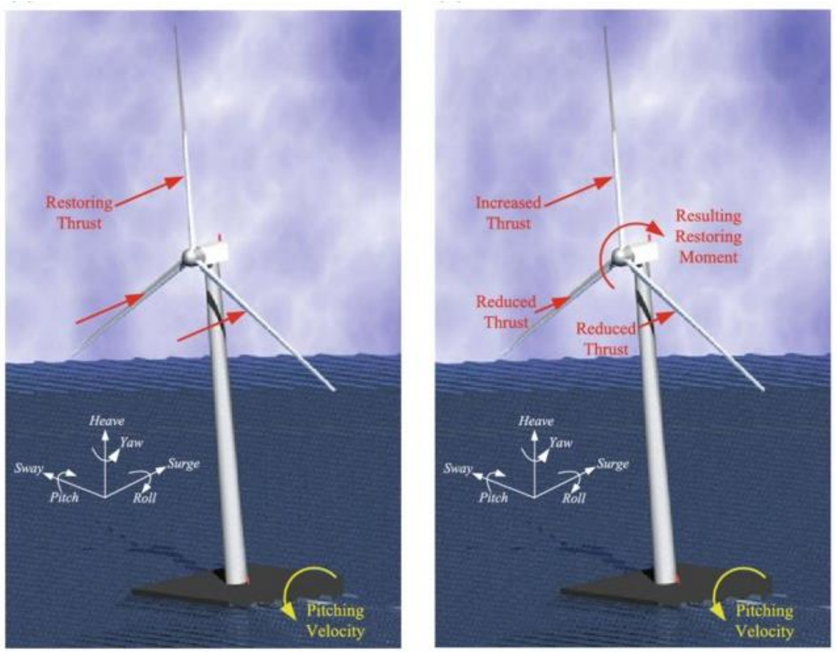
Feasible designs for complex optimal design problems

- **Pre-calibration** *(PhDs C. Duhamel, A. Hirvoas)* for wind turbine
  find a set of structure parameters x, such that,
  for environmental conditions $\mathbf{U}$

$$\Gamma^{\star} := \left\{ x \;\; s.t.\; \mathbb{P}_{\mathbf{U}}\left(\left\| D^{sim}(\mathbf{U}, x) - D^{meas}(\mathbf{U}) \right\| < seuil \right) > 1 - \alpha \right\}$$



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APPLICATIONS OF EXCURSION SET ESTIMATION

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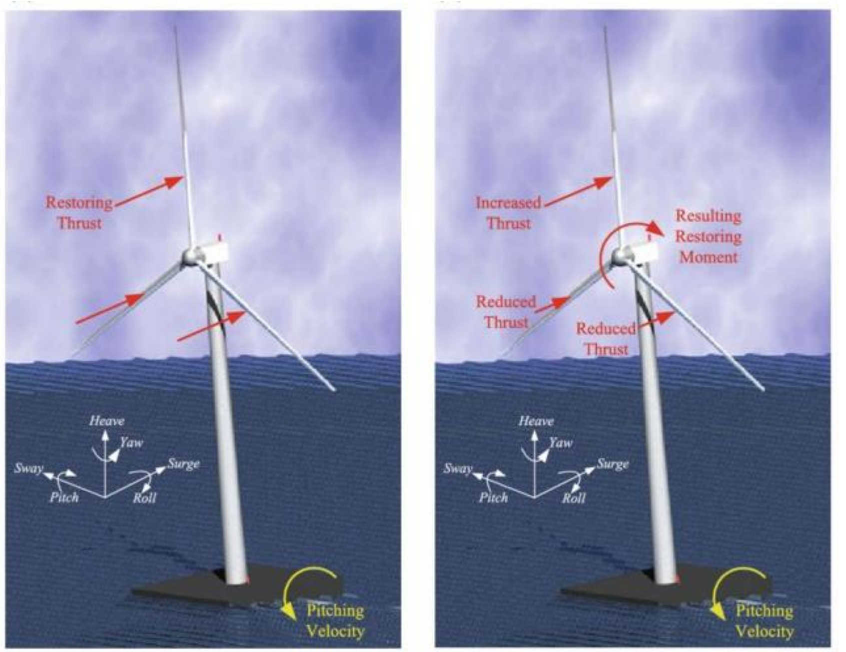
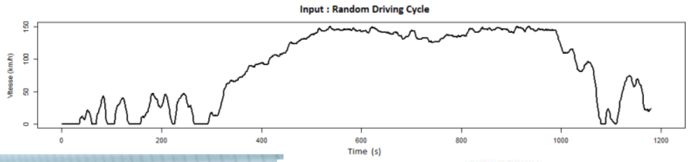
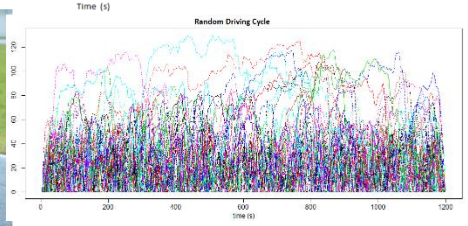
- **Robust tuning of control systems**
  - **for offshore wind turbines**: avoid an unstable float-push system while staying above a minimum production level *(ANR Samourai)*
  - **for the de-pollution system of a vehicle** *(PhD. R. El Amri)*

$$\Gamma^{\star} := \{x \ \ s.t.\ \mathbb{E}_{\mathbf{U}}(g_1(x,U)) \leq s\}$$







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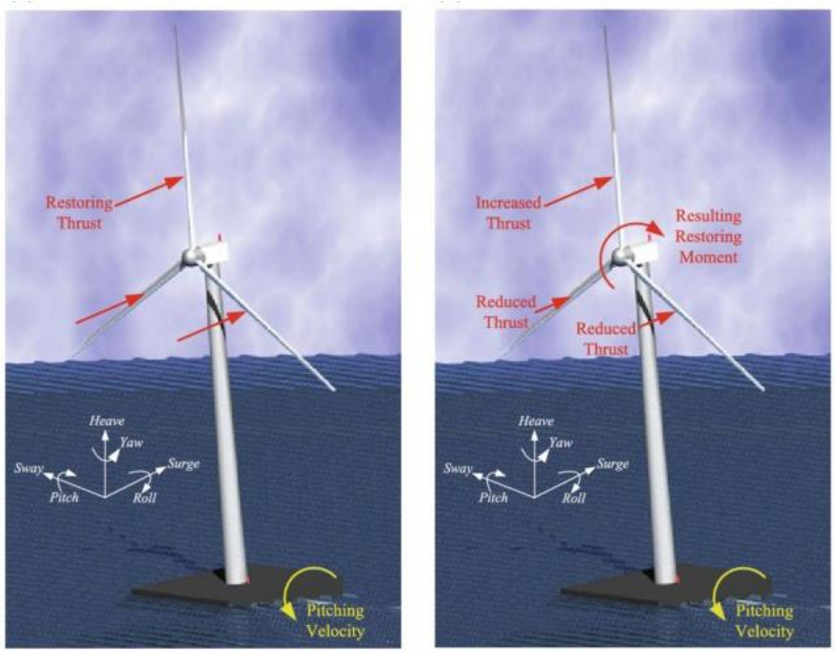
APPLICATIONS OF EXCURSION SET ESTIMATION



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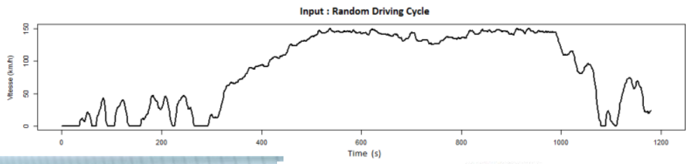

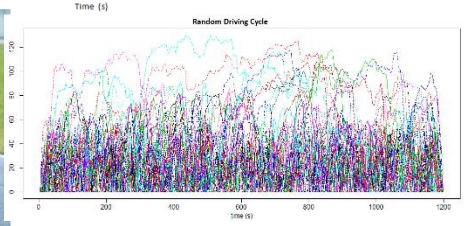

Feasible input set for complex simulators

- **Hidden constraints leading to simulation crashes**
  $$\Gamma^{*} = \{x \in \Omega : f(x) \neq NAN\} = \{x \in \Omega : \mathbb{1}_{f(x)\neq NAN} = 1\}$$

(ANR Samourai)

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OUTLINE

- Robust tuning of control systems
  for the de-pollution system of a vehicle (PhD. R. El Amri)

- Feasible input set for complex simulators
  hidden constraints leading to simulation crashes

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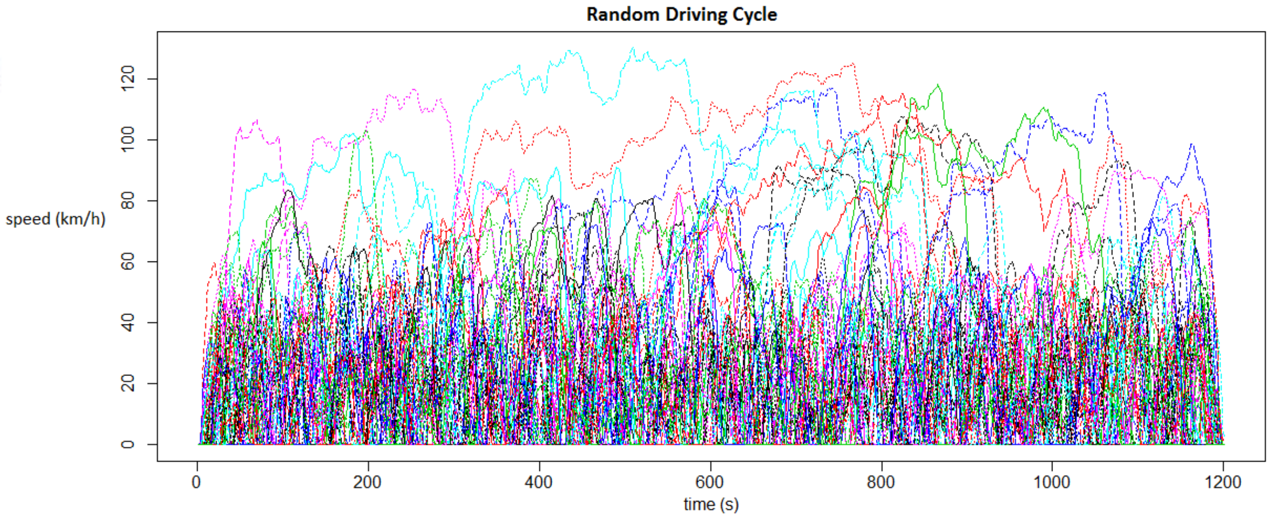
ROBUST TUNING OF CONTROL SYSTEMS

IFPEN test case : control strategy for an automotive depollution system

- $\mathbf{v}^1, \ldots, v^{100}$ random driving cycles.



Control parameters of the depollution system
(SCR: Selective Catalytic Reduction)

- $\mathrm{NH}_3^{\max}$ function of x_1 and x_2, $D = [0, 0.6]^2$

$$\Gamma^* = \{\mathbf{x} = (x_1, x_2) \in D \ : \ \mathbb{E}[\mathrm{NH}_3^{\max}(\mathbf{x}, \mathbf{V})] \leq s\}.$$

Ammoniac spike must be smaller than **30** ppm

The model is expensive to evaluate (chemical kinetic model).

El Amri et al, Data-driven stochastic inversion via functional quantization, Statistics and Computing, **30**, pages 525–541(2020)
El Amri et al, Set inversion under functional uncertainties with Gaussian Process Regression defined in the joint space of control and uncertain, hal-02986558

ROBUST INVERSION WITH FUNCTIONAL INPUTS

$$\Gamma^* \quad := \quad \{\mathbf{x} \in D \ s.t. \ f(x) = \mathbb{E}[g(\mathbf{x}, \mathbf{V})] \leq s\}$$

Objective:
estimate $\Gamma^* \subset \mathbb{R}^p$ from model evaluations.

Issues :

- each evaluation $f(\mathbf{x})$ requires the estimation of $\mathbb{E}[g(\mathbf{x}, \mathbf{V})]$,
- $\mathbf{V}$ is known through κ realizations $\mathbf{v}^1, \ldots \mathbf{v}^\kappa$,
- each evaluation $g(\mathbf{x}, \mathbf{v})$ is costful.

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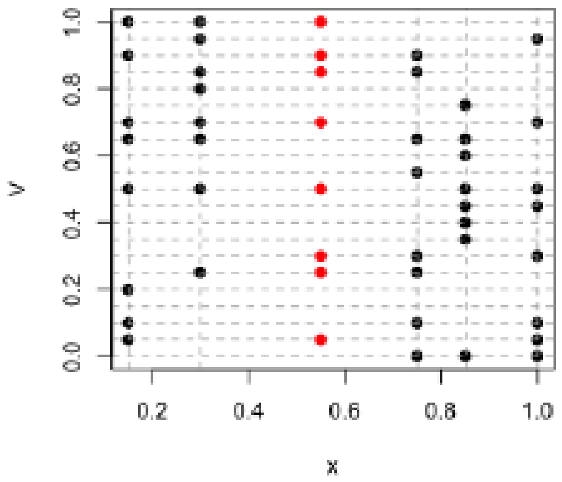
TWO STRATEGIES

$$\Gamma^* := \{\mathbf{x} \in D \ s.t. \ f(x) = \mathbb{E}[g(\mathbf{x}, \mathbf{V})] \leq s\}$$

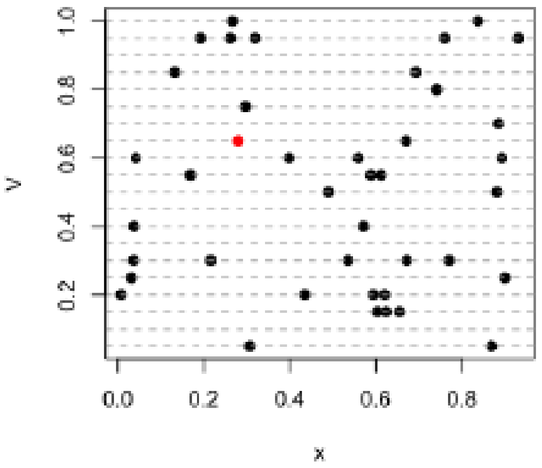
Strategy I

- Build a meta-model of $f(x)$
- Choose $x_{n+1} \in D$,
- Estimate $f(\mathbf{x}_{n+1}) = \mathbb{E}[g(\mathbf{x}_{n+1}, \mathbf{V})]$ with l evaluations of $g(\mathbf{x}_{n+1}, .)$ selected by quantization in ($\mathbf{v}^1$, $\mathbf{v}^2$,…, $\mathbf{v}^K$)



Strategy II

- Build a meta-model of $g(x, \boldsymbol{V})$
- Choose $(x_{n+1}, \mathbf{v}^{n+1})$,
- Evaluate $\mathbb{E}[\hat{g}(\mathbf{x}_{n+1}, \mathbf{V})]$ at this new point



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DIMENSION REDUCTION OF FUNCTIONAL VARIABLES

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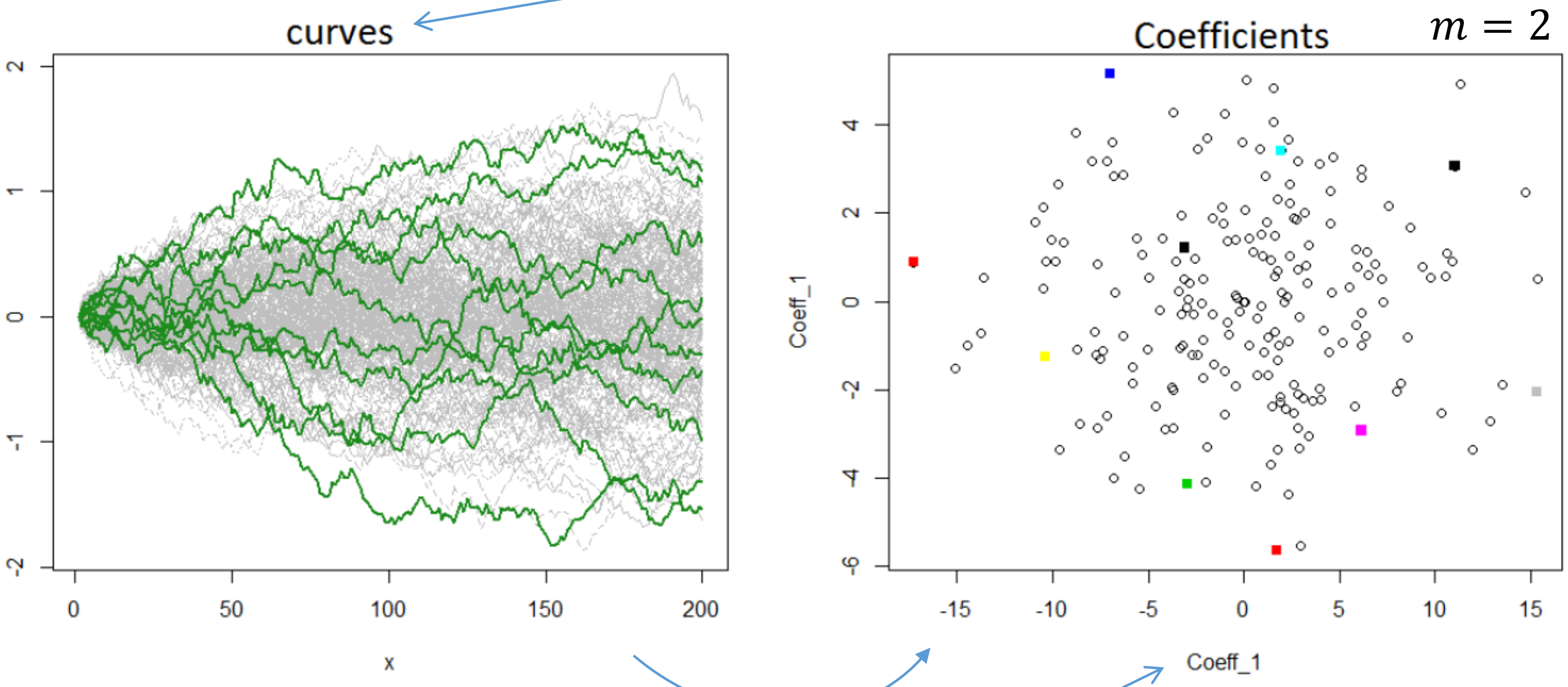

Karhunen-Loève (KL) expansion

$$V(t) = \mu_{\mathbf{V}}(t) + \sum_{k=1}^{m} \sqrt{\lambda_k} \eta_k \phi_k(t).$$

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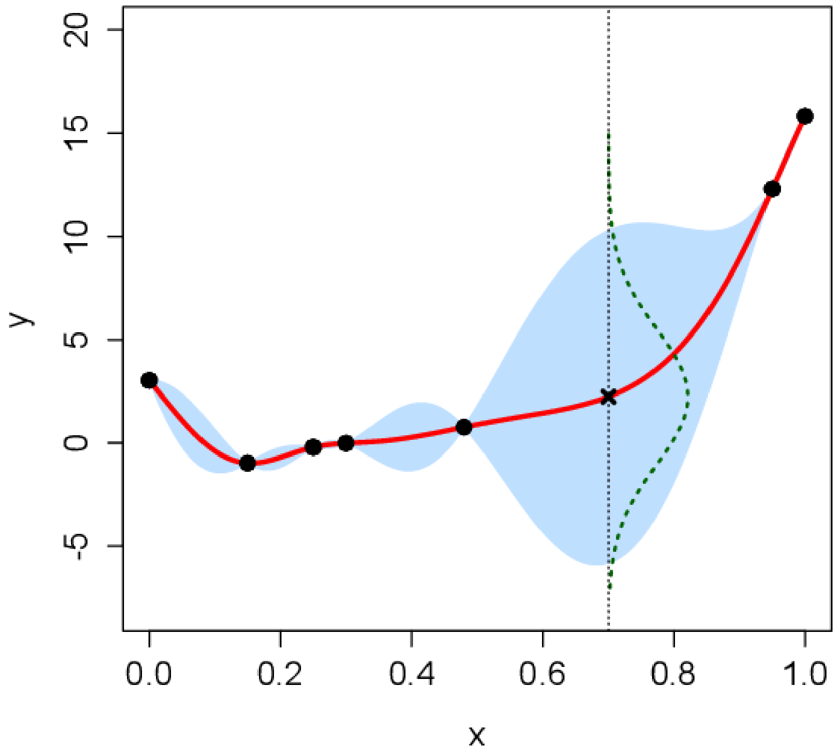
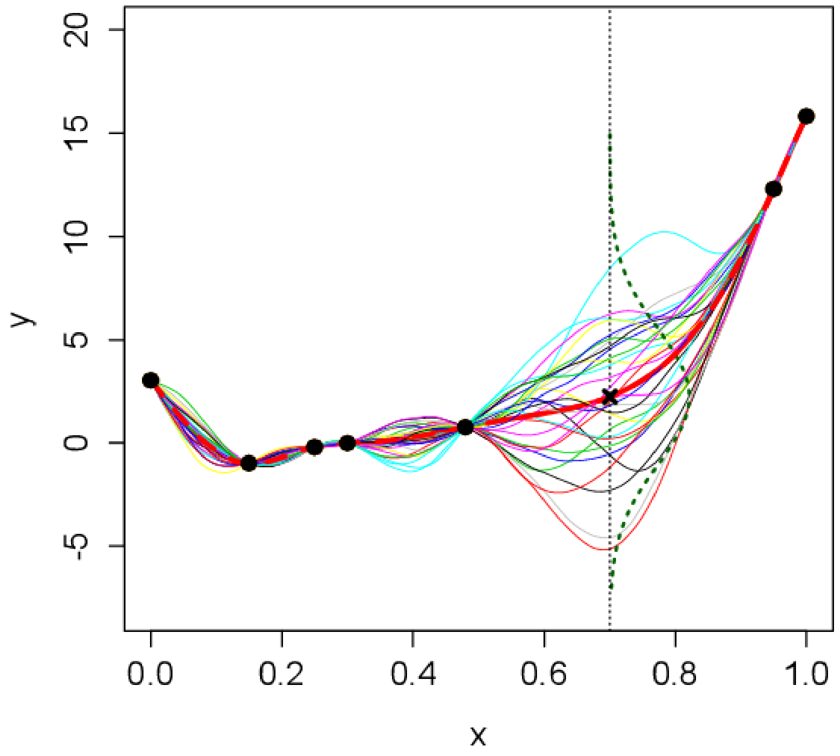
GAUSSIAN PROCESS METAMODELING





Meta-models based on **Gaussian Process** that provides **uncertainty estimation**

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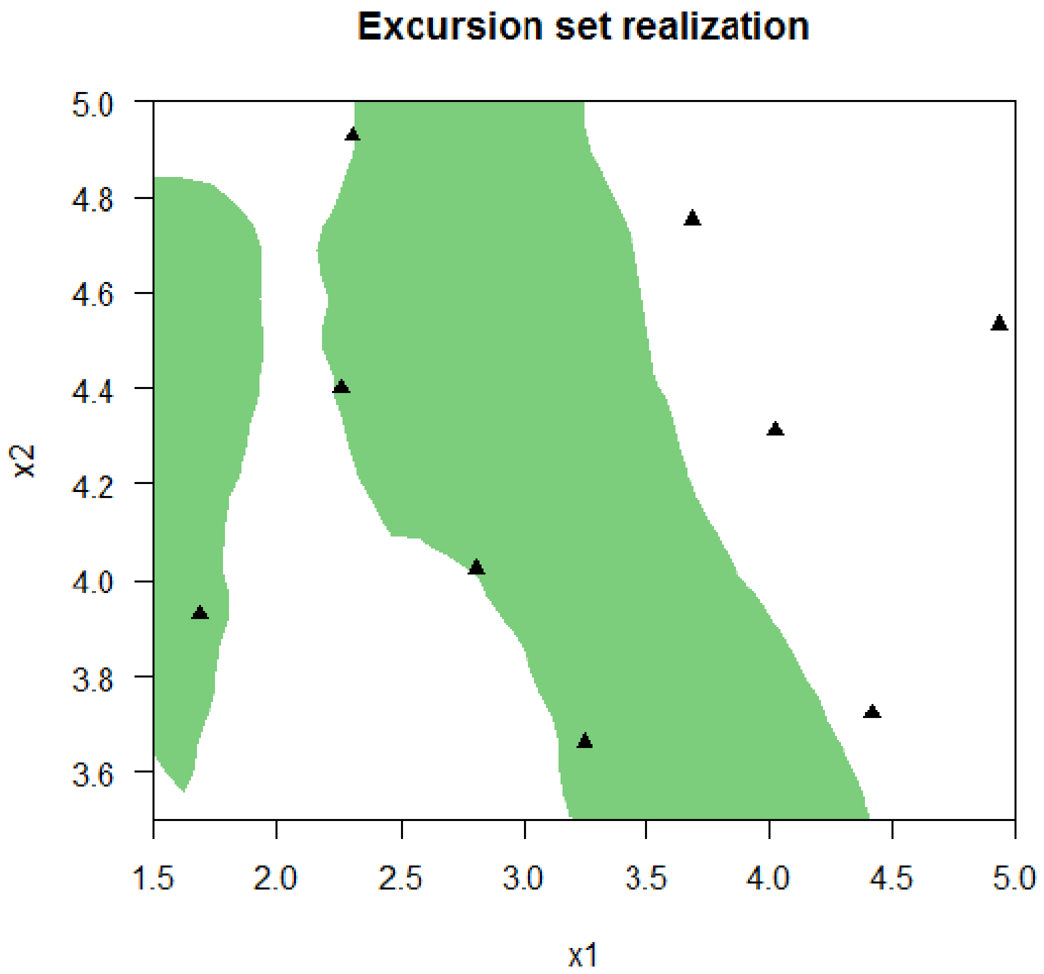
GP INDUCES RANDOM EXCURSION SET

$$\Gamma := \{x \in D: Z_x | Z_{\chi_n} \leq s\}$$



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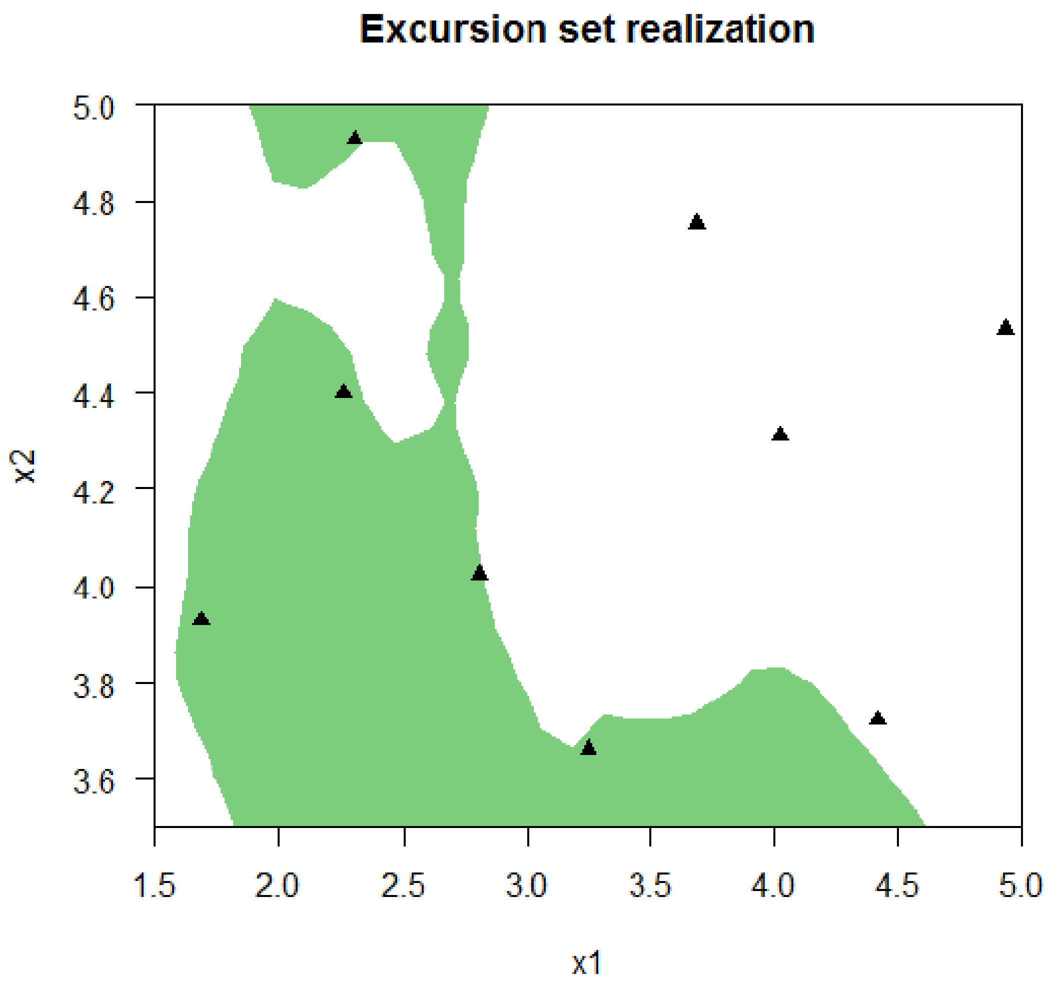

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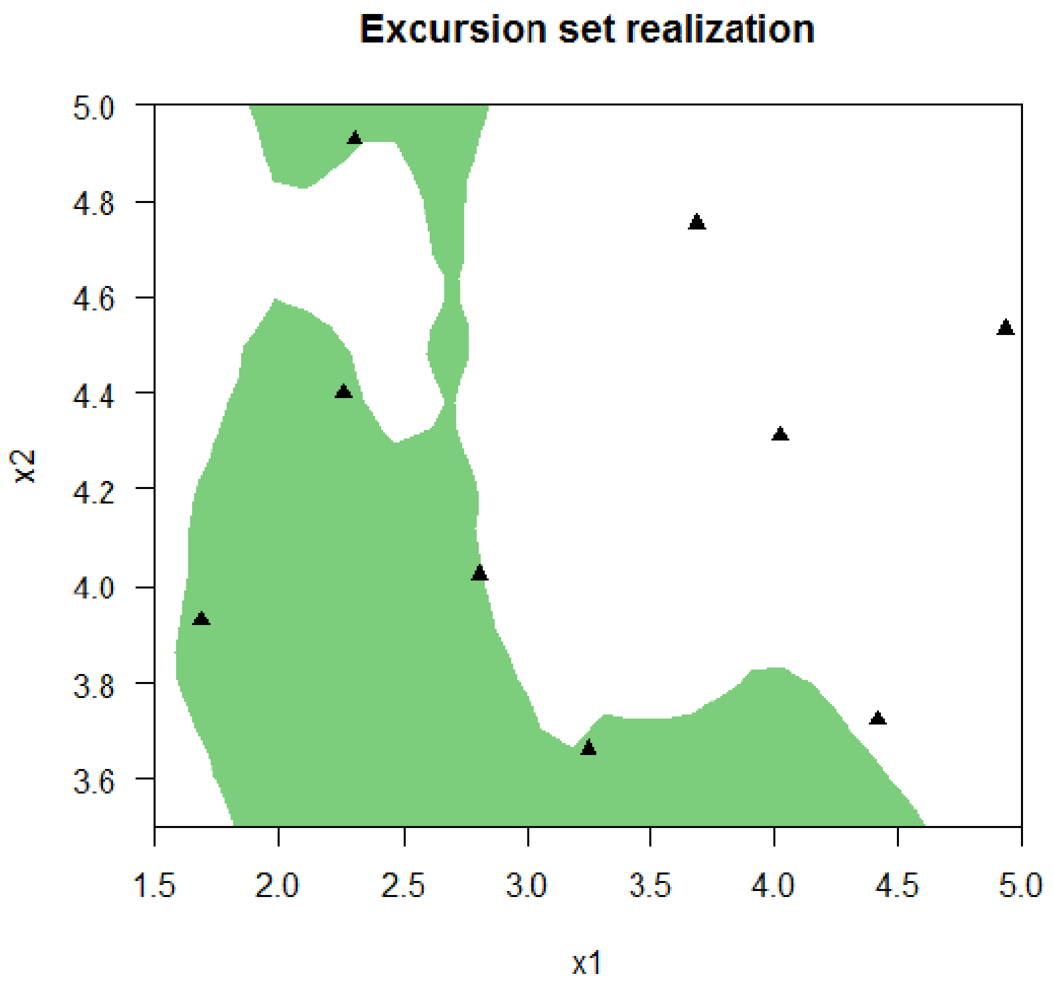
GP INDUCES RANDOM EXCURSION SET

How to summarize the distribution on sets?

- **Estimate** Γ^* with Expectation of random closed sets (Molchanov, 2006)



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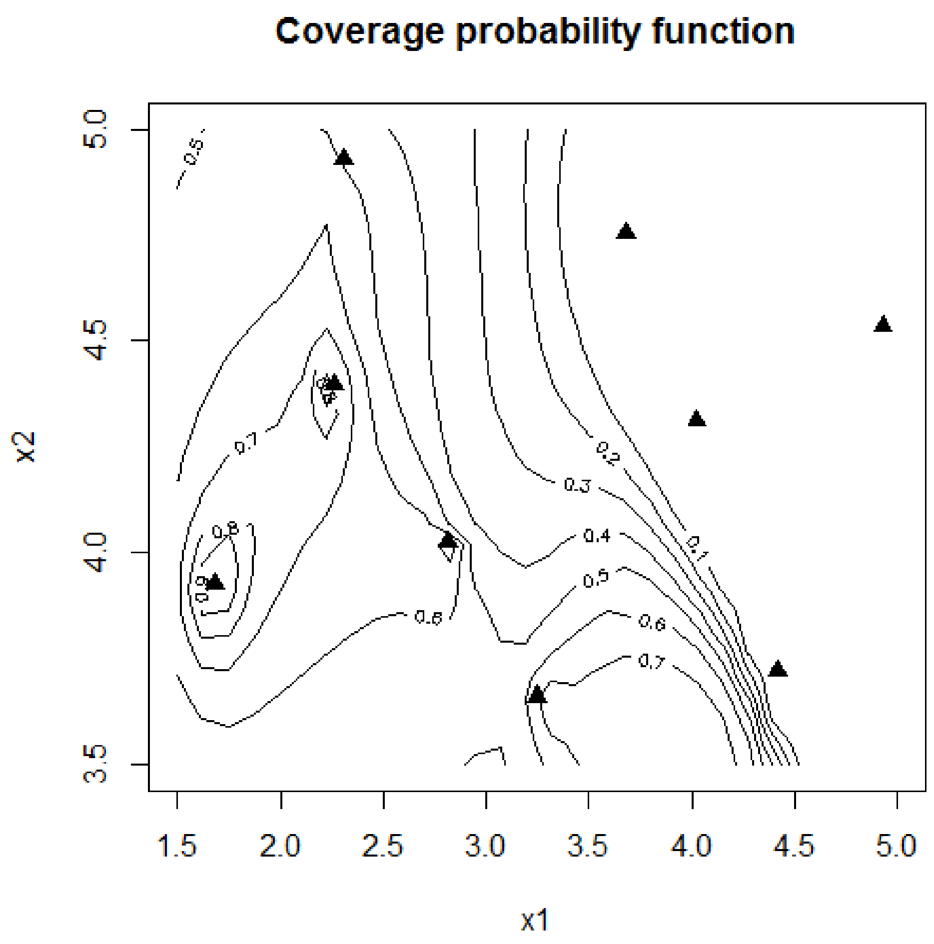
- The coverage probability of Γ is given by

$$
\begin{aligned}
p_n(x) &= \mathbb{P}(\, Z_n(x) \leq s \mid \mathcal{X}_n, \mathcal{Y}_n \,) \\
&= \phi\left(\frac{c - m_n(x)}{\sqrt{k_n(x,x)}}\right)
\end{aligned}
$$



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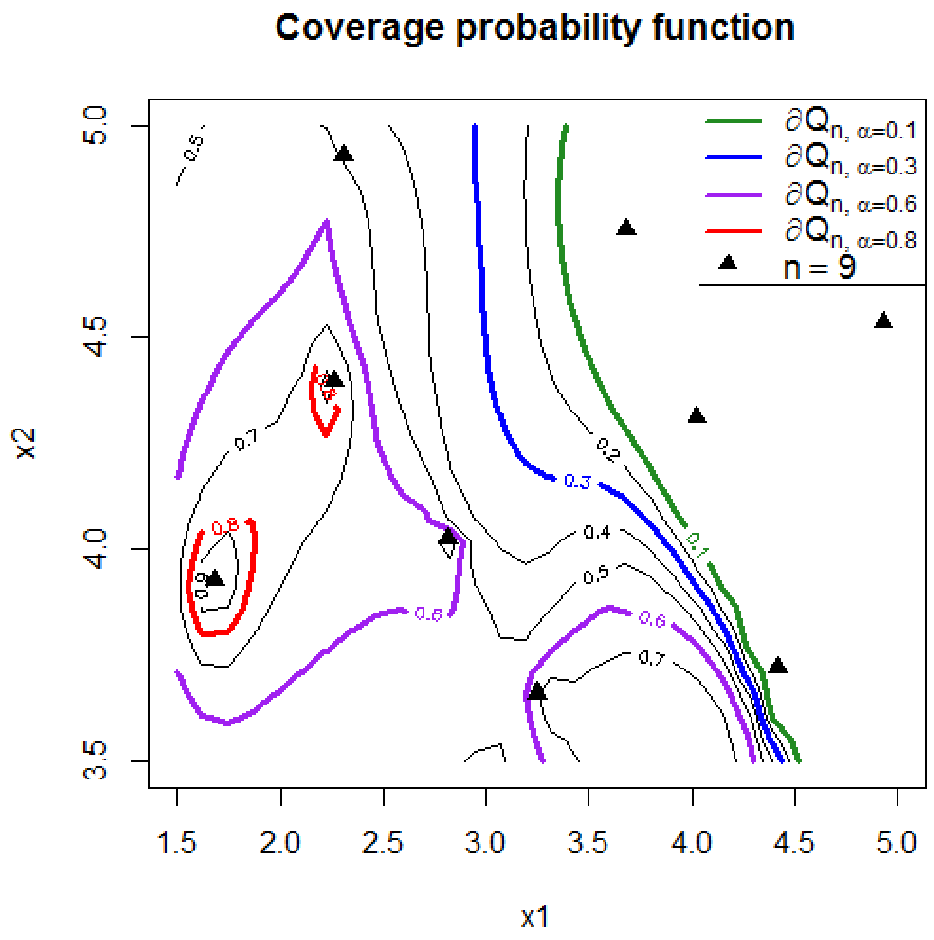
- It creates a family of sets $\boldsymbol{Q_{n,\alpha}} = \{\boldsymbol{x} \in \mathbb{X}: \boldsymbol{p_n}(\boldsymbol{x}) \geq \boldsymbol{\alpha}\}$



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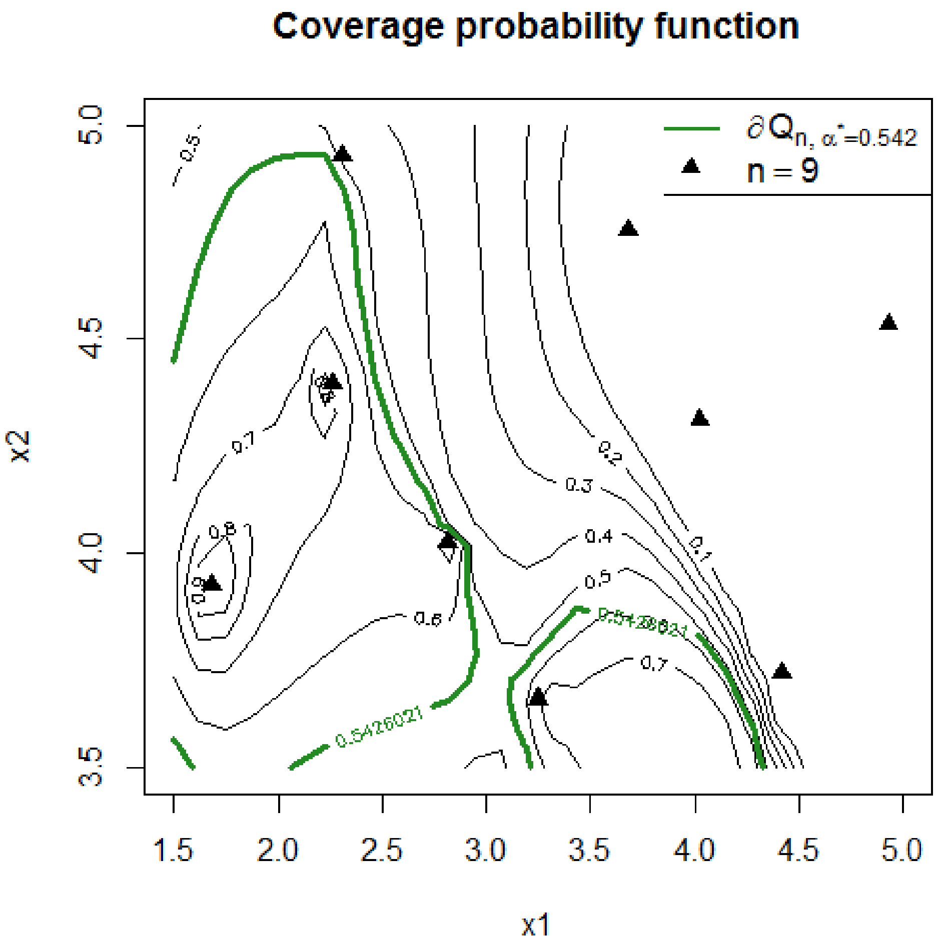
  α^* chosen such that $\mathbb{E}(\mu(\Gamma)) = \mu(Q_{n,\alpha^*})$



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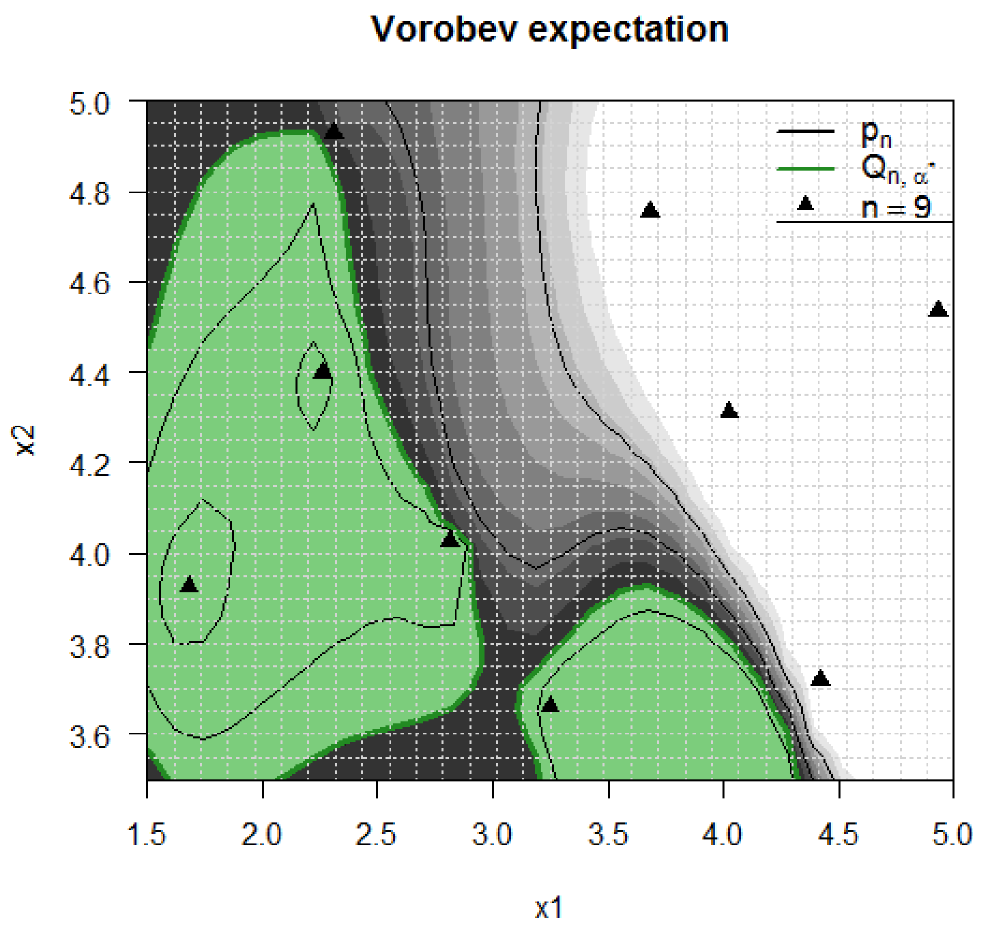

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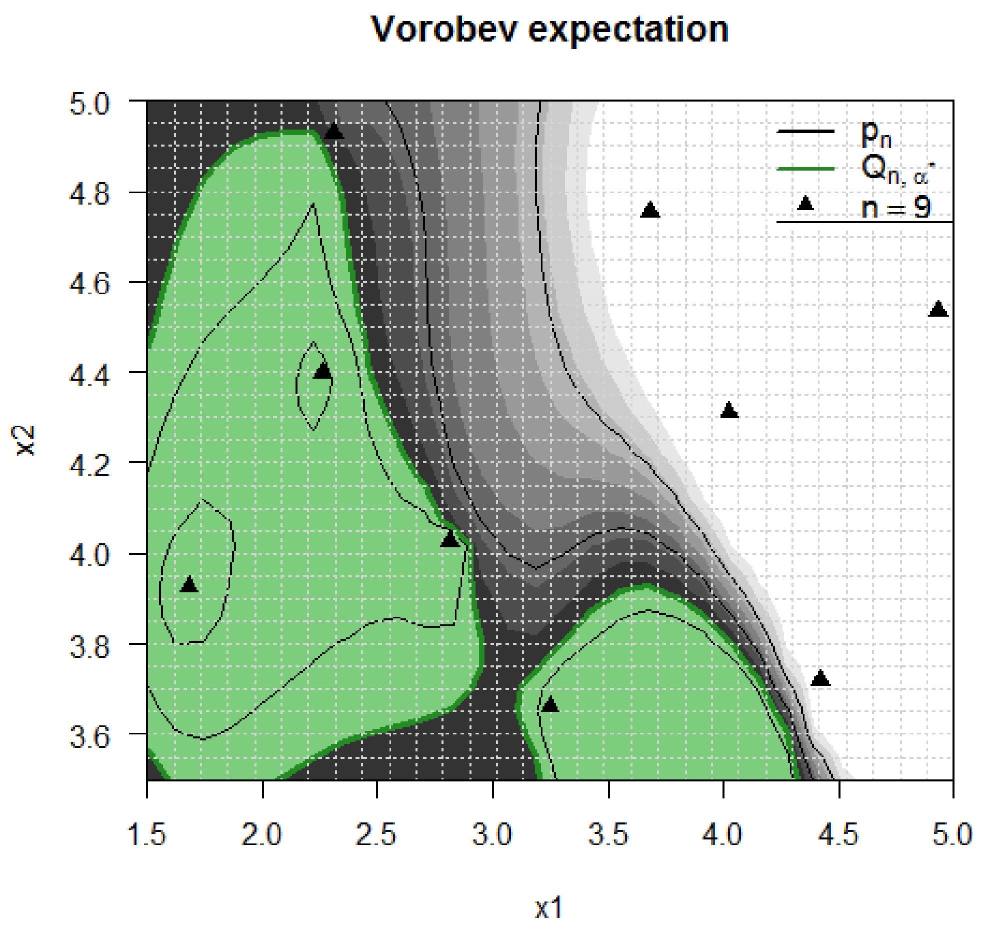
- **Vorob'ev deviation :** $\boldsymbol{Var_n(\Gamma)} = \mathbb{E}\left(\boldsymbol{\mu}(\boldsymbol{Q_{n,\alpha^*}\Delta\Gamma})\right)$



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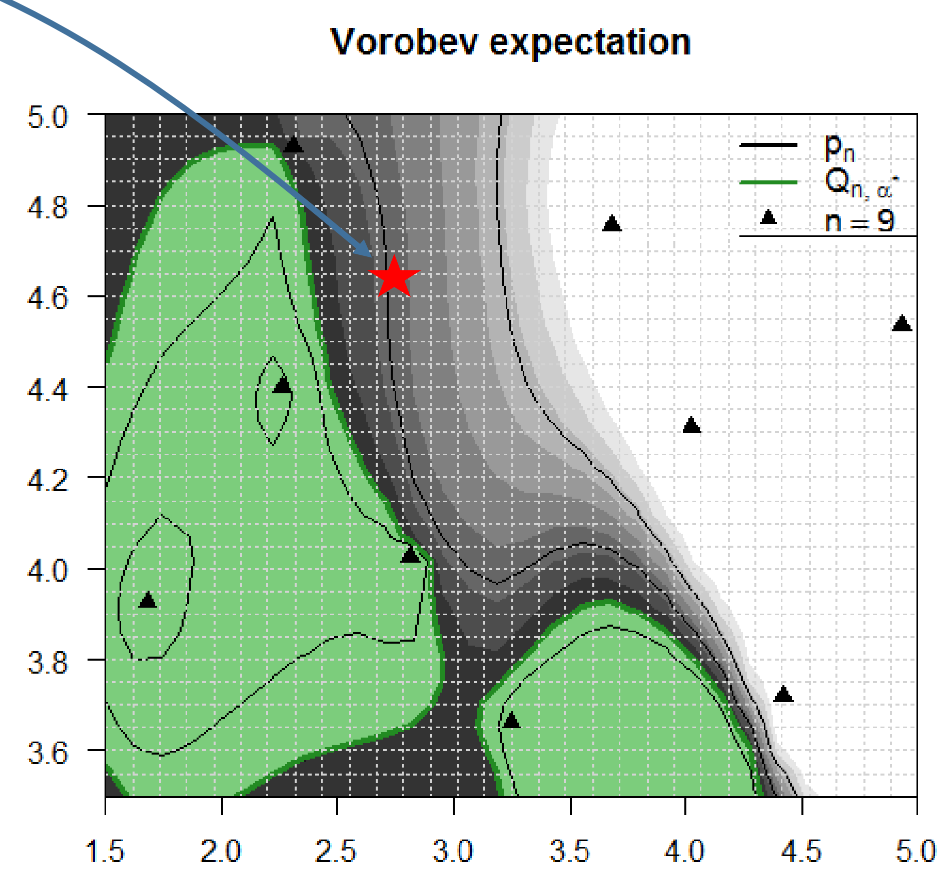
STEPWISE UNCERTAINTY REDUCTION BASED ON VOROB'EV THEORY

- Choose next point x_{n+1} to reduce expected uncertainty H_{n+1} on the future model:

$$\boldsymbol{x}_{n+1} = \underset{x \in D}{argmin}\; \mathbb{E}_{n,Y_{n+1}(x)}[H_{n+1}]$$

Uncertainty function : Vorob'ev deviation

$$\mathcal{H}_n^{\text{uncert}} = \mathbb{E}_n[\mu(Q_{\alpha_n^*} \Delta \Gamma)]$$



- Choose next curve
  (Strategy II)

$$\mathbf{V}_{(n+1)} \leftarrow \arg\min \mathbb{VAR}(Y^{n+1}_{\mathbf{x}_{(n+1)}})$$

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APPLICATION ON AN ANALYTICAL EXAMPLE WITH V A BROWNIAN MOTION

$$f : (\mathbf{x}, v) \mapsto \max_t v_t . |0.1 \cos(x_1 \max_t v_t) \sin(x_2).(x_1 + x_2 \min_t v_t)^2|. \int_0^T (30 + v_t)^{\frac{x_1 . x_2}{20}} \mathrm{dt},$$

Excursion set to retrieve

$$\Gamma^* := \{\mathbf{x} \in [1.5, 5] \times [3.5, 5] \ : \ f(\mathbf{x}) = \mathbb{E}[g(\mathbf{x}, \mathbf{V})] \leq c\}.$$

For the experiments we chose:

- a threshold $c = 1.2$,
- $\mathrm{card}(\Xi) = 200$,
- a constant mean function m, a Matérn 5/2 covariance kernel,
- an initial DoE of size $n = 30$,
- a KL truncation argument $m_{KL} = 2, 4, 8$.

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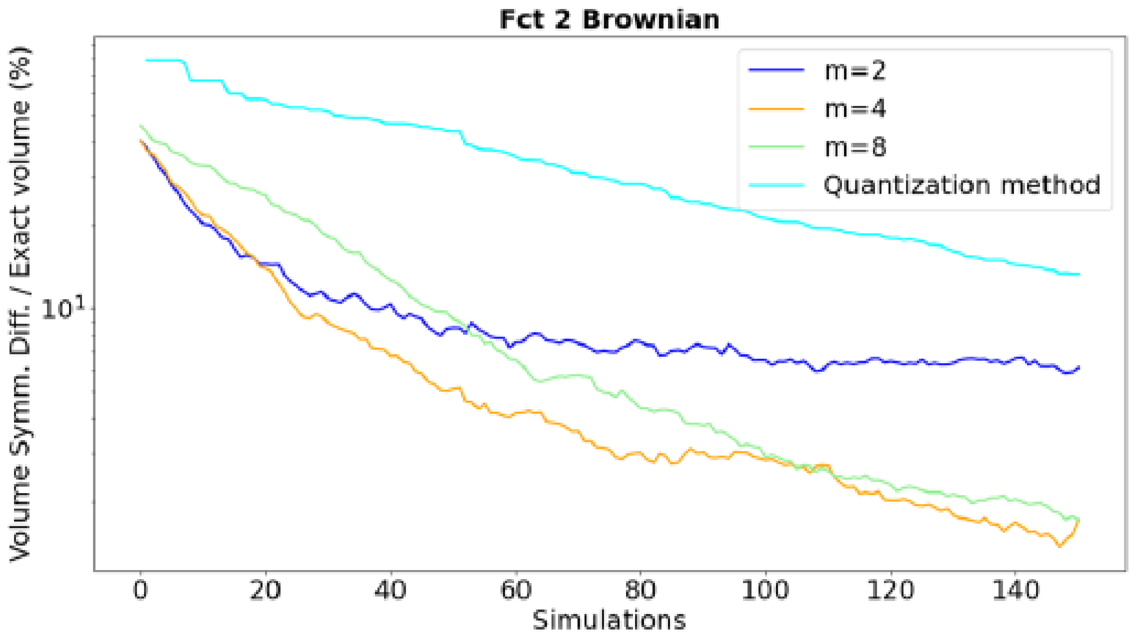
APPLICATION ON AN ANALYTICAL EXAMPLE WITH V A BROWNIAN MOTION

COMPARISON STRATEGY I (QUANTIZATION) AND STRATEGY II (MM IN JOINT SPACE)



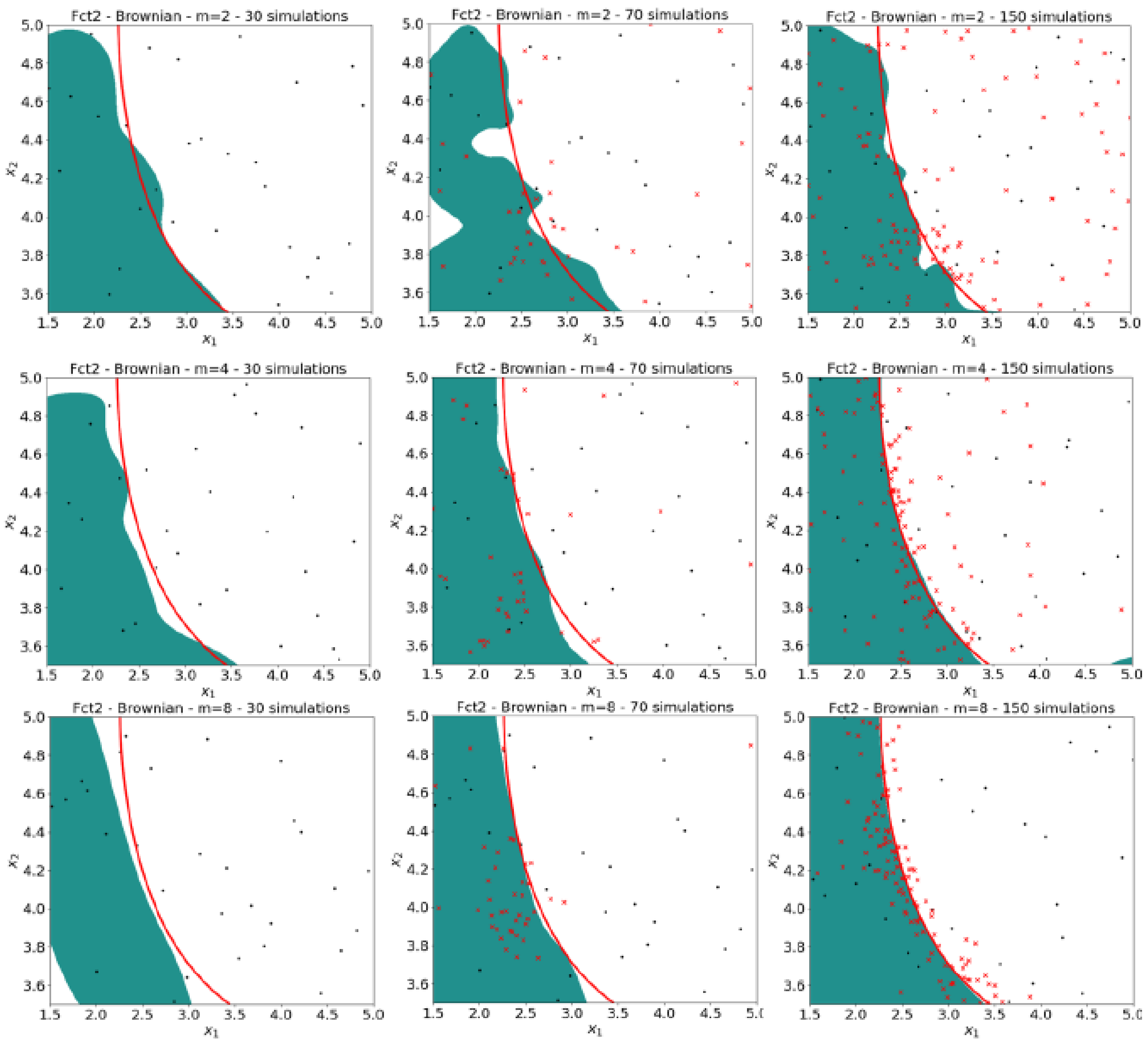
For the approach based on quantization, we chose an initial DoE in $\mathbb{X}$ of size 9. We have neglected the cost due to the quantization on this initial DoE. Indeed, around 20 points in average are required to estimate the expectation at each of these 9 points.

APPLICATION ON AN ANALYTICAL EXAMPLE WITH V A BROWNIAN MOTION

STRATEGY II (MM IN JOINT SPACE)

simulations →

KL truncation
Argument m ↓



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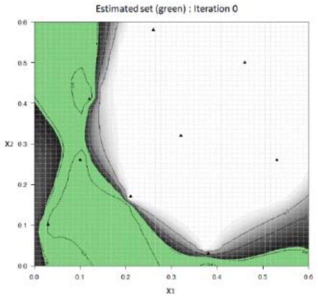
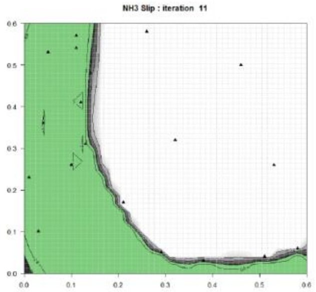
NUMERICAL RESULTS

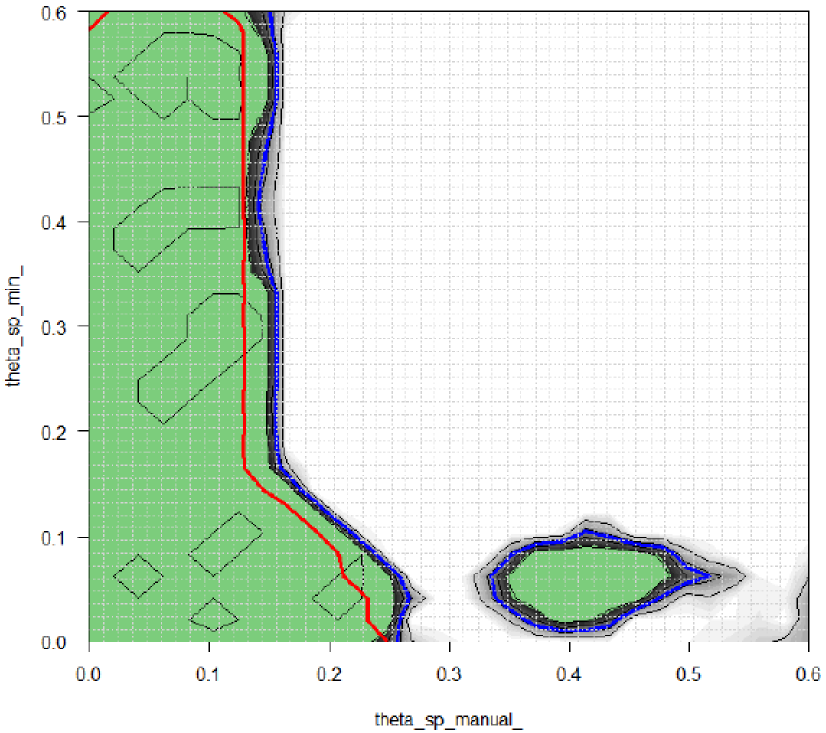
IFPEN test case: control strategy for an automotive NO_x depollution system

- $\mathrm{NH}_3^{\mathrm{out}}$ function of '*theta.sp.min*' and '*theta.sp.manual*', $\mathbb{X} = [0, 0.6] \times [0, 0.6]$,
- $n =$ **510** calls to f,

The estimated set by **Algorithm I (green set)** and **Algorithm II (red boundary)**







- Small dimension
  Algo II > Algo I
- Larger dimension
  Algo I > Algo II

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CONCLUSIONS FOR ROBUST INVERSION PART

- Two strategies for robust inversion strategy based on GP regression
  - MM in control space with expectation estimated by quantization (El Amri et al, 2020)
  - **MM in joint space of control and uncertain variables (**El Amri et al, 2021)
- Application to a depollution control system

Perspectives : phD thesis of Clément Duhamel (INRIA AIRSEA team, IFPEN)

- Extend strategies to correlated responses (multiple objectives)
- Deal with other measures of robustness : quantiles …
- Other applications : offshore wind turbines

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OUTLINE

- Robust tuning of control systems
  for the de-pollution system of a vehicle (PhD. R. El Amri)

- Feasible input set for complex simulators
  hidden constraints leading to simulation crashes

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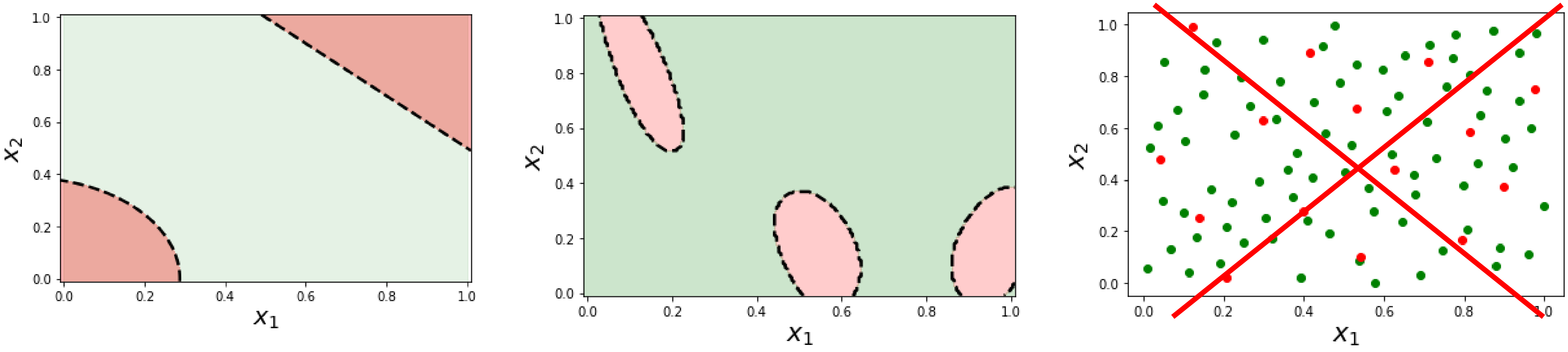
SECOND PART: LEARNING HIDDEN CONSTRAINTS

Context

- crash of expensive simulator

➔ **Learn hidden constraints with limited number of evaluations**



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PROBLEM STATEMENT

- f: a simulator with inputs $x \in \Omega \subset \mathbb{R}^m$ with simulation failures on Ω
- Our objective: determine the feasible set

$$\Gamma^* = \{x \in \Omega : f(x) \neq NAN\} = \{x \in \Omega : \mathbb{1}_{f(x) \neq NAN} = 1\}$$

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GAUSSIAN PROCESS BASED CLASSIFICATION

Learning hidden constraint is a binary classification problem

- We have binary observations $(\mathcal{X}, \mathcal{Y}) = (x_j, y_j)_{j=1,\ldots,n}$
  with $y_j = \mathbb{1}_{f(x_j) \neq NAN}$

- Objective: predict the probability of belonging to the failure/non-failure class

The formulation of the classification model is based on a Gaussian Process (GP) surrogate

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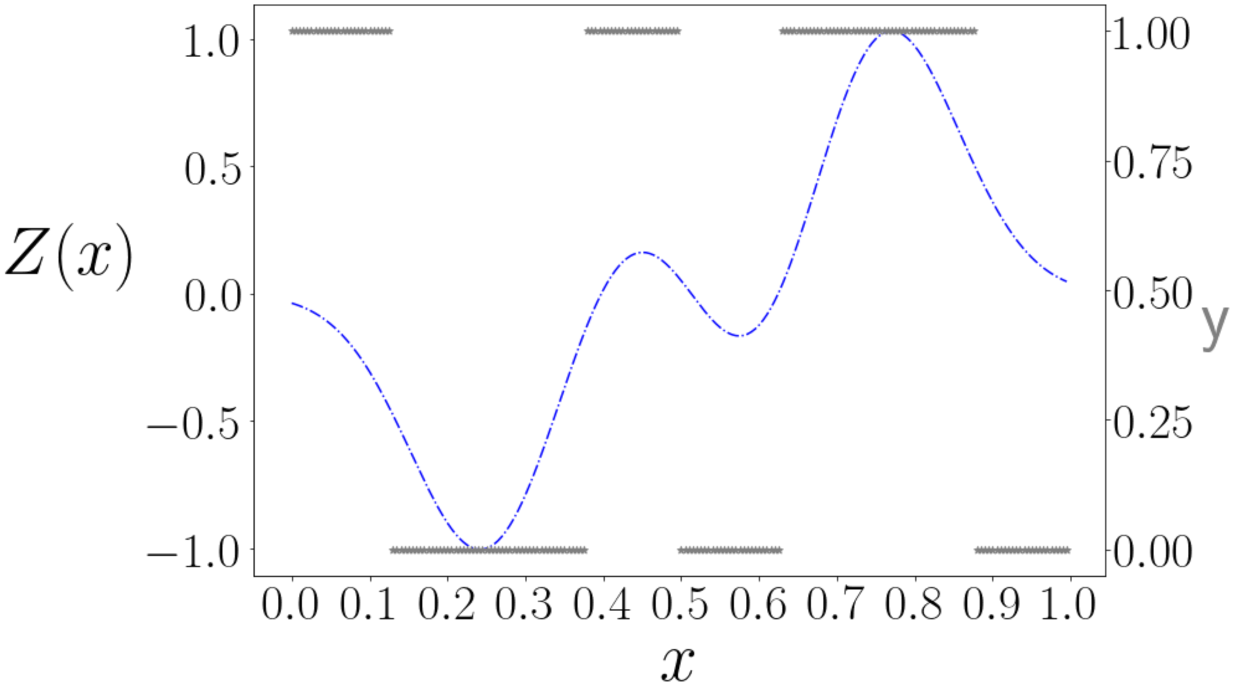
GAUSSIAN PROCESS CLASSIFIER (GPC) FORMULATION

- A GPC is based on a latent GP Z conditioned on observations $(\mathcal{X}, \mathcal{Y})$ (as $Z_n = (Z(x_1), ..., Z(x_n))$ is not available)



$Z(x) \sim GP(m_n(\cdot), k_n(\cdot,\cdot))$

$m_n(\cdot),\ k_n(\cdot,\cdot)$:

conditioned mean and kernel of $Z(x)$

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GAUSSIAN PROCESS CLASSIFIER (GPC) FORMULATION

The GPC model allows to predict the probability of non failure of a simulation:

$$p_n(x) = \mathbb{P}[Y_n(x) = 1] = \mathbb{P}[Y(x) = 1|\mathcal{X}, \mathcal{Y}]$$

This probability $p_n(x)$ is modeled on the basis of [Bachoc et al., 2020] by using the sign of the latent process Z:

$$p_n(x) = \mathbb{P}[\mathbb{1}_{Z(x)>0} = 1|x, \mathcal{X}, \mathcal{Y}] = \int_{\mathbb{R}^n} \phi_{\mathcal{Y}}^{Z_n}(z_n)\bar{\Phi}(\frac{-m_n(x, z_n)}{\sqrt{k_n(x)}})\, \mathrm{d}z_n$$

with $\phi_{\mathcal{Y}}^{Z_n}(z_n)$ the conditioned p.d.f of Z_n truncated to respect $sign(Z_n) = \mathcal{Y}$, and:

$$\bar{\Phi}(\frac{a}{b}) = \begin{cases} 1 - \Phi(\frac{a}{b}) & \text{si } b \neq 0 \\ \mathbb{1}_{-a>0} & \text{si } b = 0 \end{cases}$$

where Φ is the c.d.f. of the normal standard distribution.

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GAUSSIAN PROCESS CLASSIFIER (GPC) FORMULATION

Practical building of the GPC model $p_n(x)$ for any x:

- Optimization of the hyperparameters of the latent GP to maximize the likelihood: $\mathbb{P}[sign(Z_n) = \mathcal{Y}]$
- Generation of realizations $z_n^{(i)}$ of $Z_n | sign(Z_n) = \mathcal{Y}$
  ➜ Approximation of $p_n(x)$:

$$\widehat{p_n}(x) = \frac{1}{N} \sum_{i=1}^{N} \bar{\Phi} \left(\frac{-m_n(x, z_n^{(i)})}{\sqrt{k_n(x)}} \right)$$

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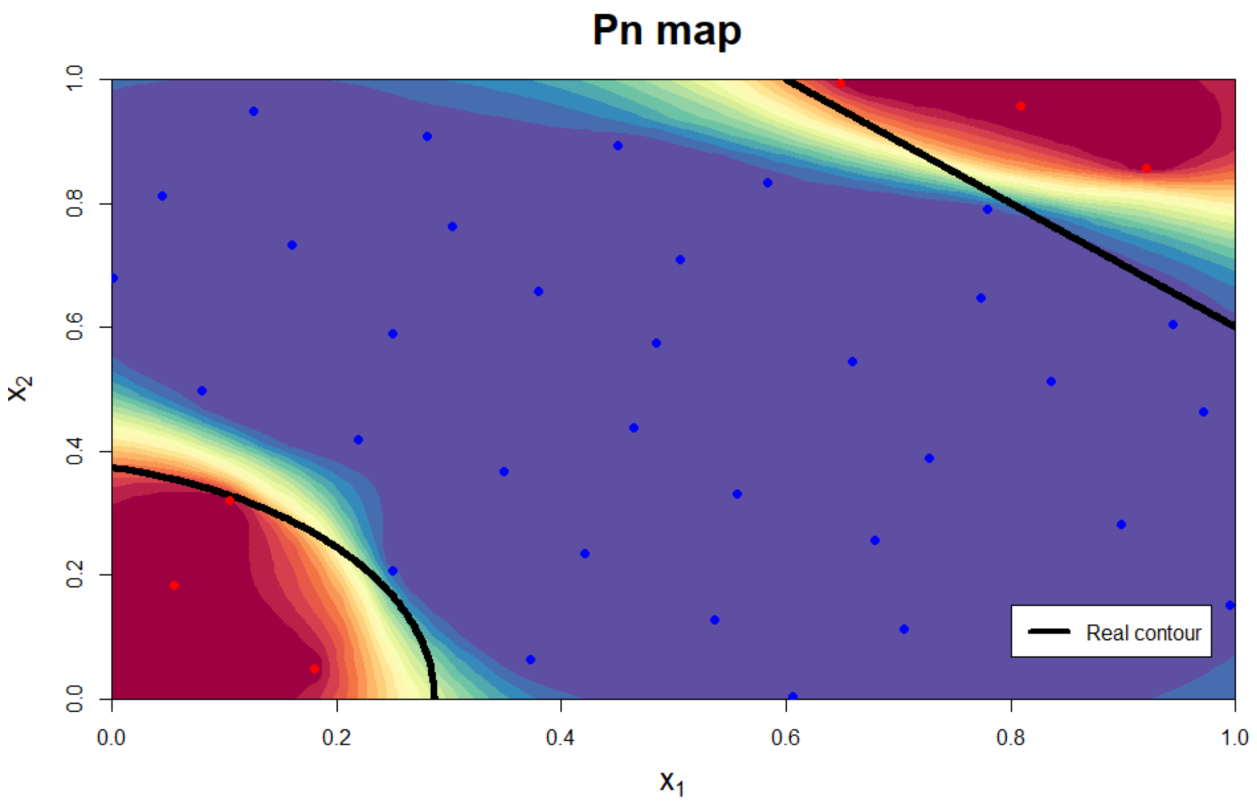
EXAMPLE OF A GPC FOR HIDDEN CONSTRAINT



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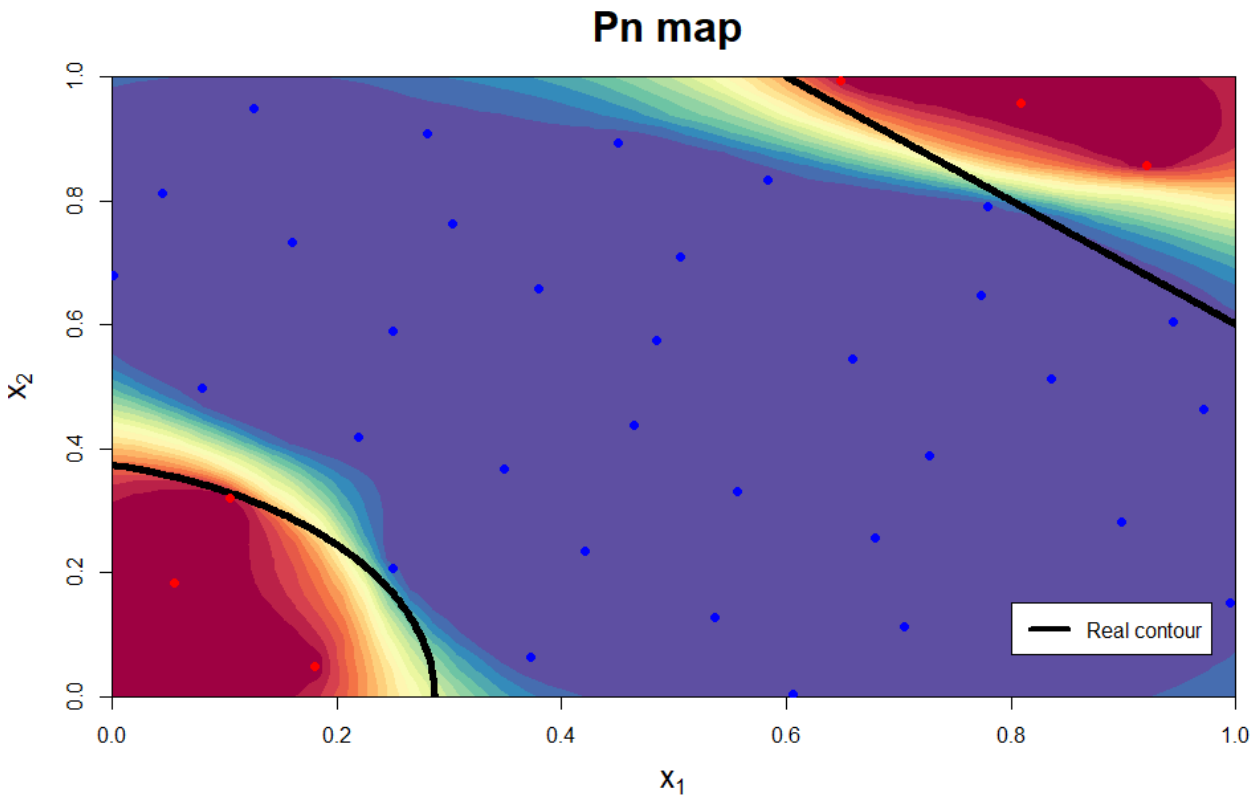
EXAMPLE OF A GPC FOR HIDDEN CONSTRAINT



- Characterization of the feasible set by quantiles

$$Q_\alpha = \{x \in \Omega : p_n(x) \geq \alpha\}, \alpha \in (0,1]$$

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STEPWISE UNCERTAINTY REDUCTION STRATEGY

The *Stepwise Uncertainty Reduction* strategy based on the uncertainty defined by the **vorob'ev deviation** $Var_n(\Gamma)$ [Chevalier, 2013, El Amri et al., 2021, Vorobyev and Lukyanova, 2013] is based on the following learning criterion:

$$J_n(x_{n+1}) = \mathbb{E}_n[Var_{n+1}(\Gamma)]$$

$$J_n(x_{n+1}) = \mathbb{E}_{Z(x_{n+1})}\left[\int (1 - p_{n+1}(x))\mathbb{1}_{p_{n+1}(x)\geq\alpha^*}\mu(dx) + \int p_{n+1}(x)\mathbb{1}_{p_{n+1}(x)<\alpha^*}\mu(dx)\right]$$

This expression can be developed using the expression of $p_n(x)$ given for the GPC model [Bachoc et al., 2020] and GP update formulae provided in [Chevalier, 2013]

- To reduce the computational time, we can get rid of the integration w.r.t. the realizations of the latent GP, using the conditional Bernouilli process $Y_n(x) = Y(x)|\mathcal{X}, \mathbf{Y_n} = \mathcal{Y}$

→ **ARCHISSUR criterion:** *Active Recovery of Constrained and Hidden Subset by SUR*

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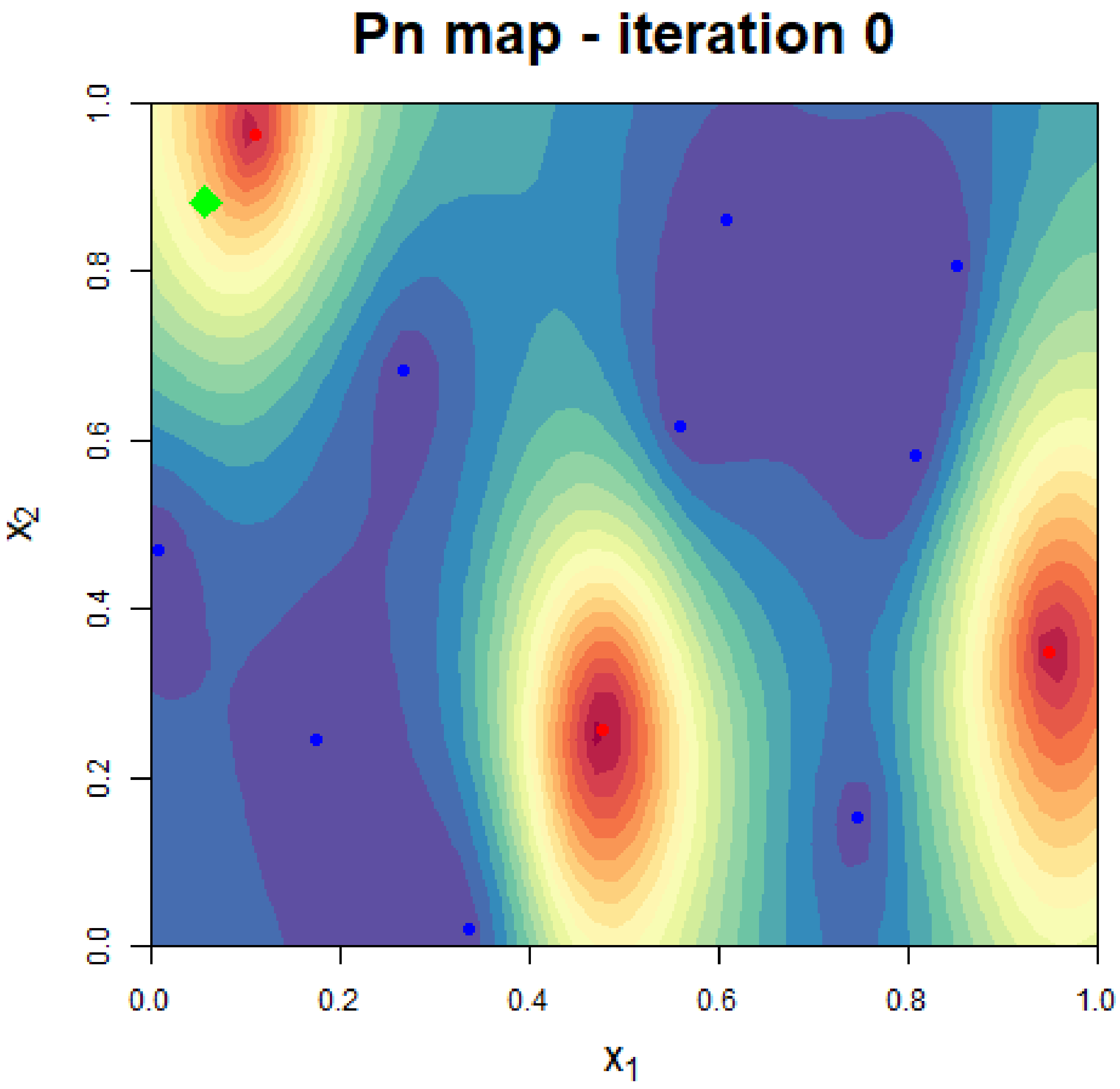
ARCHISSUR ON A 2D EXAMPLE (Branin function)



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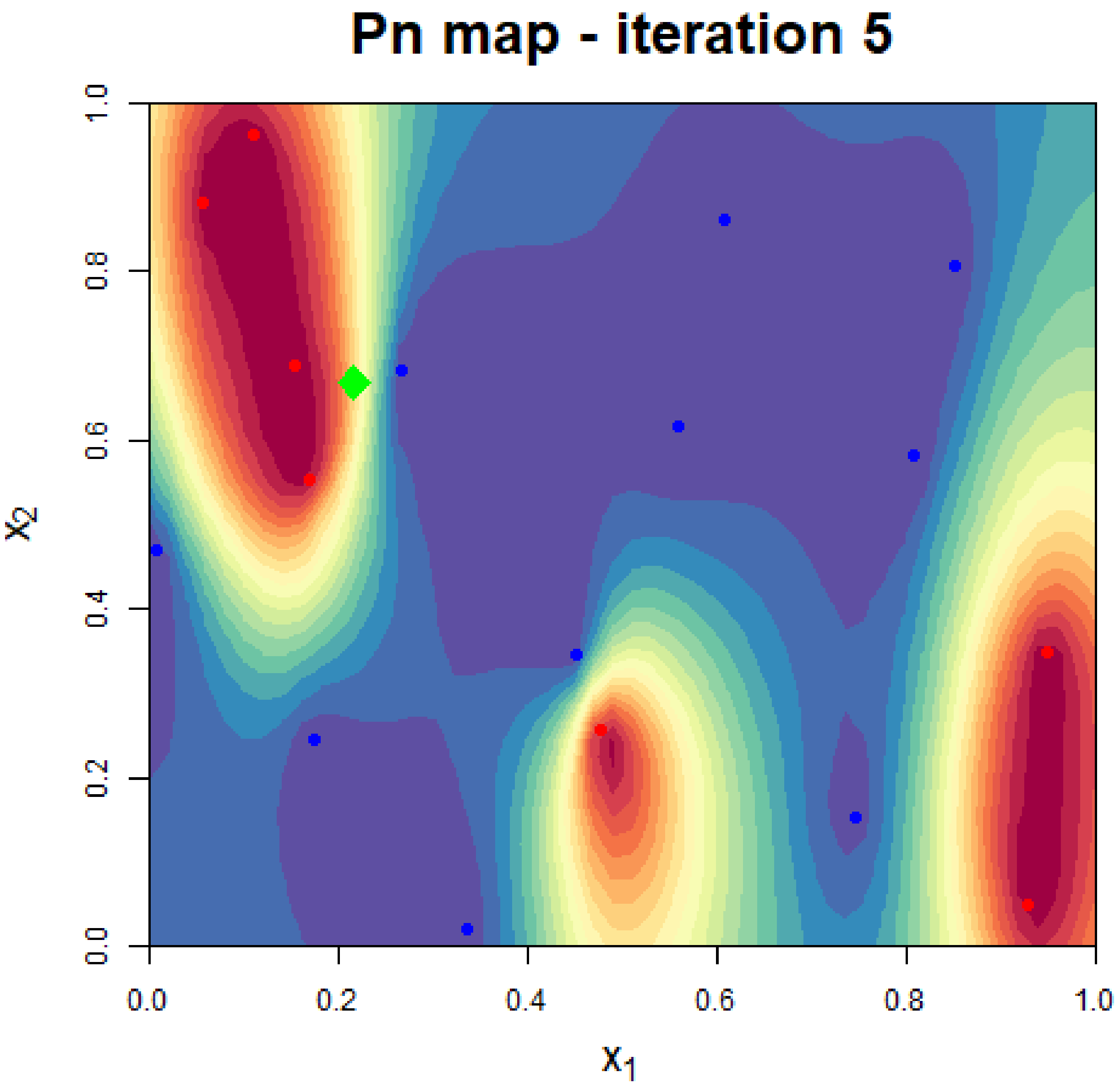

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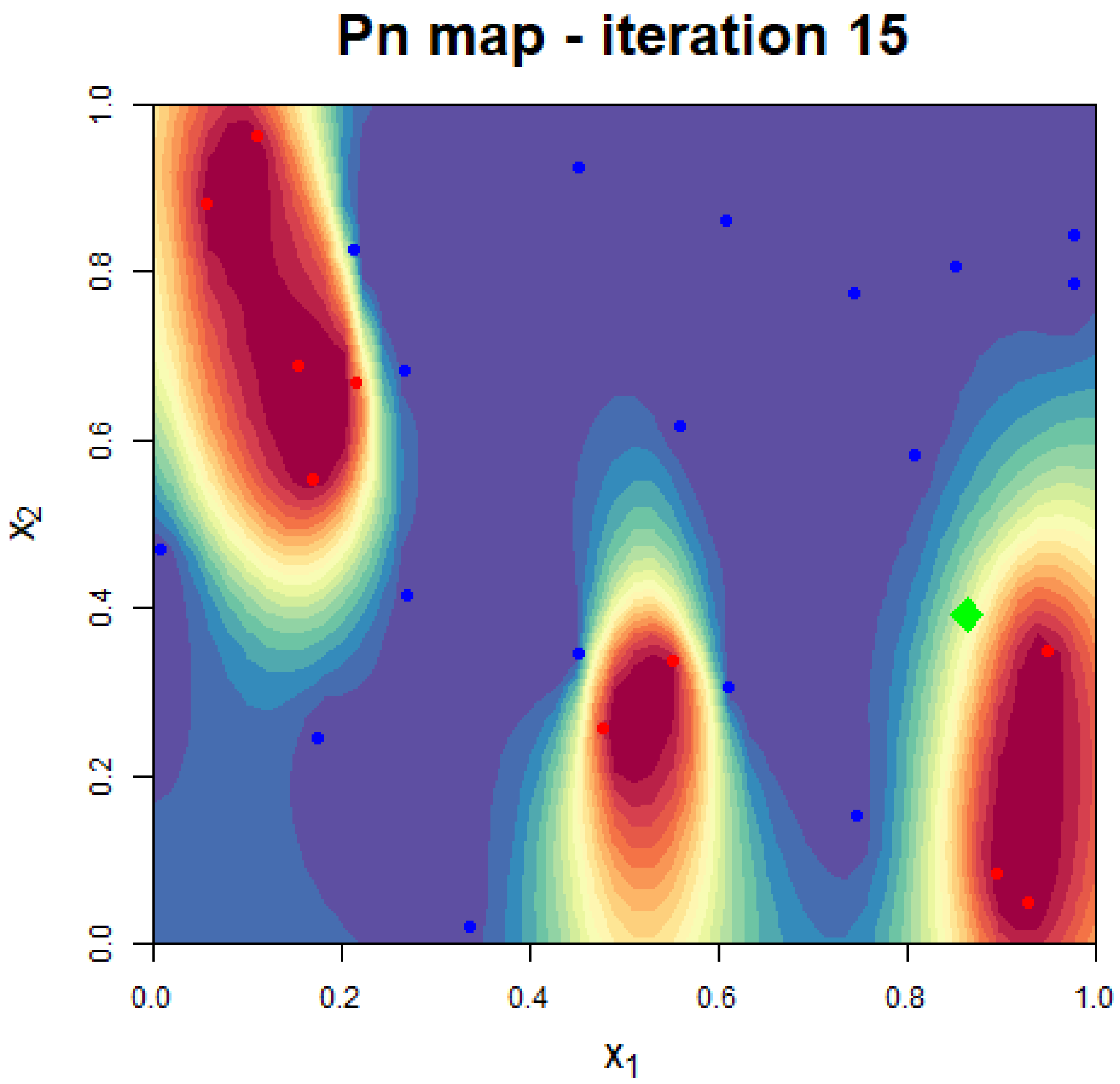
ARCHISSUR ON A 2D EXAMPLE (Branin function)



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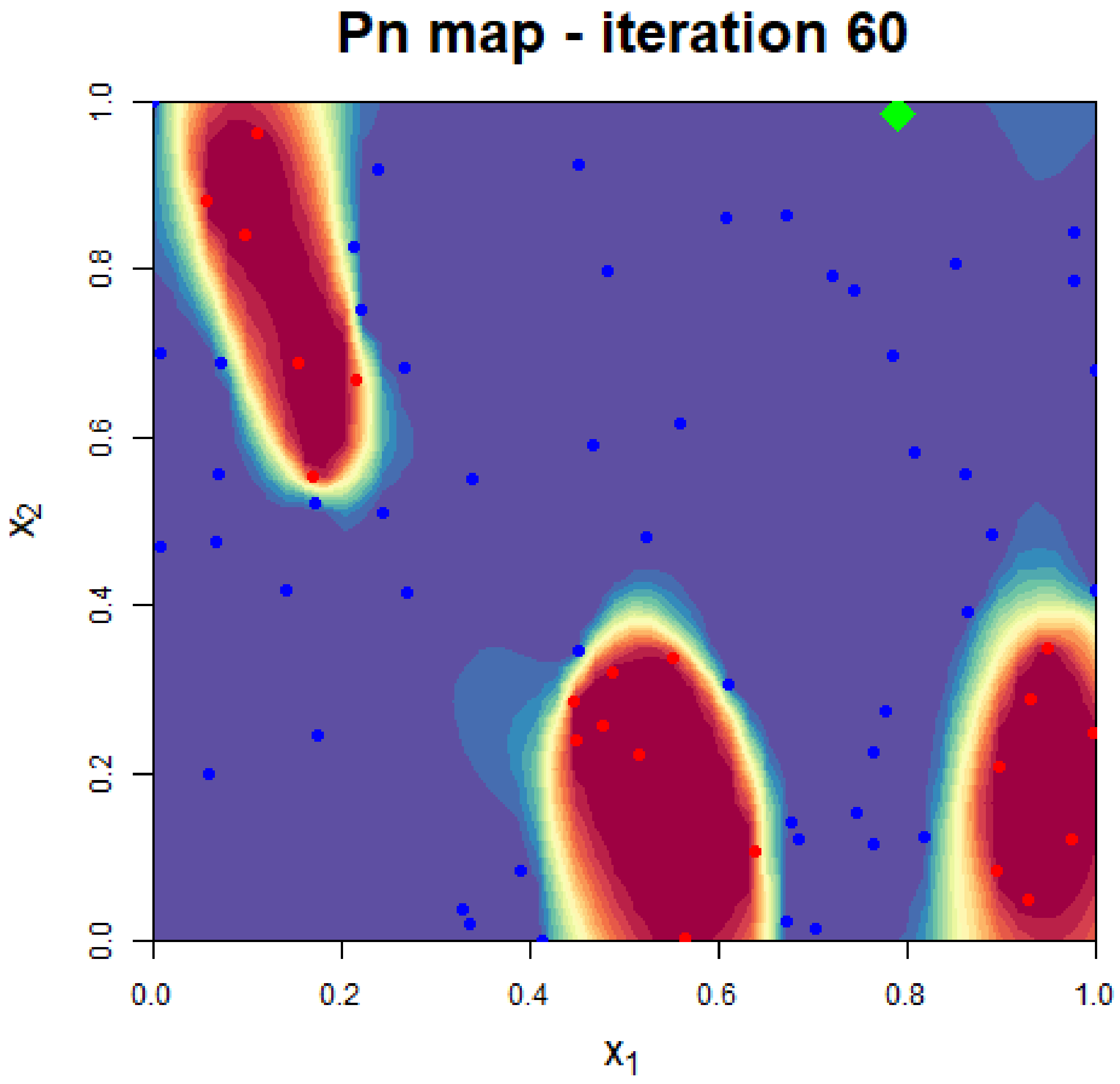
ARCHISSUR ON A 2D EXAMPLE (Branin function)



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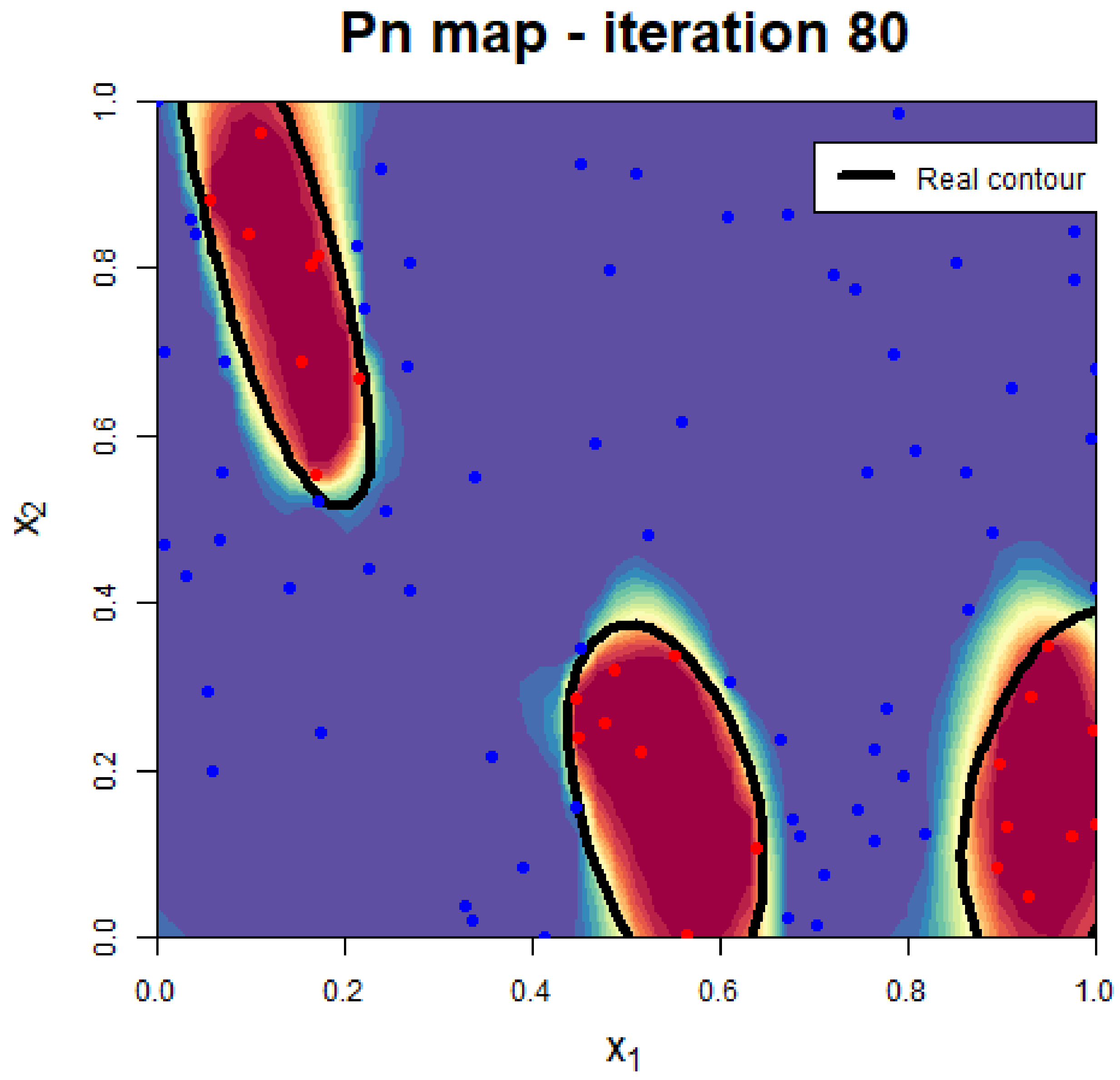

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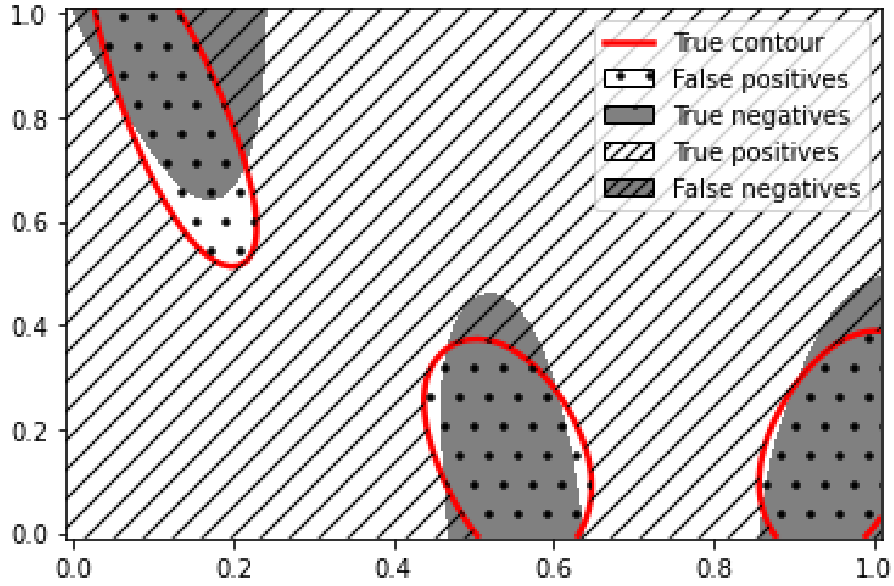
Compared strategies

- ARCHISSUR criterion: *Active Recovery of Constrained and Hidden Subset by SUR*
- Mixed enrichment criterion: add the point corresponding to the maximum of the GP variance (exploration) and the one where $p_n(x)$ value is the closest to $\frac{1}{2}$ (exploitation) simultaneously
- SMOCU enrichment measure: Soft-MOCU (Mean Objective Cost of Uncertainty) method [Zhao et al., 2021]

Comparison criterion

$$\frac{\mu(\Gamma^* \Delta Q_{\alpha^*})}{\mu(\Gamma^*)} = \frac{FN + FP}{TP + FN}$$



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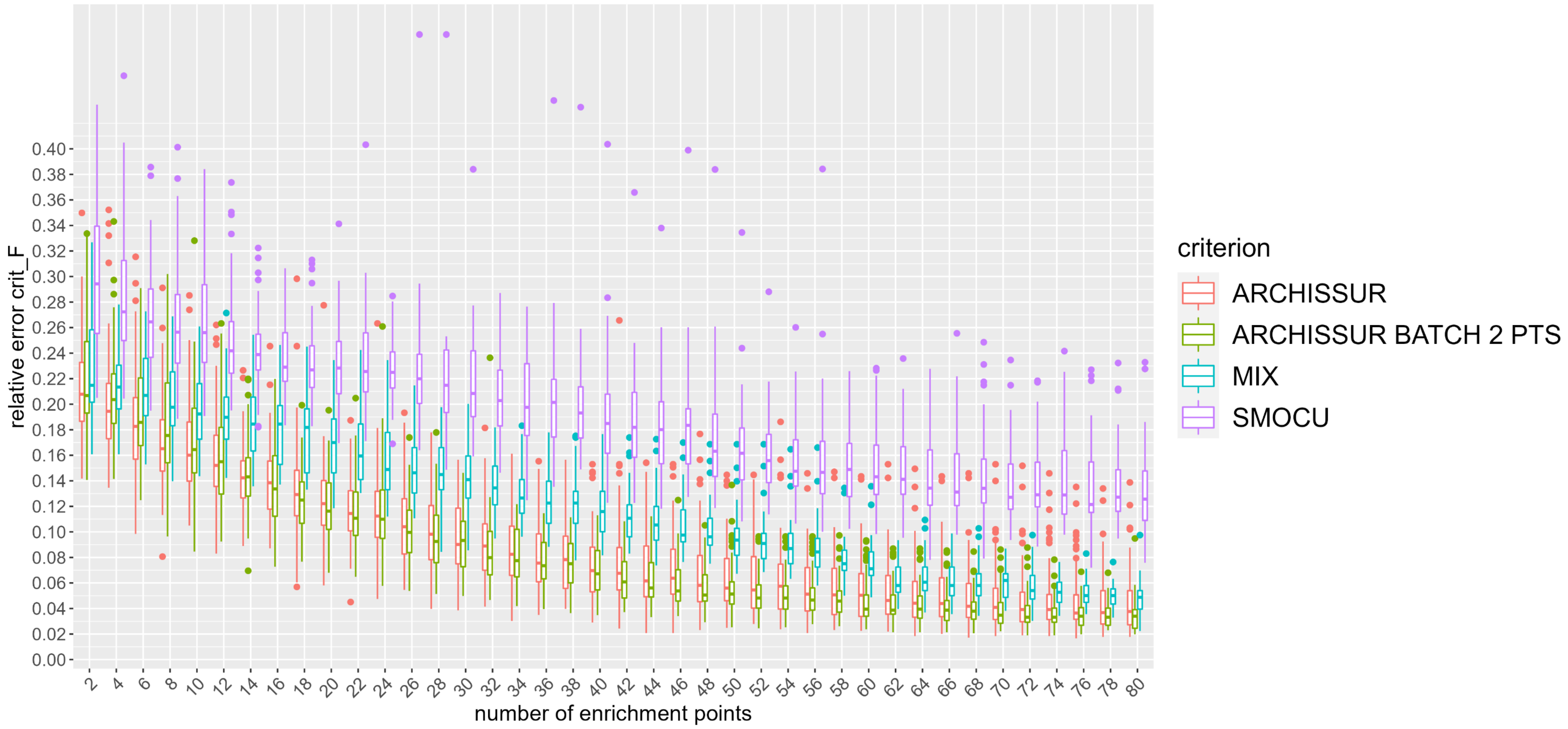
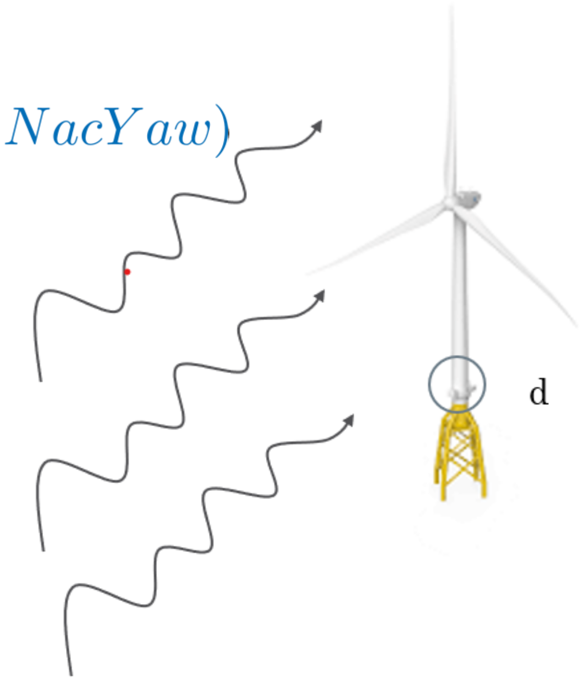
RESULTS ON BRANIN FUNCTION (2D)



RESULTS FOR DAMAGE PREDICTION OF A WIND TURBINE

$x = (\bar{U}, TI, NacYaw)$



TurbSim to simulate multiple realizations $(\bar{U}, TI, NacYaw)$

\+

FAST simulator
\+ Python scripts

↓

Predictions of damage at the bottom of the tower

Wind turbine subject to wind loads described by 3 parameters:
$\bar{U}$ mean of wind speed (10mn), TI turbulence intensity,
$NacYaw$ misalignment angle

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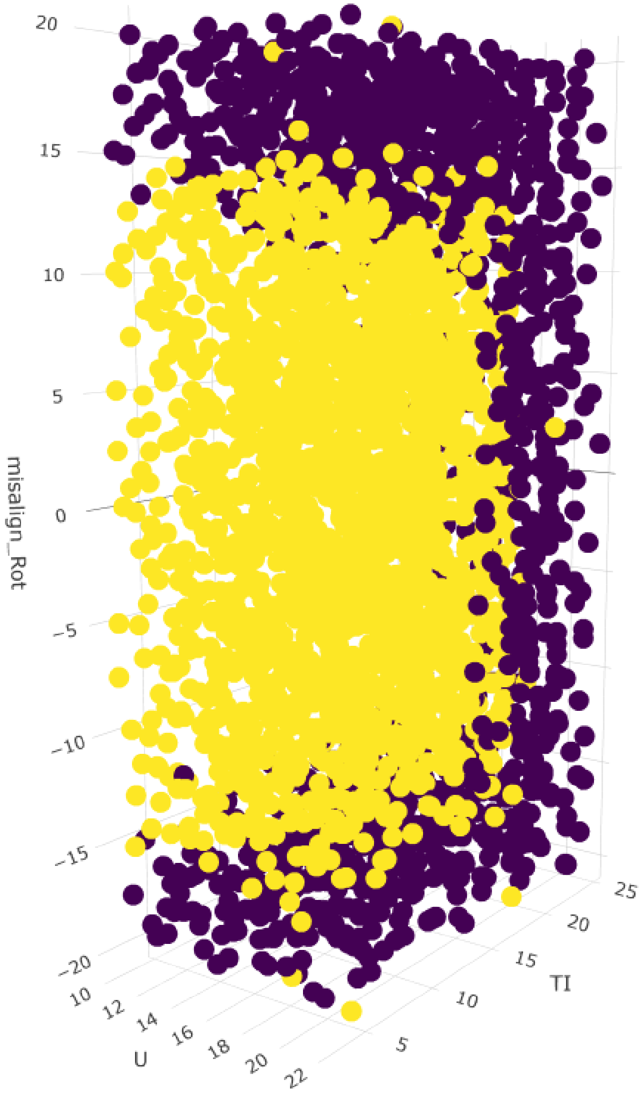
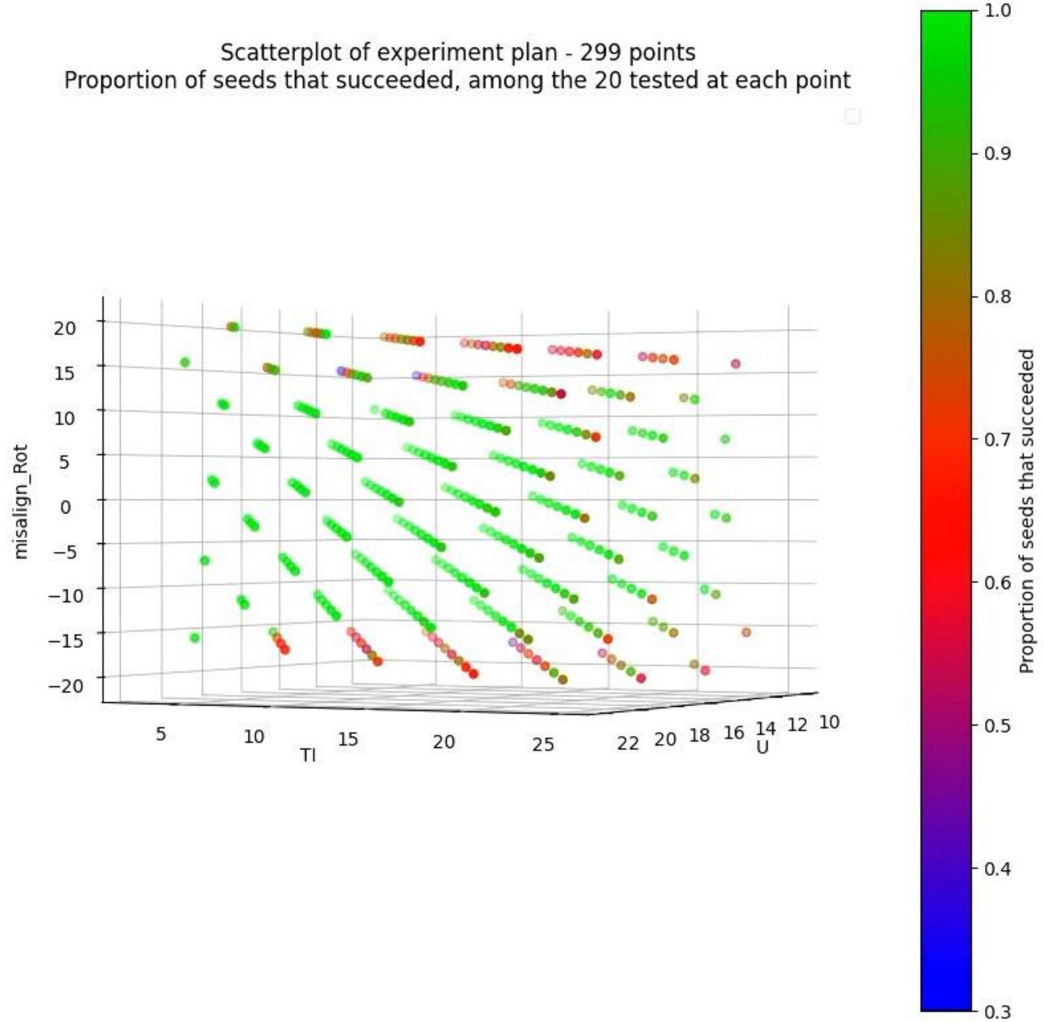
RESULTS FOR DAMAGE PREDICTION OF A WIND TURBINE





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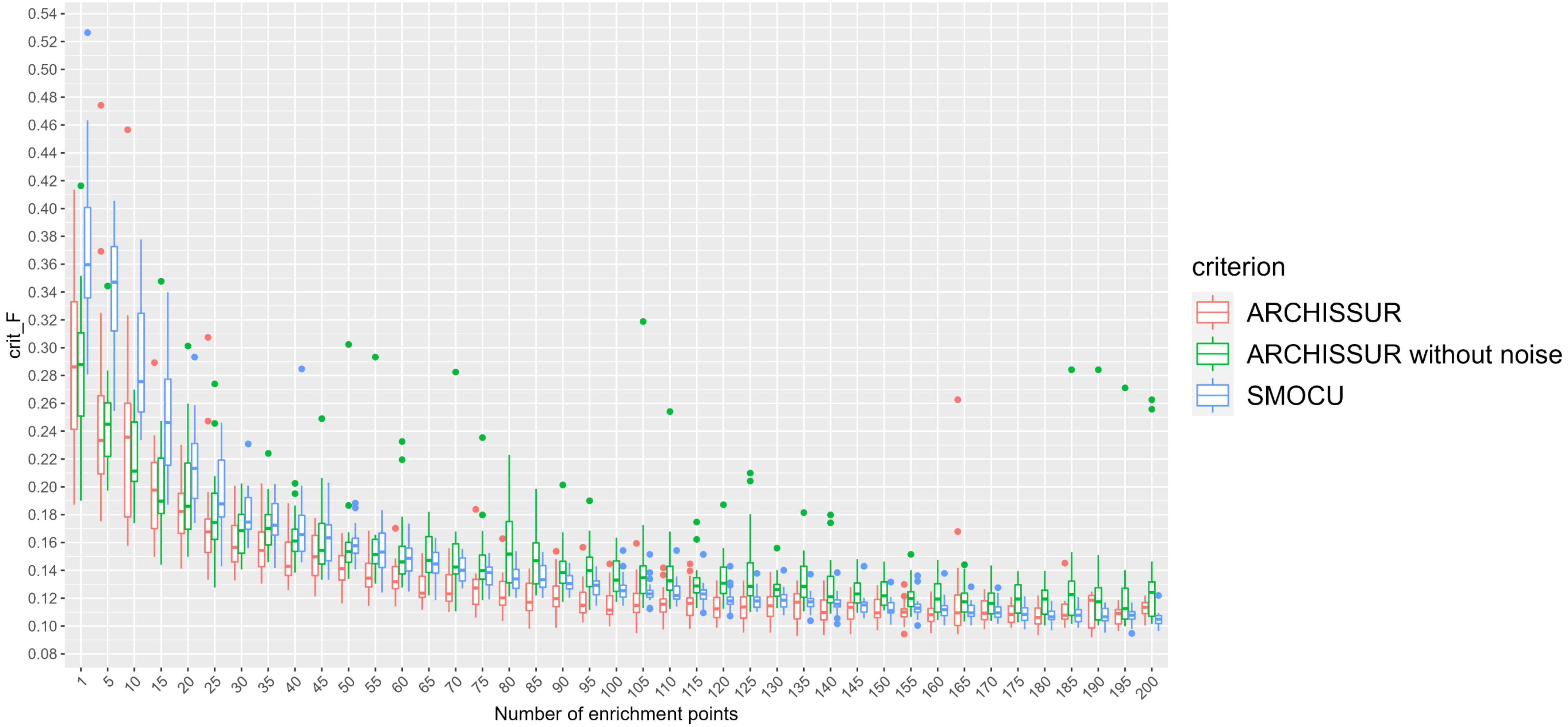

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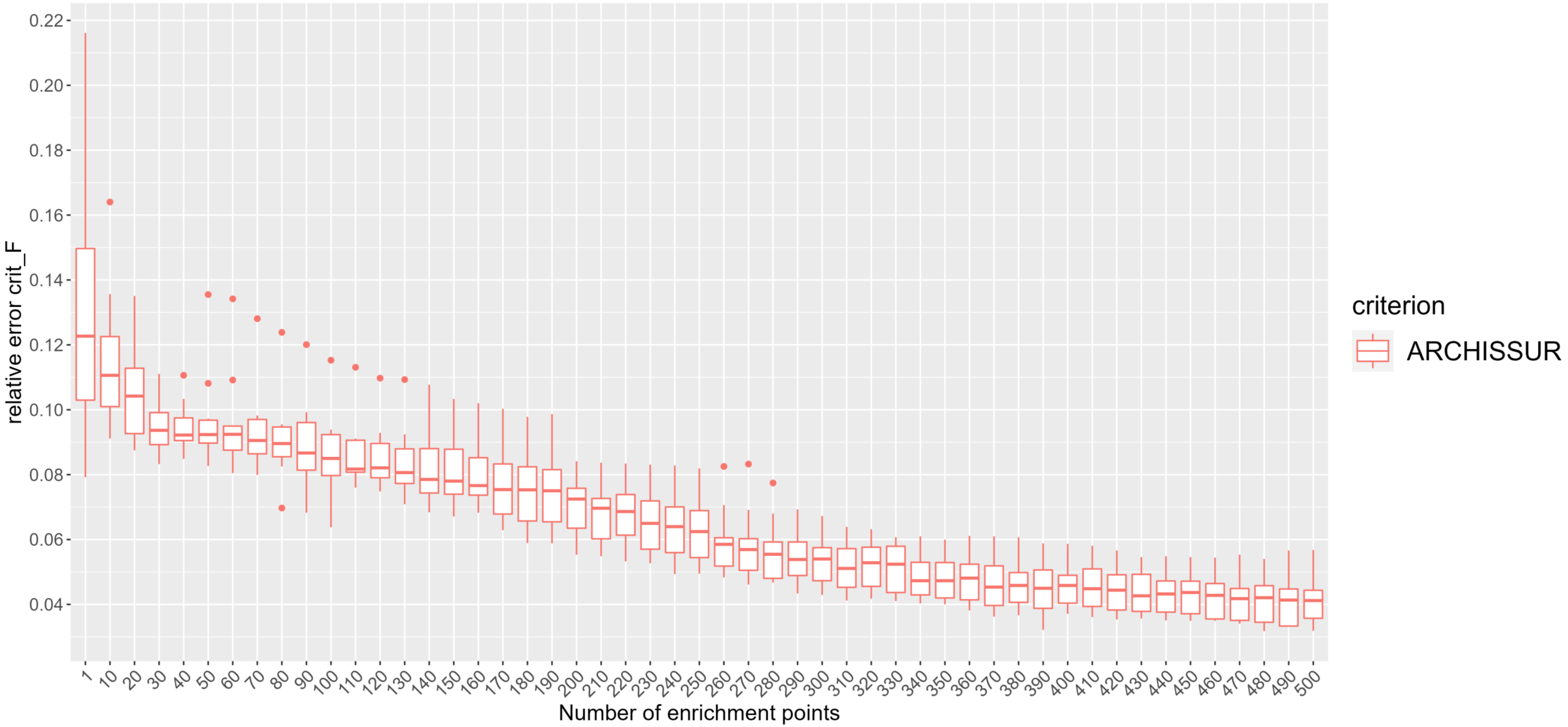
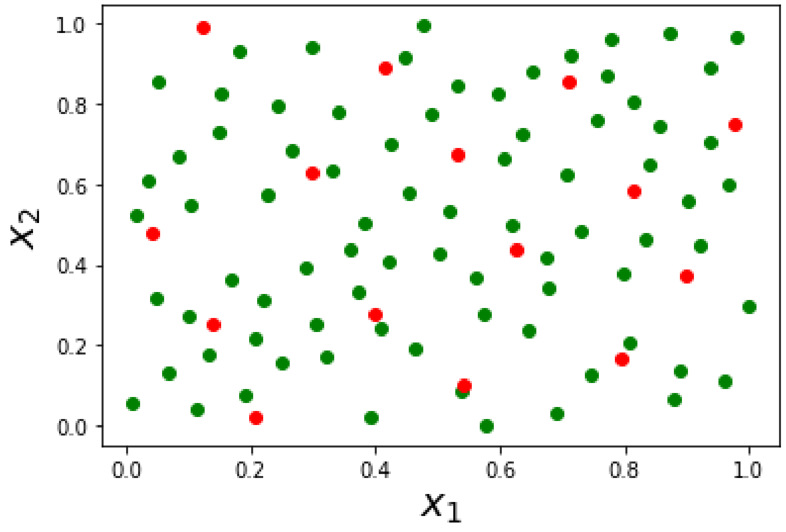
RESULTS ON A 10D FUNCTION



CONCLUSIONS

- Archissur has a good potential to learn non-convex feasible sets regarding crash constraints
- Optimization of the computation time for the criterion

But Archissur is not suited for



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CONCLUSIONS

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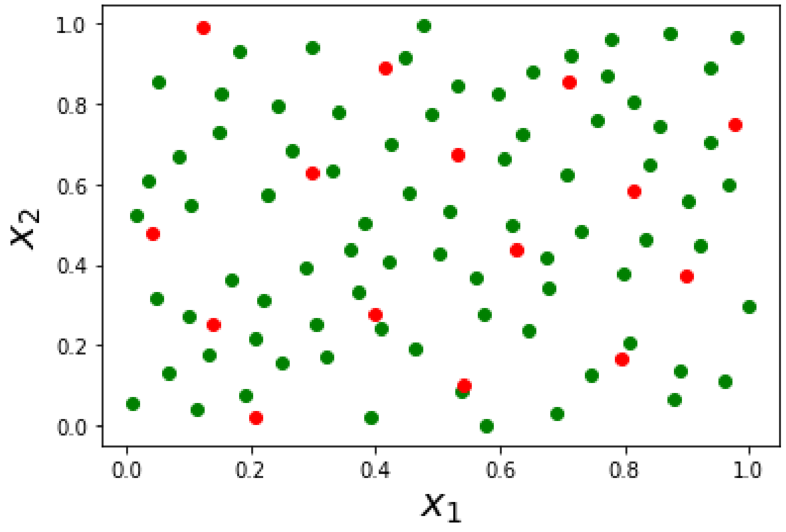

Perspectives

- Coupling with optimization: Bayesian optimization and Direct Search methods
  → ANR Samourai (with Polytechnique Montréal)
- More than 2 classes: multiple robustness or convergence levels

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