Learning hidden constraints using a Stepwise Uncertainty Reduction strategy with Gaussian Process Classifiers

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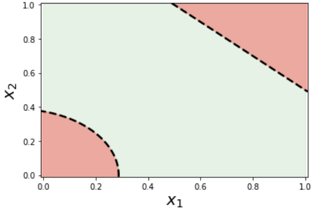
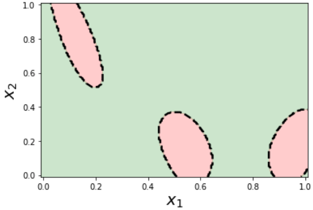
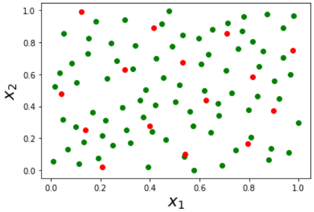
Problem statement: hidden constraints

Context: Expensive simulator outputs evaluation
➜ simulations crash: hidden constraints







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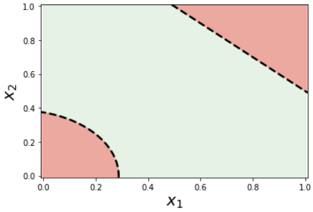
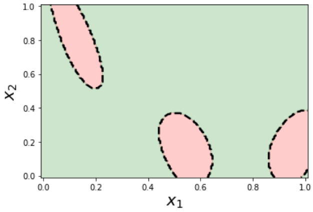
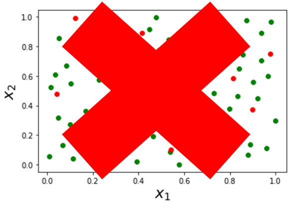






Problem statement: hidden constraints

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

Objective: determination of the feasible set:

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

Gaussian process based classification

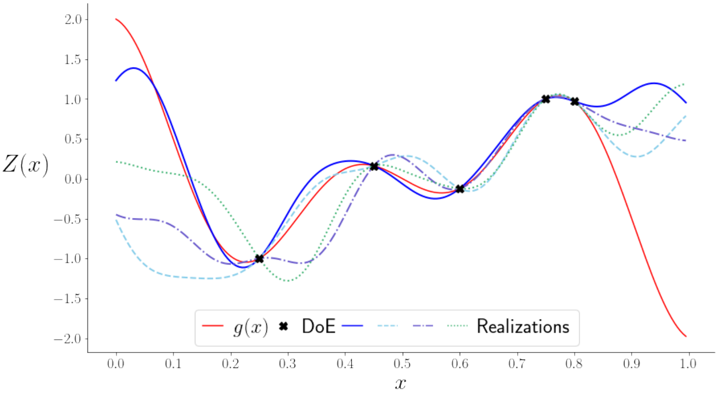
Learning hidden constraint is a binary classification problem:

- We have binary observations: $(\mathcal{X}, \mathcal{Y}) = (x_j, y_j)_{j=1,\dots,n}$, 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

Function approximation by Gaussian process model

Approximation of a function g by a GP $Z(x)$ conditioned on observations of g [Forrester et al., 2008, Rasmussen and Williams, 2006]

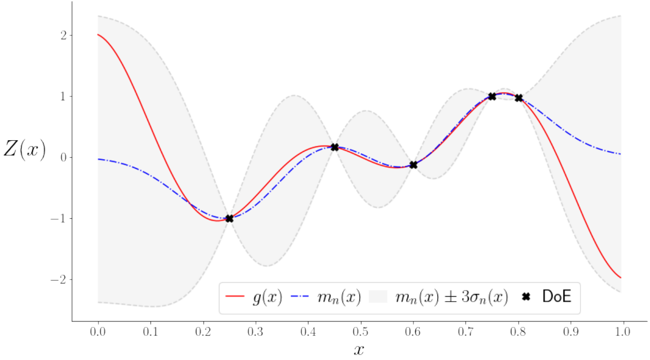


Function approximation by Gaussian process model

Approximation of a function g by a Gaussian process conditioned on observations of g defined by:

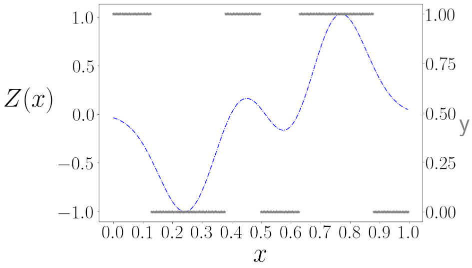
$$Z(x) \sim GP(m_n(\cdot), k_n(\cdot, \cdot))$$

$m_n(\cdot)$, $k_n(\cdot, \cdot)$ conditioned mean and kernel of $Z(x)$



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).



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:

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

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:

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

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

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: $\mathbb{P}[sign(Z_n) = \mathcal{Y}]$

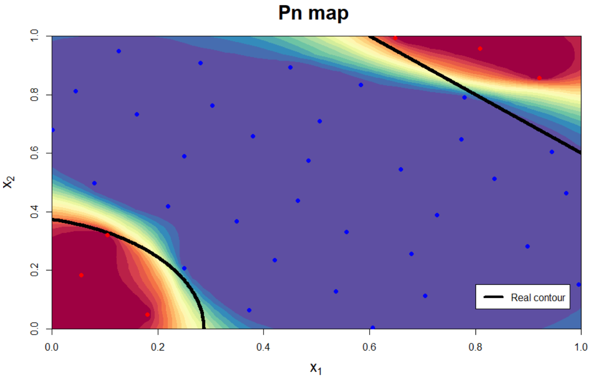
Gaussian process classifier (GPC) formulation

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

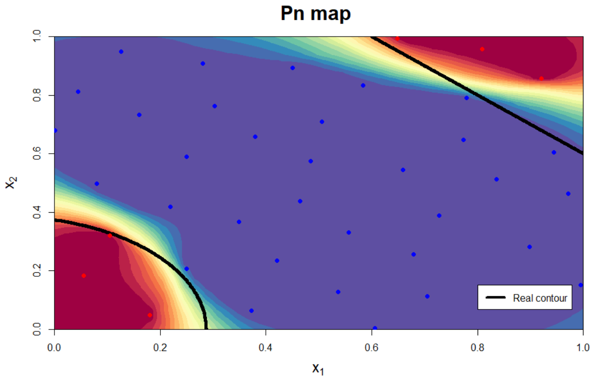
- Optimization of the hyperparameters of the latent GP to maximize the likelihood: $\mathbb{P}[sign(Z_n) = \mathcal{Y}]$
- Generation of realizations $z_n^{(i)}$ of $Z_n | sign(Z_n) = \mathcal{Y}$
  ➜ Approximation of $p_n(x)$:

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

Example of a GPC for hidden constraint learning



Example of a GPC for hidden constraint learning



Characterisation of the feasible set:

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

GPC based active learning

Principle: adaptively enrich the GPC using a learning criterion in order to obtain an accurate approximation of the set Γ^* contour

GPC based active learning

Principle: adaptively enrich the GPC using a learning criterion in order to obtain an accurate approximation of the set Γ^* contour

Idea: draw a methodology from existing criteria 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 strategies

Let $\mathcal{U}_n$ be a measure of uncertainty about the excursion set knowing observations at points $\mathcal{X}$

Stepwise Uncertainty Reduction (SUR) strategies aim to minimize at each step:

$$J_n(x_{n+1}) = \mathbb{E}_n[\mathcal{U}_{n+1}(x_{n+1}, Z(x_{n+1}))] := \mathbb{E}_{Z(x_{n+1})}[\mathcal{U}_{n+1}(x_{n+1})|\mathcal{X}, Z(\mathcal{X})]$$

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:

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

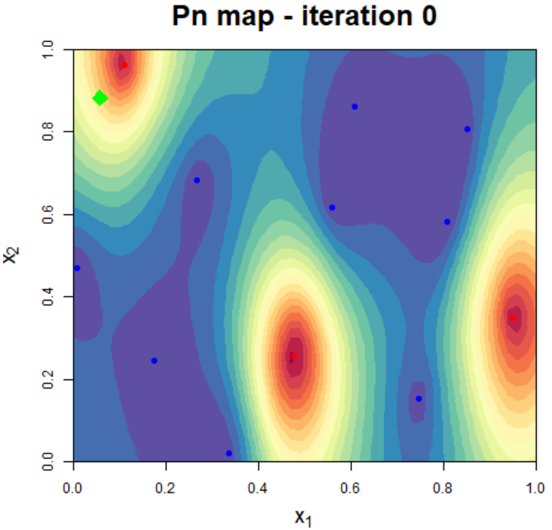
i.e.

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

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]

Example - Active learning based on Vorob'ev criterion

Classification problem based on the Branin function



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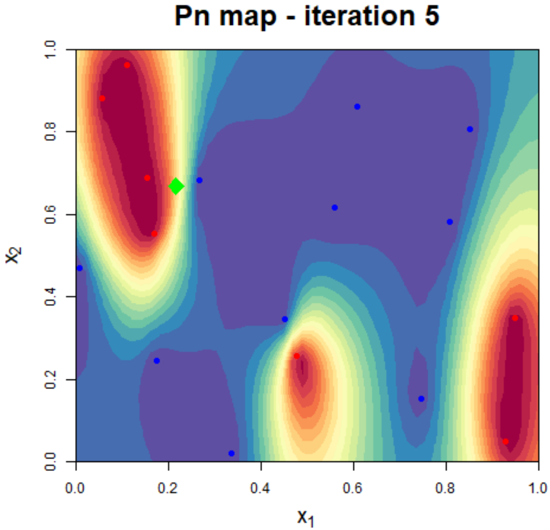

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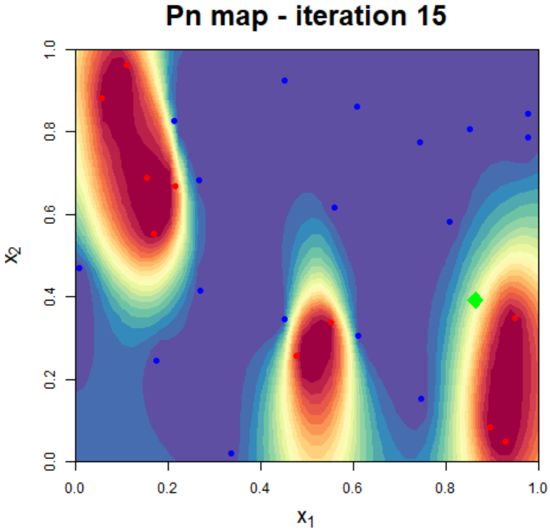

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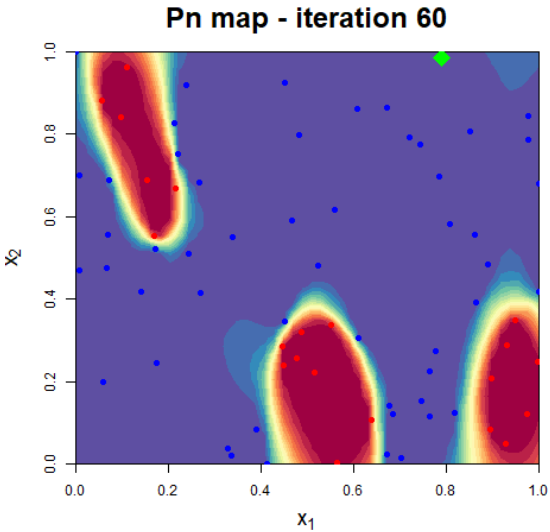

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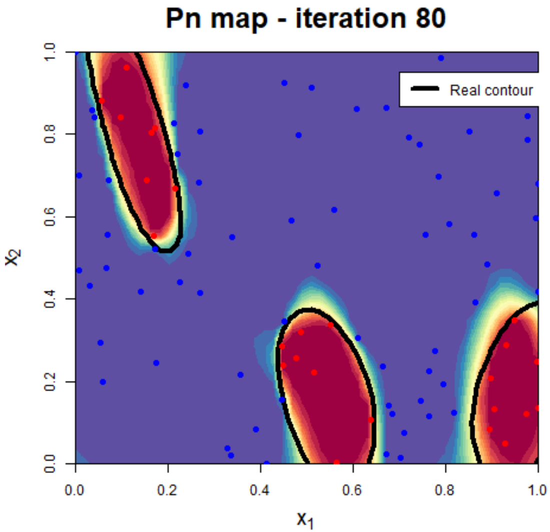


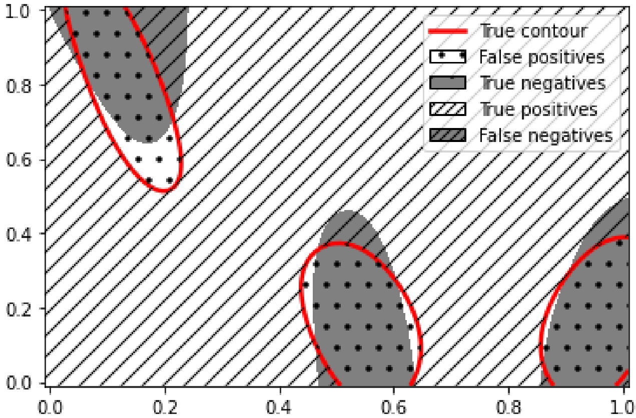
Results: comparison of different enrichment criteria

Compared strategies:

- SUR criterion for classification
- Mixed enrichment criterion: add of 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) simultanously
- SMOCU enrichment measure: Soft-MOCU (Mean Objective Cost of Uncertainty) method [Zhao et al., 2021]

Results: comparison criteria

1 - Number of true positives ($Q_\alpha \cap \Gamma^*$) and true negatives ($\Omega \setminus (Q_\alpha \cap \Gamma^*)$)

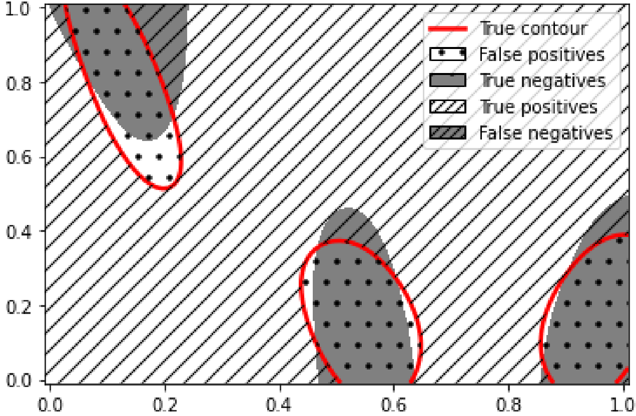


$$crit_P = \frac{TP}{P}$$

$$crit_N = \frac{TN}{N}$$

Results: comparison criteria

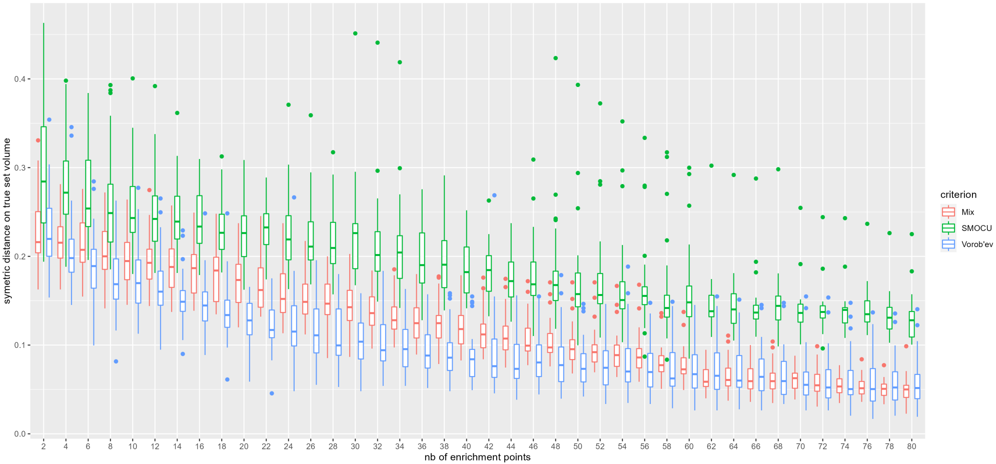
2 - Relative error of the feasible set estimation



$$crit_F = \frac{FN + FP}{P}$$

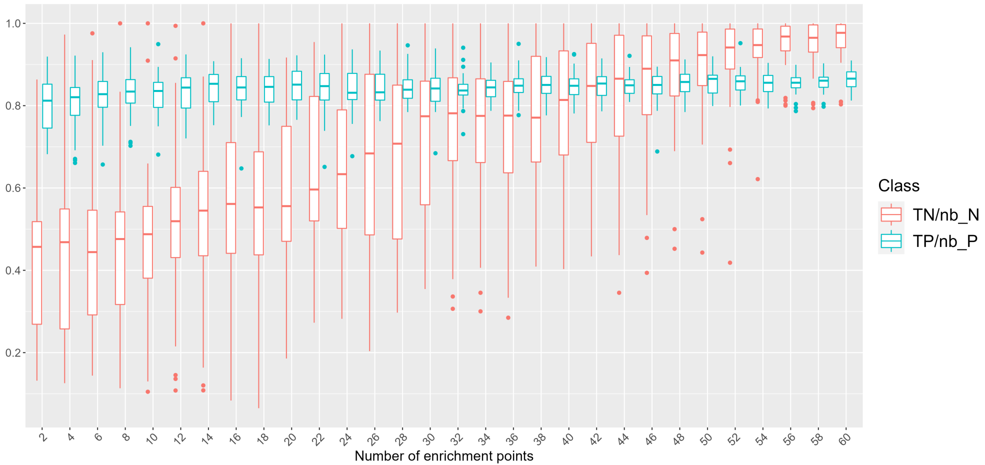
Results on the classification problem based on Branin function

Evolution of $crit_F$ for mixed, SMOCU and SUR criteria



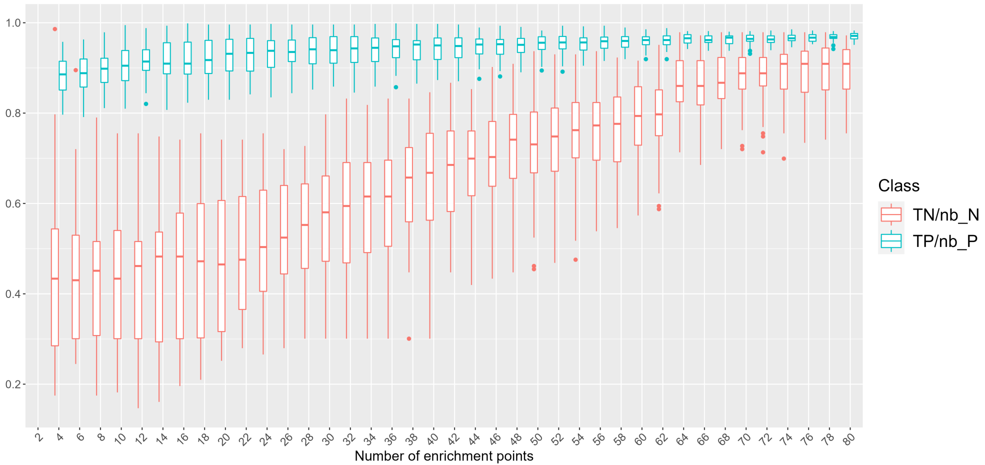
Results on the classification problem based on Branin function

Evolution of the number of true positives/negatives for SMOCU method



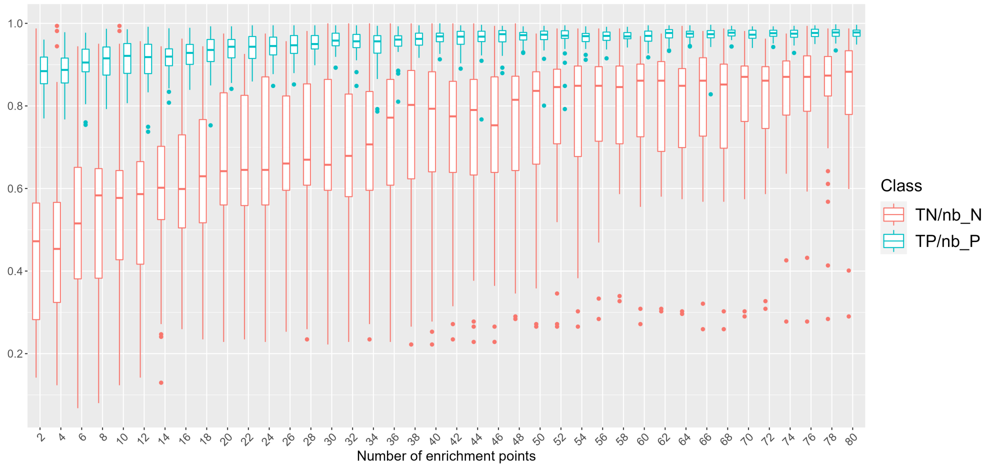
Results on the classification problem based on Branin function

Evolution of the number of true positives/negatives for mixed criterion



Results on the classification problem based on Branin function

Evolution of the number of true positives/negatives for SUR criterion



Example in 4 dimensions

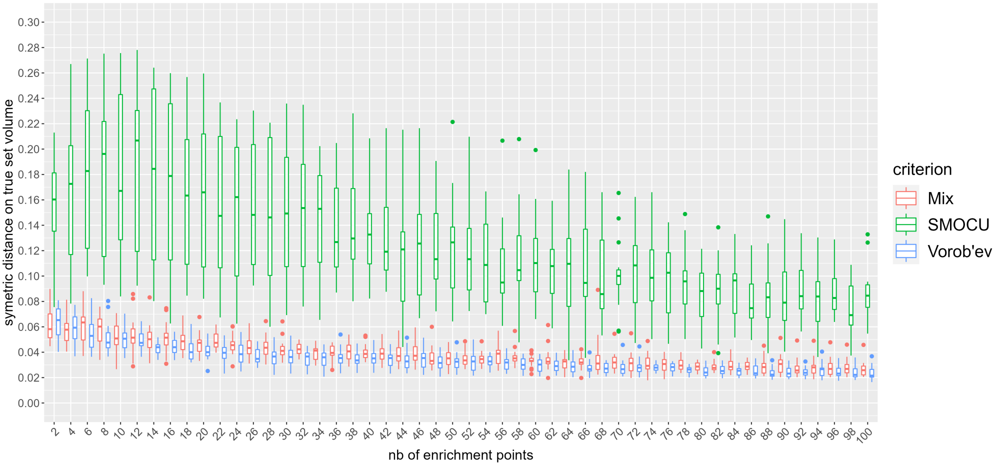
Classification problem with two constraints defined in $[0,1]^4$:

$$f_1(x_1, x_2, x_3, x_4) = x_2 + x_1 - 1.6 + 0.1 * x_3$$

$$f_2(x_1, x_2, x_3, x_4) = 0.15 - (x_2^2 + (x_1 + 0.1)^2)$$

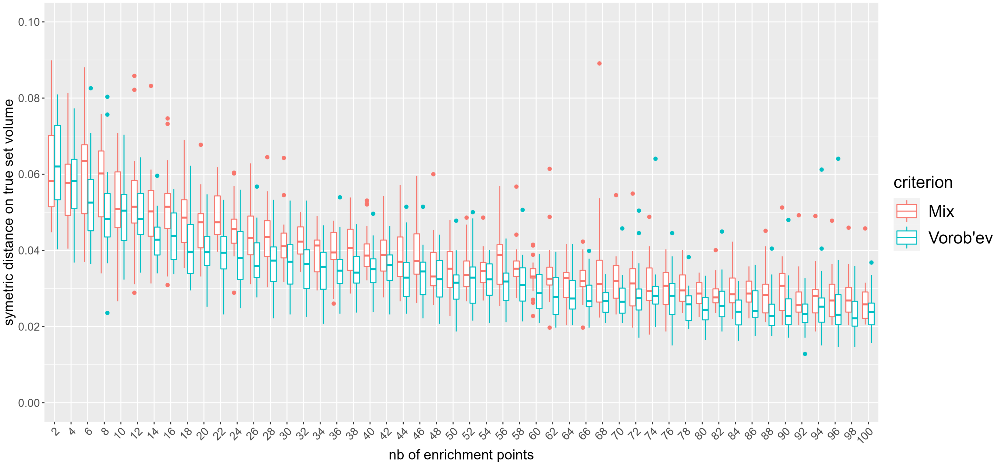
Results on the classification problem in 4 dimensions

Evolution of $crit_F$ for mixed, SMOCU and SUR criteria



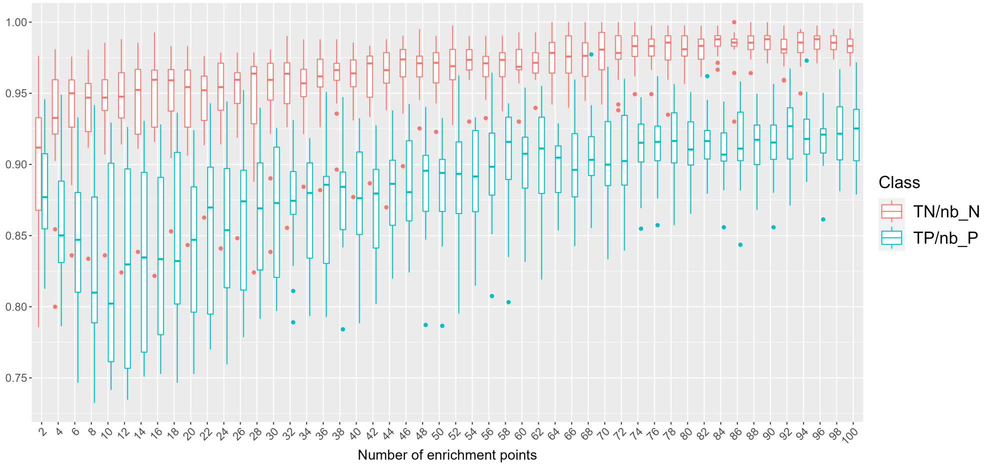
Results on the classification problem in 4 dimensions

Evolution of $crit_F$ for mixed, SMOCU and SUR criteria



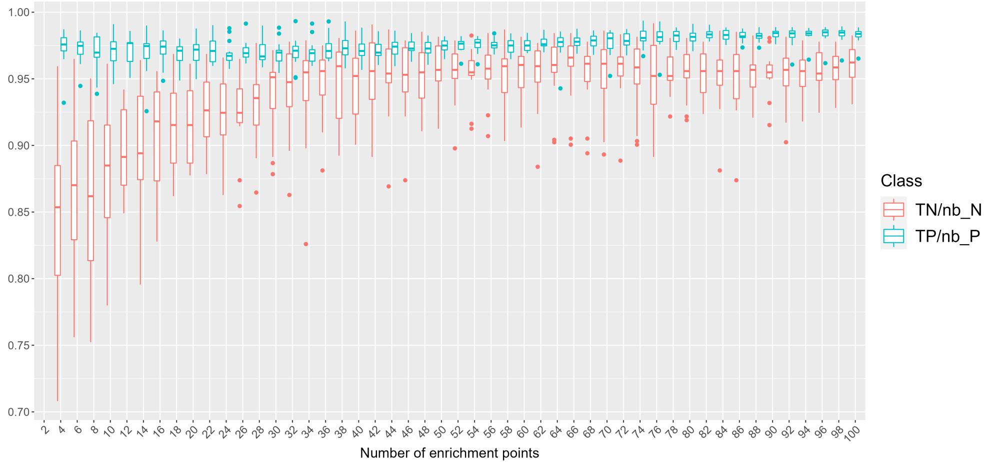
Results on the classification problem in 4 dimensions

Evolution of the number of true positives/negatives for SMOCU method



Results on the classification problem in 4 dimensions

Evolution of the number of true positives/negatives for mixed criterion



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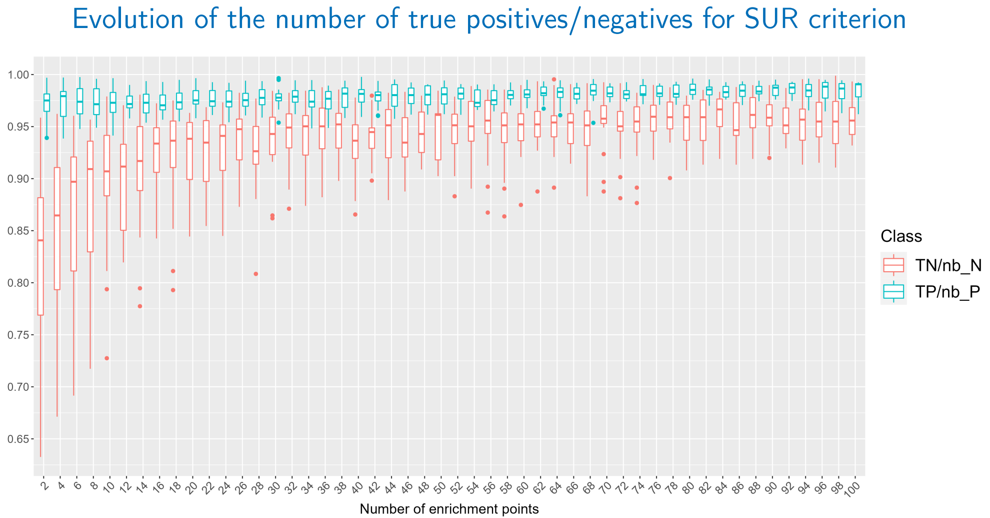

Conclusions and outlook

Conclusions:

- great potential to learn feasible sets in terms of crash constraints
- drawbacks: enrichement criterion computation (integration) and optimization time in high dimension

Perspectives:

- Coupling with an optimization ➜ e.g. NOMAD, see session MB8: Stéphane Jacquet's presentation (at 15h30)
- Take into account the simulation robustness or convergence level (more than two classes)

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Expressions of m_n and k_n for the GPC model

$$m_n(x, z_n^{(i)}) = \mu_Z + k_\theta^Z(x, \mathcal{X})(k_\theta^Z(\mathcal{X}, \mathcal{X}))^{-1}(z_n^{(i)} - \mu_Z)$$

and

$$k_n(x, x') = k_\theta^Z(x, x') + k_\theta^Z(x, \mathcal{X})(k_\theta^Z(\mathcal{X}, \mathcal{X}))^{-1}k_\theta^Z(\mathcal{X}, x')$$

GP update formulae

Updated GP mean for r new points $x^{(r)} = (x_{n+1}, \ldots, x_{n+r})$:

$$m_{n+r}(x) = m_n(x) + \lambda_{new}(x)^T Z_c(x^{(r)})$$

with:

- $Z_c(x^{(r)}) = Z(x^{(r)}) - m_n(x^{(r)})$ le vecteur des réponses centrées de distribution $\mathcal{N}(0, \Sigma)$, où Σ est la matrice de covariance de $(Z_n(x_{n+1}), \ldots, Z(x_{n+r}))$
- $\lambda_{new}(x) = K_{new}^{-T} k_n(x, x^{(r)})$ et $K_{new} = k_n(x^{(r)}, x^{(r)})$

Updated covariance function of GP Z:

$$k_{n+r}(x, x') = k_n(x, x') - k_n(x, x^{(r)})^T K_{new}^{-1} k_n(x', x^{(r)})$$

Vorob'ev expectation and deviation

Vorob'ev deviation can be expressed as follows:

$$
\begin{aligned}
var_n(\Gamma) &= \mathbb{E}[\mu(Q_\alpha \Delta \Gamma)|z] \\
&= \int_{Q_\alpha} (1 - p_n(x))\mu(dx) + \int_{Q_\alpha^C} p_n(x)\mu(dx) \\
&= \int (1 - p_n(x)) \mathbb{1}_{p_n(x) \geq \alpha^*} \mu(dx) + \int p_n(x) \mathbb{1}_{p_n(x) < \alpha^*} \mu(dx)
\end{aligned}
$$

with Δ such that $A \Delta B = (A \cup B) \setminus (A \cap B)$

GPC and *Jn* criterion

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Expression of the first term of J_n criterion in the integral on x:

$$\mathbb{E}_n\left[p_{n+1}(x)\mathbb{1}_{p_{n+1}(x)<\alpha^*}\right]$$

$$= \mathbb{E}_n\left[\frac{1}{N}\sum_{i=1}^{N}\bar{\Phi}\left(\frac{-m_{n+1}(x,z_n^{(i)})}{\sqrt{k_{n+1}(x)}}\right)\mathbb{1}_{\frac{1}{N}\sum_{j=1}^{N}\bar{\Phi}\left(\frac{-m_{n+1}(x,z_n^{(j)})}{\sqrt{k_{n+1}(x)}}\right)<\alpha^*}\right]$$

$$= \mathbb{E}_n\left[\frac{1}{N}\sum_{i}\bar{\Phi}\left(\frac{-(m_n(x,z_n^{(i)})+\lambda_{new}(x)^T\mathrm{U})}{\sqrt{k_{n+1}(x)}}\right)\mathbb{1}_{\frac{1}{N}\sum_{j}\bar{\Phi}\left(\frac{-(m_n(x,z_n^{(j)})+\lambda_{new}(x)^T\mathrm{U})}{\sqrt{k_{n+1}(x)}}\right)<\alpha^*}\right]$$

avec $\mathrm{U} \sim \mathcal{N}(0,\Sigma)$, où Σ est la matrice de covariance de $(Z_n(x_{n+1}),\ldots,Z(x_{n+r}))$.

Remark: The realizations $z_n^{(i)}$ are not updated because $sign(Z(x_{n+1}))$ do not provide any information on Z_n.

GPC and Vorob'ev based *Jn* criterion

The third can be expressed as follows:

$$\mathbb{E}_n\left[\mathbb{1}_{p_{n+q}(x)\geq\alpha^*}\right]$$

$$= \mathbb{E}_n\left[\mathbb{1}_{\frac{1}{N}\sum_j \bar{\Phi}\left(\frac{-(m_n(x,z_n^{(i)})+\lambda_{new}(x)^T\mathbf{U})}{\sqrt{k_{n+q}(x)}}\right)<\alpha^*}\right]$$

Update of the realizations $z_n^{(i)}$

MOBILITÉ DURABLE

$$z_{n+q}^{(i)} = z_n^{(i)} + \lambda_{new}^Z(\mathcal{X})^T (Z_n(x_{new})_{real} - Z_n(x_{new})_{simu})$$

$$\begin{pmatrix} Z(x_1)^{(i)} \\ \vdots \\ Z(x_n)^{(i)} \end{pmatrix}_{n+q} = \begin{pmatrix} Z(x_1)^{(i)} \\ \vdots \\ Z(x_n)^{(i)} \end{pmatrix}_n + \lambda_{new}^Z(\mathcal{X})^T Z_{n,c}(x_{new})$$

with $Z_{n,c}(x_{new}) \sim \mathcal{N}(0, k^Z(x_{new}, x_{new}))$ and $\lambda_{new}^Z(\mathcal{X}) = k^Z(x_{new}, x_{new})^{-T} k^Z(x_{new}, \mathcal{X})$.

Yet:

- we do not guarantee that the signs of $z_{n+q}^{(i)}$ correspond to the observed values $y_1, \ldots, y_n$ anymore,
- it can be verified that as for Z_n, Z_{n+q} can be modeled by a GP with constant mean μ_Z and a stationary covariance function k_θ^Z

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Vorob'ev expectation and deviation

MOBILITÉ DURABLE

Let us consider the random set:

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

The function

$$\begin{aligned} P_\Gamma(x) &= \mathbb{P}[x \in \Gamma] \\ &= p_n(x) \end{aligned}$$

is the cover function of Γ and its level sets are the α-percentiles of Γ:

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

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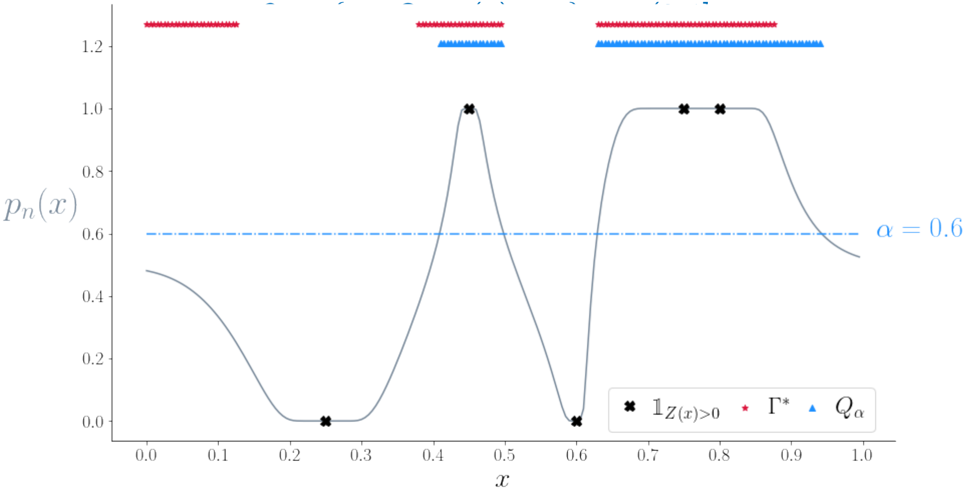

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Vorob'ev expectation and deviation

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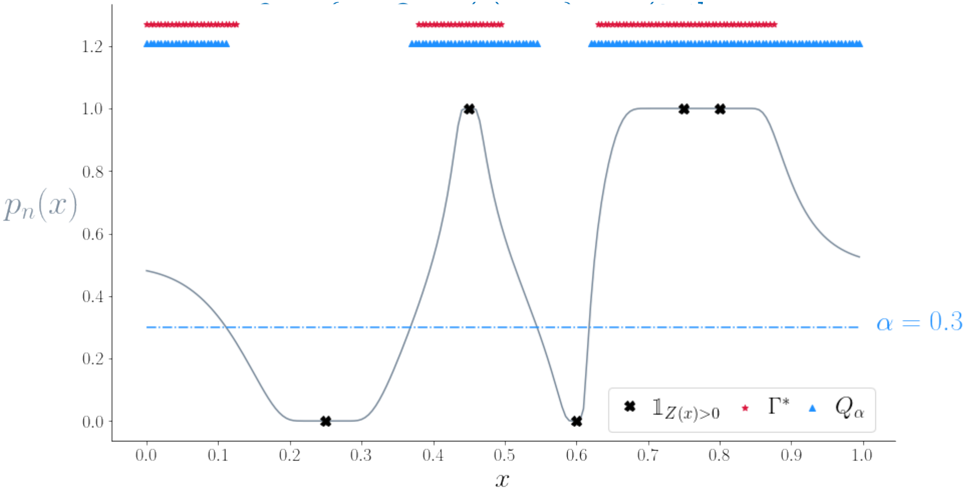


Vorob'ev expectation and deviation

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.

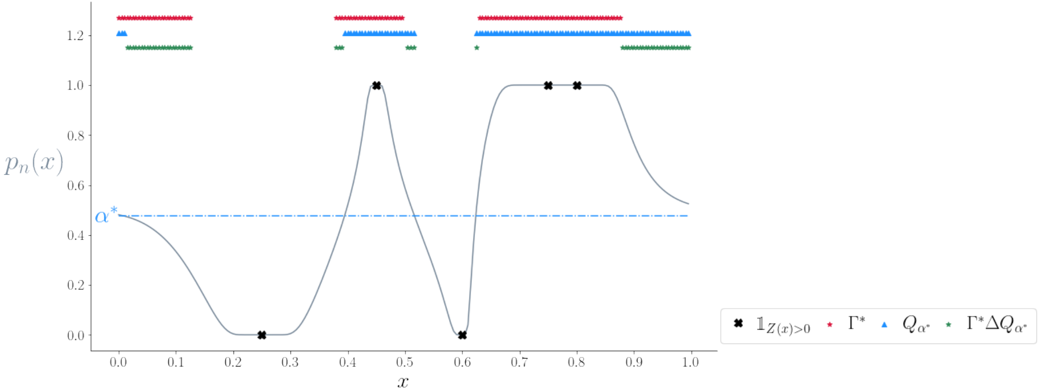
Vorob'ev expectation is a global minimiser of the vorob'ev deviation $Var_n(\Gamma)$ among closed sets of volume equal to the mean volume of Γ:

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

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

Vorob'ev expectation and deviation

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



MOCU/SMOCU criteria

$$U^{MOCU}(x) = \mathbb{E}_{x_s}[\mathbb{E}_n[max(p_{n+1}(x_s), 1 - p_{n+1}(x_s))] - max(p_n(x_s), 1 - p_n(x_s))]$$

i.e.

$$U^{MOCU}(x) = \mathbb{E}_{x_s}[1 - max(p_n(x_s), 1 - p_n(x_s))] - \mathbb{E}_n[\mathbb{E}_{x_s}[1 - max(p_{n+1}(x_s), 1 - p_{n+1}(x_s))]$$

et

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

