RECOVERING HIDDEN CONSTRAINED SUBSETS BY A GAUSSIAN PROCESS CLASSIFIER ACTIVE LEARNING METHOD BASED ON THE STEPWISE UNCERTAINTY REDUCTION STRATEGY

Morgane Menz, Miguel Munoz Zuniga, Delphine Sinoquet

HIDDEN CONSTRAINTS LEARNING PROBLEM

f: a computer code with inputs $x \in \Omega \subset \mathbb{R}^m$ with simulation failures on Ω.

Objective: determination of the feasible set:

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

Learning hidden constraints is a binary classification problem:

- We have binary observations: $(\mathcal{X}, \mathcal{Y}) = (x_j, y_j)_{j=1,\dots,n}$, with $y_j = \mathbb{1}_{f(x_j) \neq NAN}$.
- Objective: predict the probability of belonging to the failure/non-failure class

OVERVIEW OF HIDDEN CONSTRAINTS LEARNING STRATEGIES

Expensive numerical simulators

Classifiers

Support Vector Classifier

Naive Bayes Classifier

Gaussian Process Classifier

Neural Networks

K-Nearest Neighbors

Random Forest Classifier

…

Active learning

Uncertainty-based query approaches

Disagreement-based query approaches

Diversity- and density-based approaches

Expected error Reduction / One-step-look-ahead

[Cacciarelli and Kulahci, 2021]

One-step-look-ahead

Expected Error Reduction
[Roy and McCallum, 2001]
[Zhao et al, 2021]

→ Generalization error

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Stepwise Uncertainty Reduction strategies ?

LEARNING HIDDEN CONSTRAINT LEARNING WITH GAUSSIAN PROCESS CLASSIFIER

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- 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

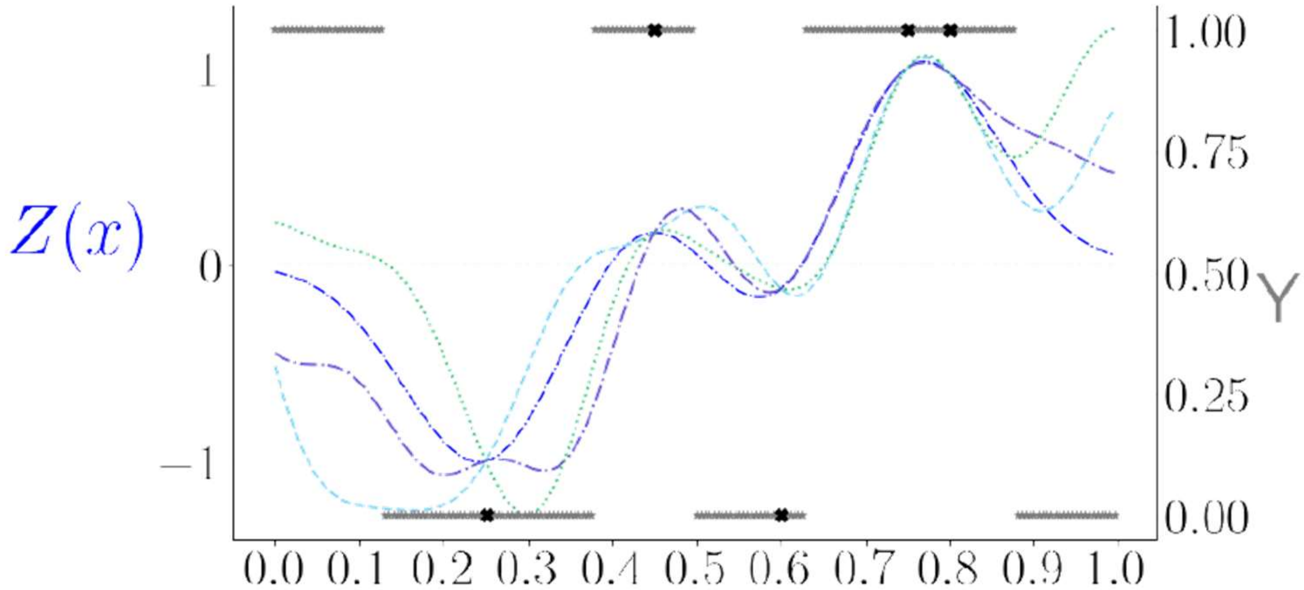
The GPC model allows to predict the probability of success of a simulation:

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

GAUSSIAN PROCESS CLASSIFIER FORMULATION

In [Bachoc et al., 2020], the probability of non-failure is modeled using the sign of a latent GP $Z(x) \sim GP(m_n(x, z_n), k_n(x))$:

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



GAUSSIAN PROCESS CLASSIFIER 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 $p_n(x)$:

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

LEARNING HIDDEN CONSTRAINT WITH GPC

The feasible set learned by a GPC model can be characterized by a percentile of the feasibility probability: $\boxed{Q_\alpha = \{x \in \Omega : p_n(x) \geq \alpha\}, \alpha \in (0,1]}$

Objective: Obtaining an accurate approximation of Q_α

Idea: draw a methodology from an existing paradigm used in Gaussian Process Regression active learning for feasible set estimation: stepwise uncertainty reduction strategy using the notion of random set [Bect et al., 2012, Molchanov, 2005]

STEPWISE UNCERTAINTY REDUCTION STRATEGY FOR HIDDEN CONSTRAINTS LEARNING

Let us consider the random set:

$$\boxed{\Gamma = \{x \in \Omega : Y_n(x) = 1\}}$$

with $Y_n(x)$ the conditional Bernoulli [Dai et al., 2013] random variable $Y(x)|\mathcal{X}, \mathrm{Y_n} = \mathcal{Y}$

The SUR strategy based on the uncertainty on Γ defined by the **vorob'ev deviation** Var_n^{Γ} [Chevalier, 2013, El Amri et al., 2020, Vorobyev and Lukyanova, 2013] aim to minimize at each step the following learning function:

$$\boxed{J_n(x_{n+1}) = \mathbb{E}_n\left[Var_{n+1}^{\Gamma}(x_{n+1}, Z(x_{n+1}))\right]}$$

STEPWISE UNCERTAINTY REDUCTION STRATEGY FOR HIDDEN CONSTRAINTS LEARNING

We propose to minimize the expectation of uncertainty using the expectation on the Bernoulli process $\mathrm{Y_n}$

$$\mathbb{E}_n[\cdot] = \mathbb{E}_{Y_n(x_{n+1})}[\cdot|\mathcal{X}, \mathrm{Y_n} = \mathcal{Y}]$$

Hence:

$$\boxed{\begin{aligned} J_n(x_{n+1}) &= (1 - p_n(x_{n+1}))\ Var^{\Gamma}_{n+1}(x_{n+1}, Y_n(x_{n+1}) = 0) \\ &\quad + p_n(x_{n+1})\ Var^{\Gamma}_{n+1}(x_{n+1}, Y_n(x_{n+1}) = 1) \end{aligned}}$$

➜ Advantage: no integration over the realizations of the latent GP $Z(x_{n+1})$

➜ Simplified computation of $Var^{\Gamma}_{n+1}(x_{n+1}, Y_n(x_{n+1}) = y_{n+1})$ with our proposed GPC update formulae

STEPWISE UNCERTAINTY REDUCTION STRATEGY FOR HIDDEN CONSTRAINTS LEARNING

The Vorob'ev deviation is given by:

$$Var^{\Gamma}_{n+1}(x_{n+1}, Y_n(x_{n+1}) = y_{n+1}) = \int (1-p_{n+1}(x))\mathbb{1}_{p_{n+1}(x)\geq\alpha^*} + p_{n+1}(x)\mathbb{1}_{p_{n+1}(x)<\alpha^*}\mu(dx)$$

with $p_{n+1}(x)$ the future feasibility probability knowing $Y_n(x_{n+1}) = y_{n+1}$ given by:

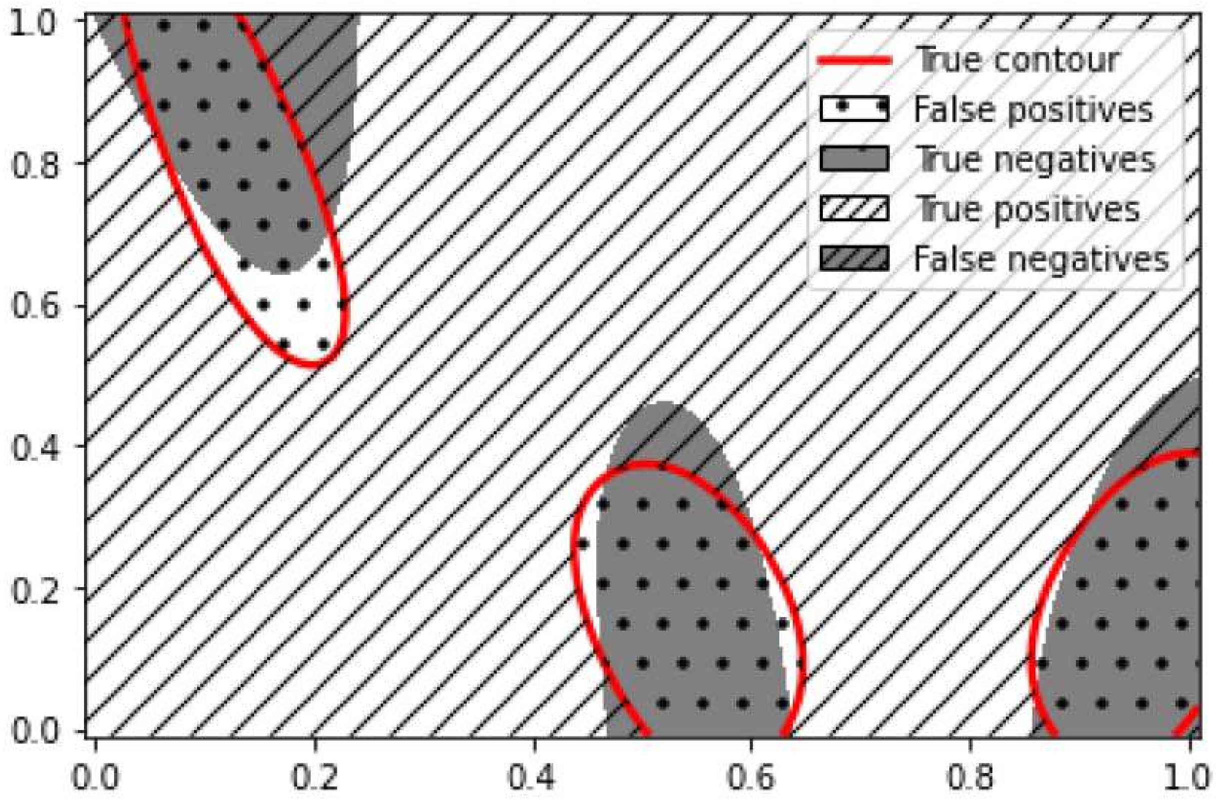
$$p_{n+1}(x) = \frac{1}{N}\sum_{i=1}^{N}\bar{\Phi}\left(\frac{-m_{n+1}(x, \mathrm{z}^{\mathrm{i}}_{\mathrm{n+1}})}{\sigma_{n+1}(x)}\right)$$

This probability can be computed by:

- using GP update formulae provided in [Chevalier, 2013]
- sampling $\mathrm{z}^{\mathrm{i}}_{\mathrm{n+1}}$ using $\mathrm{z}^{\mathrm{i}}_{\mathrm{n}}$ and:

$z(x_{n+1})^i \sim \mathcal{N}\left(m_n(x_{n+1}, \mathrm{z}^{\mathrm{i}}_{\mathrm{n}}), k_n(x_{n+1}, x_{n+1})\right)$ truncated such that $sign(z(x_{n+1})^i) = y_{n+1}$

RESULTS: COMPARISON CRITERIA



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

RESULTS: COMPARISON OF DIFFERENT ENRICHMENT CRITERIA

Compared strategies:

- ARCHISSUR: An Active Recovery of a Constrained and Hidden Subset by SUR method based on the Vorob'ev deviation $\Rightarrow$ one point and batch versions [Menz et al.,2023]
- Mix 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] `https://github.com/QianLab/Soft_MOCU`

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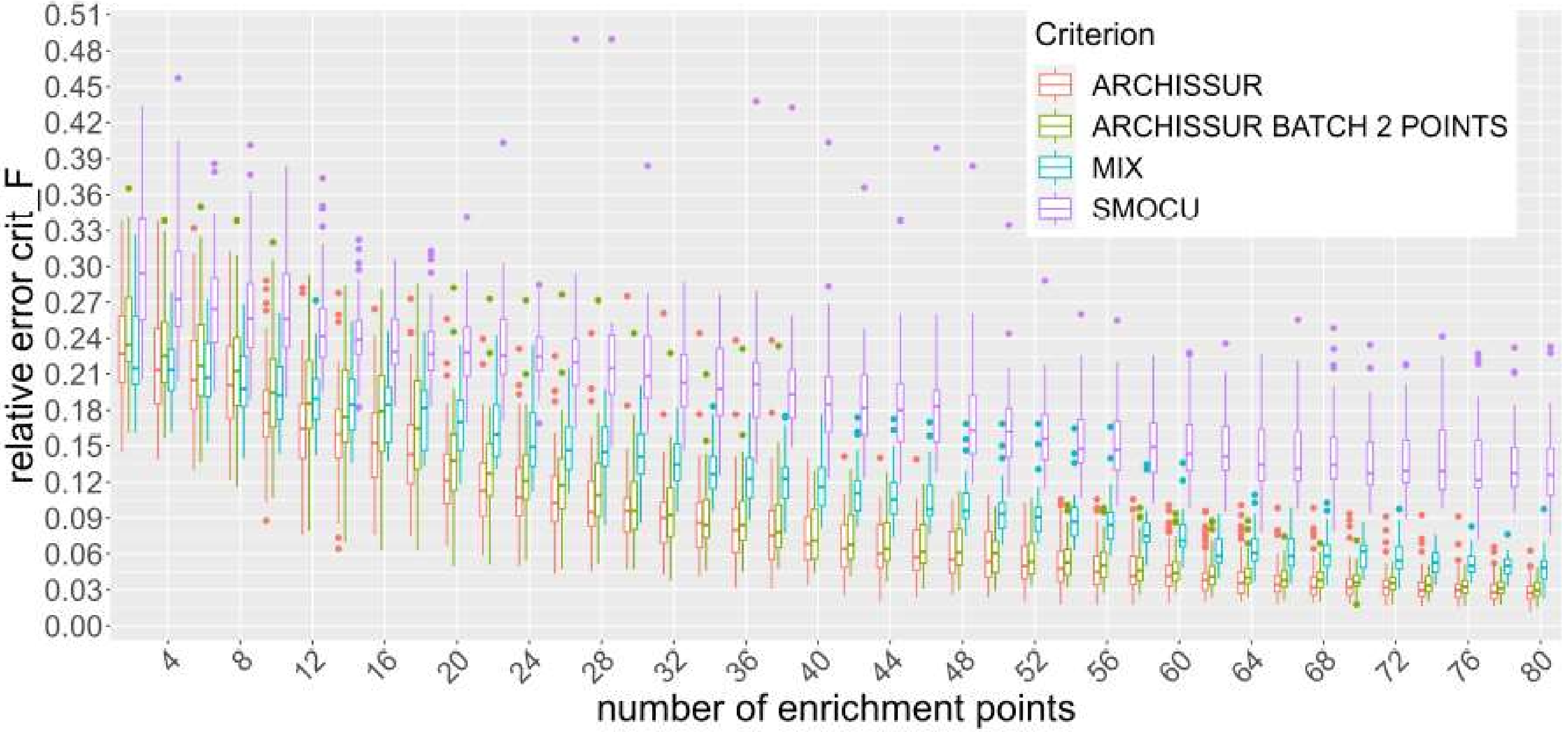
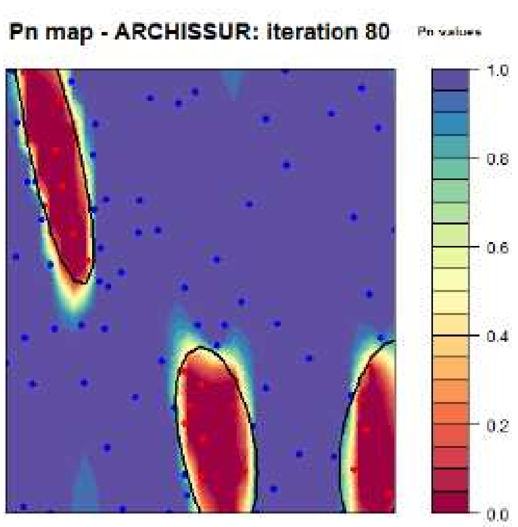
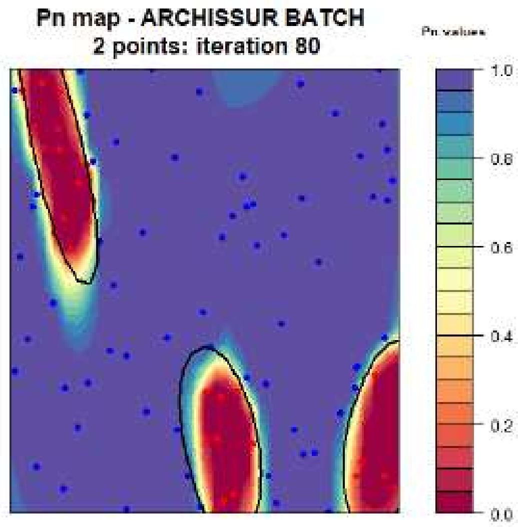
TOY EXAMPLE BASED ON BRANIN

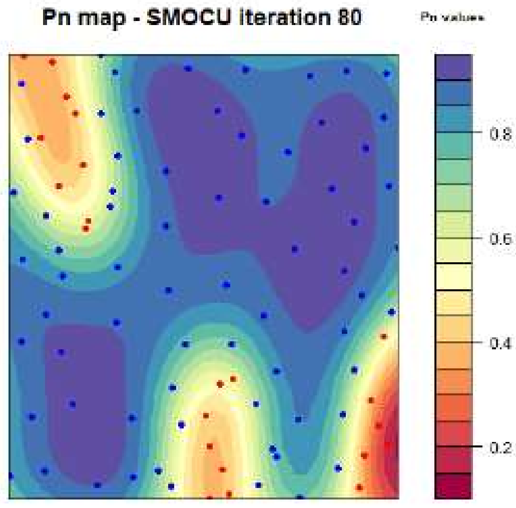
Evolution of $crit_F$ for MIX, ARCHISSUR, ARCHISSUR BATCH and SMOCU



TOY EXAMPLE BASED ON BRANIN







TOY EXAMPLE BASED ON BRANIN

Mean CPU times (in seconds) of the learning function evaluation on 20 repetitions with 2000 integration points

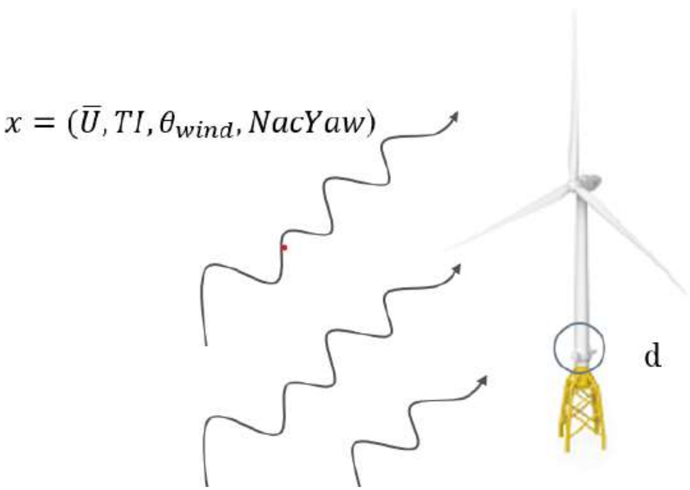
Method	ARCHISSUR with old formulation	ARCHISSUR	ARCHISSUR BATCH (2 points)	SMOCU
	0.311	0.079	0.412	0.849

* old formulation: $\mathbb{E}_n[\cdot] = \mathbb{E}_{Z_n(x_{n+1})}[\cdot|\mathcal{X}, \mathrm{Z_n} = z_n]$

DAMAGE PREDICTION OF A WIND TURBINE

Wind loads are described by 3 parameters:

- wind speed $\bar{U}$,
- turbulence intensity TI,
- misalignment angle $NacYaw$.



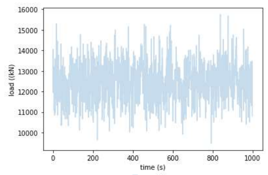
Wind parameters: $\bar{U}$, TI, $NacYaw$

↓

Turbsim

↓

n_{seed} simulations of wind



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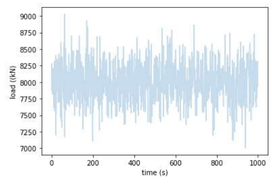

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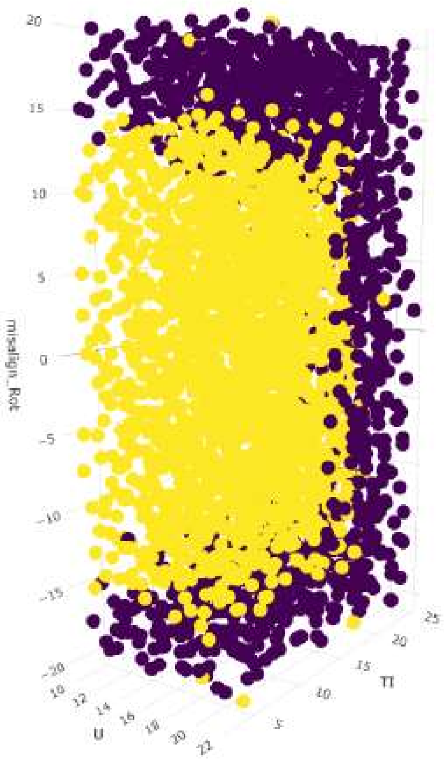
Multiphysics simulator **OpenFast** … Multiphysics simulator **OpenFast**

↓

Mean damage across wind turbine tower base

DAMAGE PREDICTION OF A WIND TURBINE



failure / success

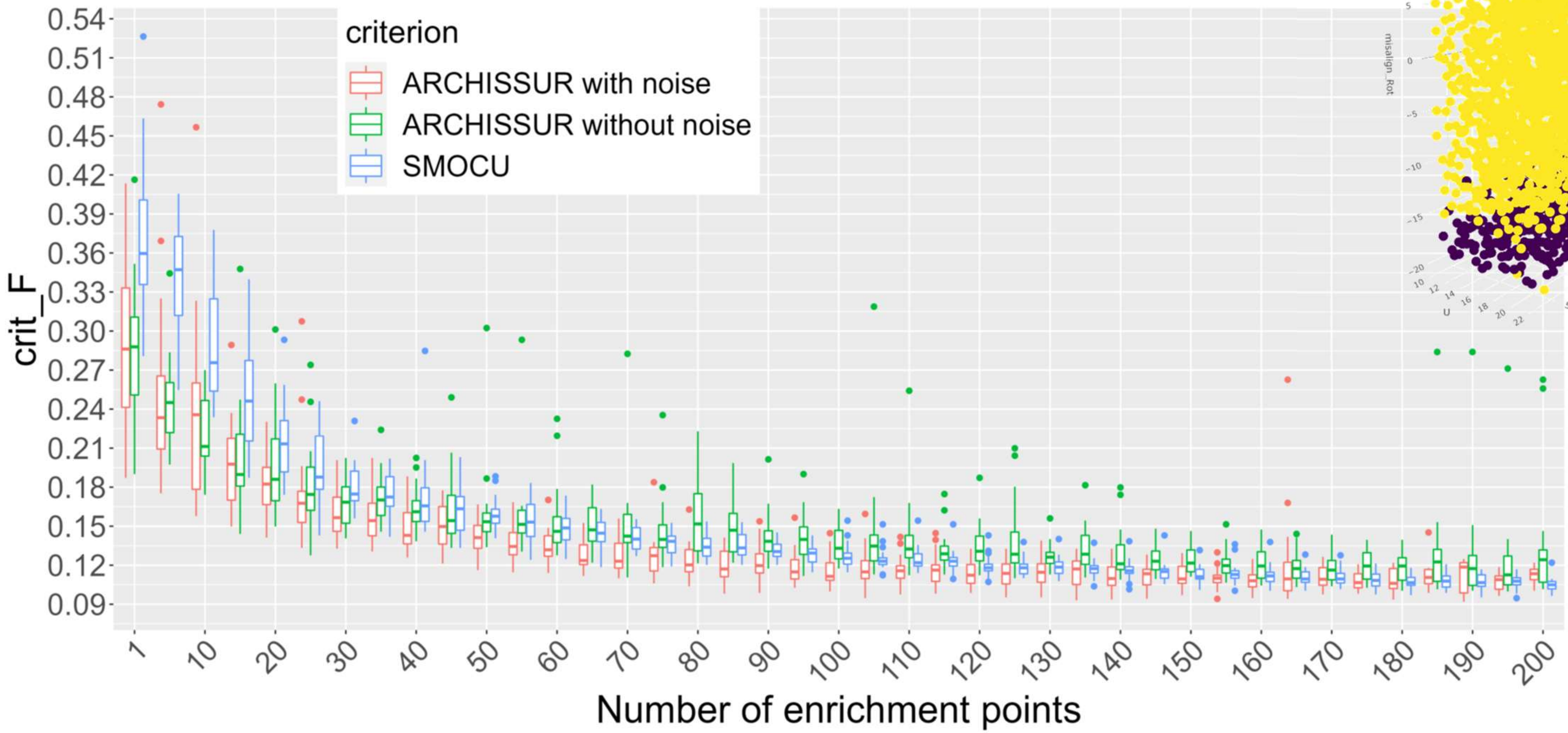
Specificity of this test case:

- non-regular frontier between feasible/unfeasible sets
- Presence of outliers

→ GPC model with noise on observed points

RESULTS FOR THE DAMAGE PREDICTION OF A WIND TURBINE

Evolution of $crit_F$ for ARCHISSUR and SMOCU



failure / success

CONCLUSIONS AND OUTLOOK

- Great potential to learn hidden constraints with application to an industrial test case
- Application on a analytic case in 10 dimensions tackled in the preprint
- Faster decrease of the error measure as a function of number of simulation on the test cases

→Can this work be integrated within space-filling or optimization strategies to help in the presence of hidden constraints?

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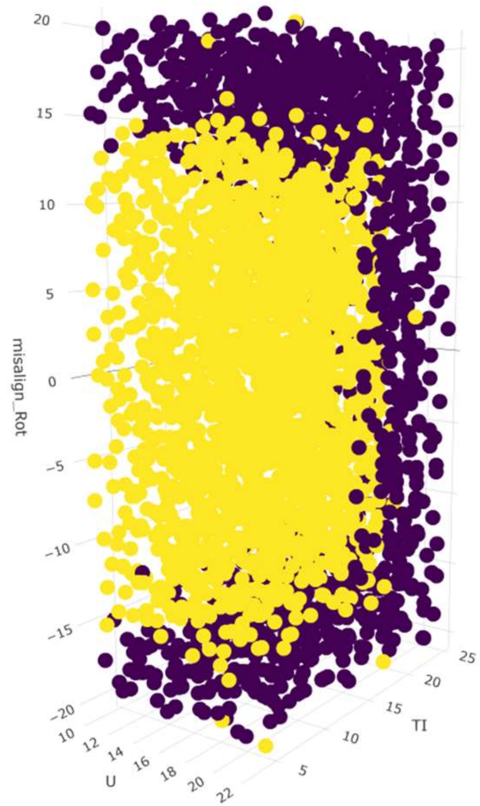
APPLICATION IFPEN : DOMMAGE EN PIED DE TOUR D'UNE ÉOLIENNE OFFSHORE

Climat, Environnement et Économie circulaire

Failure for at least one of the wind seeds n_{seed} = simulation failure

failure / success



Vorob'ev expectation and deviation

Definition

Vorob'ev expectation is defined as the α^*-percentile of Γ, where α^* is determined by:

$$\mathbb{E}[\mu(\Gamma)] = \mu(Q_{\alpha^*})$$

with μ the Lebesgue measure and $Q_\alpha = \{x \in \Omega : p_n(x) \geq \alpha\}, \alpha \in (0, 1]$.

Vorob'ev expectation is a global minimiser of the vorob'ev deviation $Var_n(\Gamma)$ among closed sets of volume equal to the mean volume of Γ:

$$Var_n(\Gamma) = \mathbb{E}[\mu(Q_\alpha \Delta \Gamma) | \mathcal{X}, \mathcal{Y}]$$

with $\Gamma \Delta Q_\alpha = (\Gamma \setminus Q_\alpha) \cup (Q_\alpha \setminus \Gamma)$

MOCU/SMOCU

The enrichment criterion based on MOCU (Mean Objective Cost of Uncertainty) formulation given in [Zhao et al., 2021] can be rewritten as:

$$U^{MOCU}(x_{n+1}) = \mathbb{E}_n[Var_{n+1}(\Gamma)] - Var_n(\Gamma) \text{ with } \alpha = 0.5$$

Soft-MOCU learning function is a smooth concave approximation of MOCU given by:

$$\begin{aligned} U^{SMOCU}(x_{n+1}) &= \mathbb{E}_X[\mathbb{E}_n[\tfrac{1}{k} ln(exp(k * p_{n+1}(X)) + exp(k(1 - p_{n+1}(X))))] \\ &- \tfrac{1}{k} ln(exp(k * p_n(X)) + exp(k(1 - p_n(X))))] \end{aligned}$$

with k a smoothness parameter.

