Learning and space-filling design space constrained from hidden failure of computer experiments

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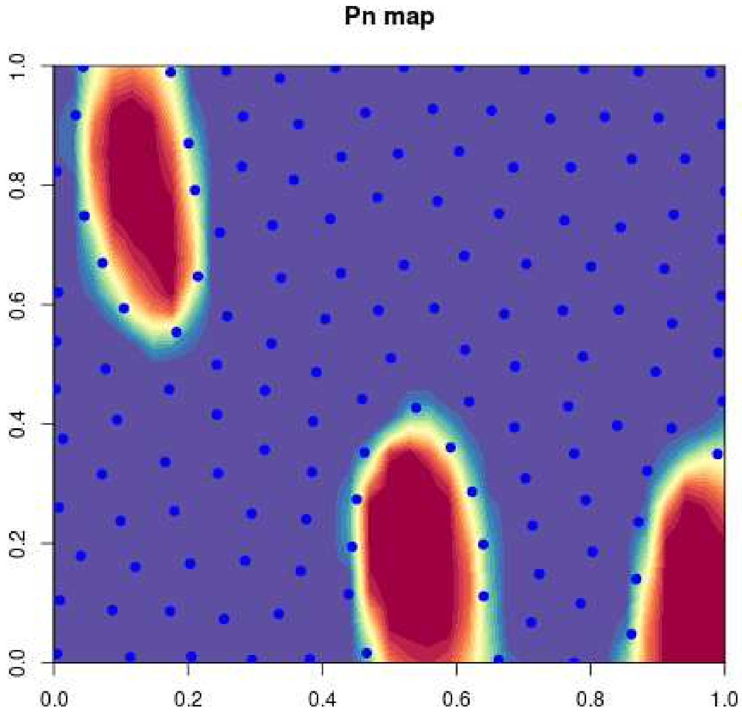
IHP, 10-11 December 2024

LEARNING AND SPACE-FILLING OBJECTIVES

- Accelerate: learning of the hidden constraint and generation of a space-filling design of experiments in the hidden constrained space
  - Sequential strategy: propose point dedicated **alternatively** to learning and space-filling
  - Coupled strategy: propose point dedicated **simultaneously** to learning and space-filling



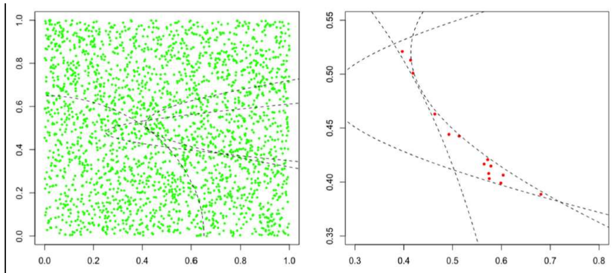
SPACE-FILLING IN CONSTRAINED SPACE

CoMinED [Huang et al.. 2021] : **Sequential** construction technique of **space-filling designs** with **continuous constraints**

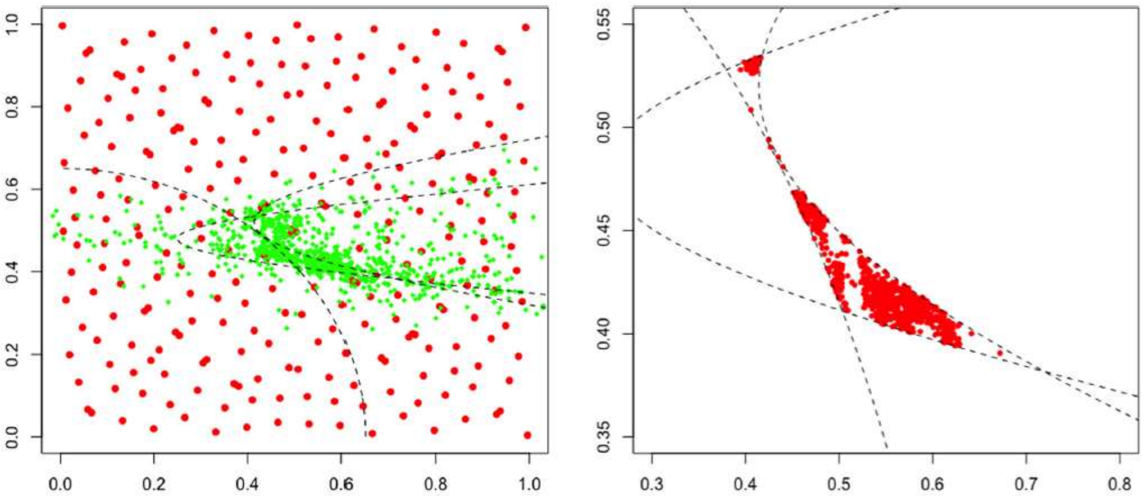
- **Candidate Generation: generate a large set of uniformly distributed candidates in X.**
- Design Construction: choose points from the set of candidates by a desired criterion.

$$\{x \in \Omega, g(x) \leq 0\}$$

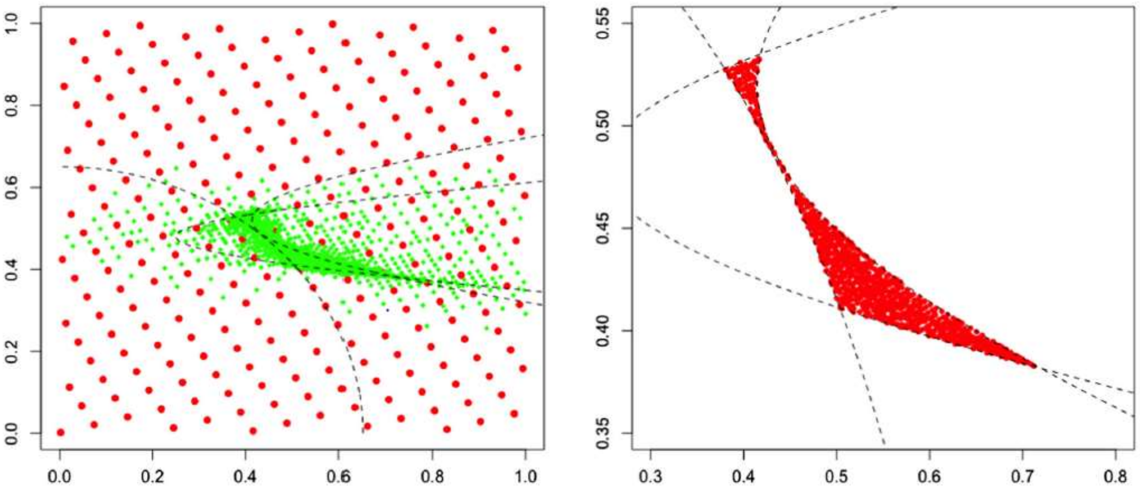
GRAPHICAL MOTIVATION [Huang et al.. 2021]



Rejection/Acceptation



Red left:
265 Sobol' points
Green left:
Adaptive Sequentially Constrained Monte Carlo
Golchi and Loeppky, 2015
Red Right:
feasible points

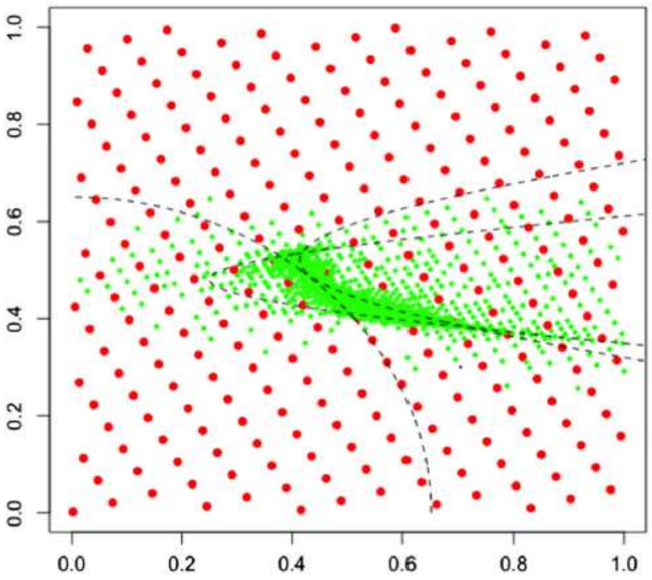


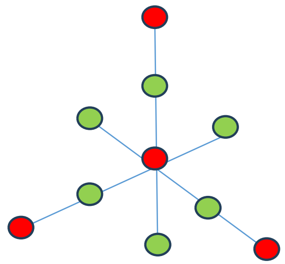
Red left:
lattice grid of points
Green left:
CoMinED population: Q-NN, middle and reflection
Red Right:
feasible points

CONSTRAINED MINIMUM ENERGY DESIGNS ALGORITHM

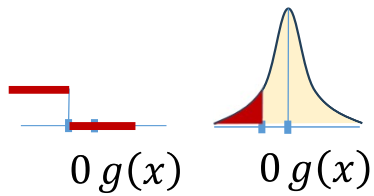
Augmentation of the set of candidate samples $\mathcal{C}^t$

Q-NN, middle point and reflection





CONSTRAINED MINIMUM ENERGY DESIGNS ALGORITHM



Constrained greedy maximin

$$\max_x \mathbb{1}_{g(x)\leq 0}\mathbb{1}_{g(x_i)\leq 0}\min_i \|x_i - x\|_s$$

$$\mathbb{1}_{g(x)\leq 0} \sim \Phi(-\tau g(x))$$

Inputs:

- sequence of rigidity parameters $(\tau_t)_{t=1,\dots,T}$.
- continuous constraints $g(x)$ -> g(x)<0
- parameters for candidate set augmentation : Q

- Initialisation of the initial candidate set $\mathcal{C}^1$
- For t= 1. … . T
  - Construction of a constrained DoE $\mathcal{D}_c$: **one-point-at-a-time Greedy-algorithm** with τ_t on candidate samples $\mathcal{C}^t$

$$x_{m+1}^t = \underset{x\in C^t\setminus\{x_l\}_{l=1}^m}{\operatorname{argmax}} \Phi(-\tau_t g(x))\left[\min_{i=1,\dots,m} \Phi(-\tau_t g(x_i))\|x_i - x\|_s^{2p}\right]$$

  - Augmentation of the set of candidate samples $\mathcal{C}^t$

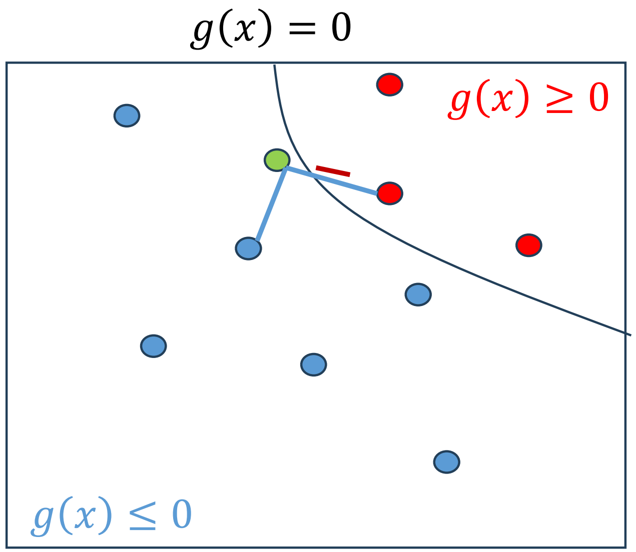
$$\|u\|_s = \left(\frac{1}{p}\sum_{l=1}^{p}|u_l|^s\right)^{\frac{1}{s}}$$ $\mathcal{D}_c = \{x_l\}_{l=1}^n$ Φ: Gaussian cumulative prob. function

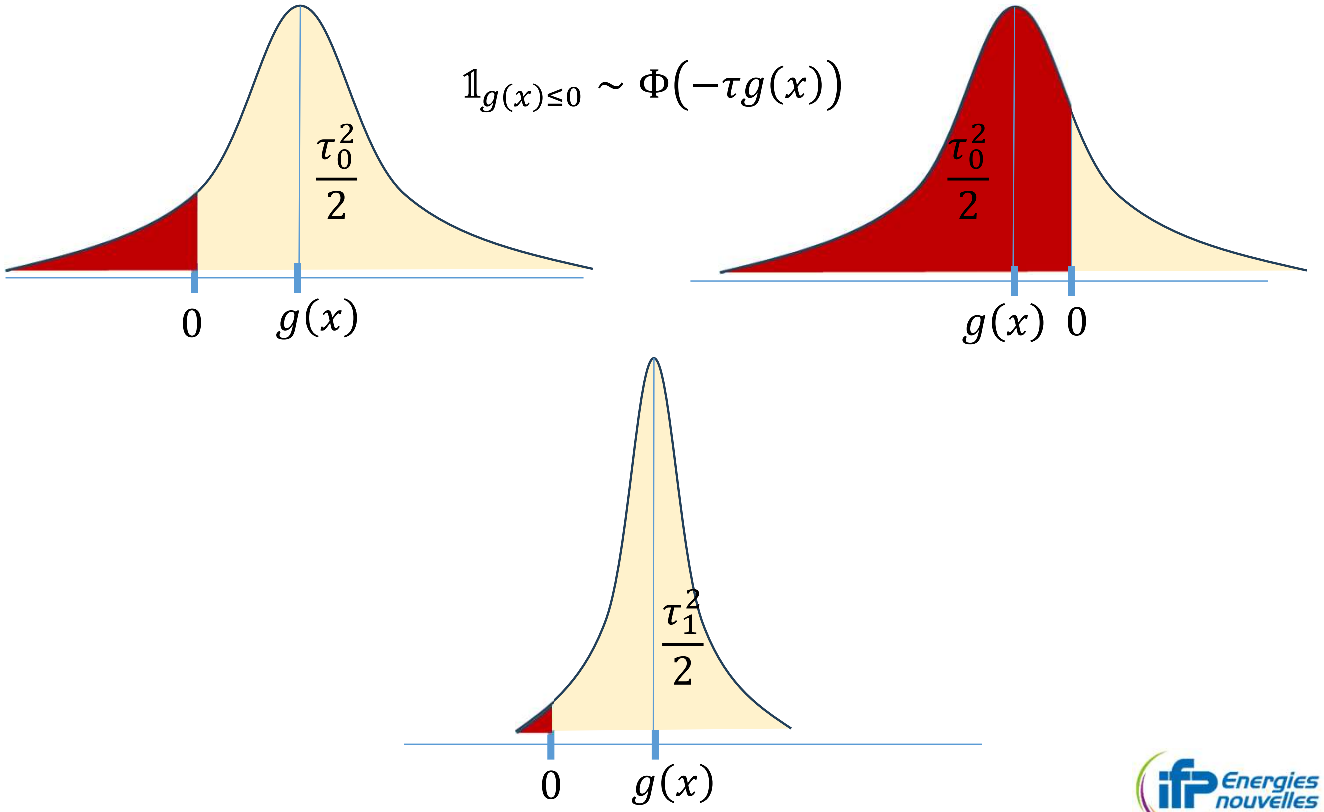
COMINED CRITERION FROM WITHIN

$0 < \tau_0 < \cdots < \tau_T$

$$x_{m+1}^t = \underset{x \in C^t \backslash \{x_l\}_{l=1}^m}{\text{argmax}} \; \Phi(-\tau_t g(x)) \left[\min_{i=1,\ldots,m} \Phi(-\tau_t g(x_i)) \|x_i - x\|_s^{2p} \right]$$

$\mathbb{1}_{g(x) \leq 0} \sim \Phi\big(-\tau g(x)\big)$

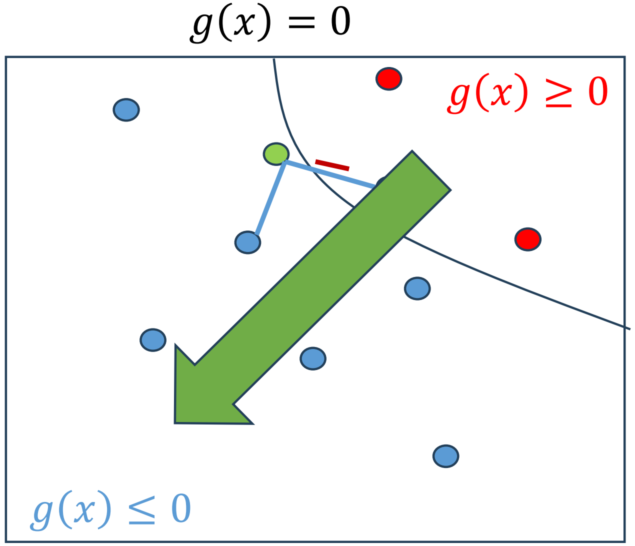


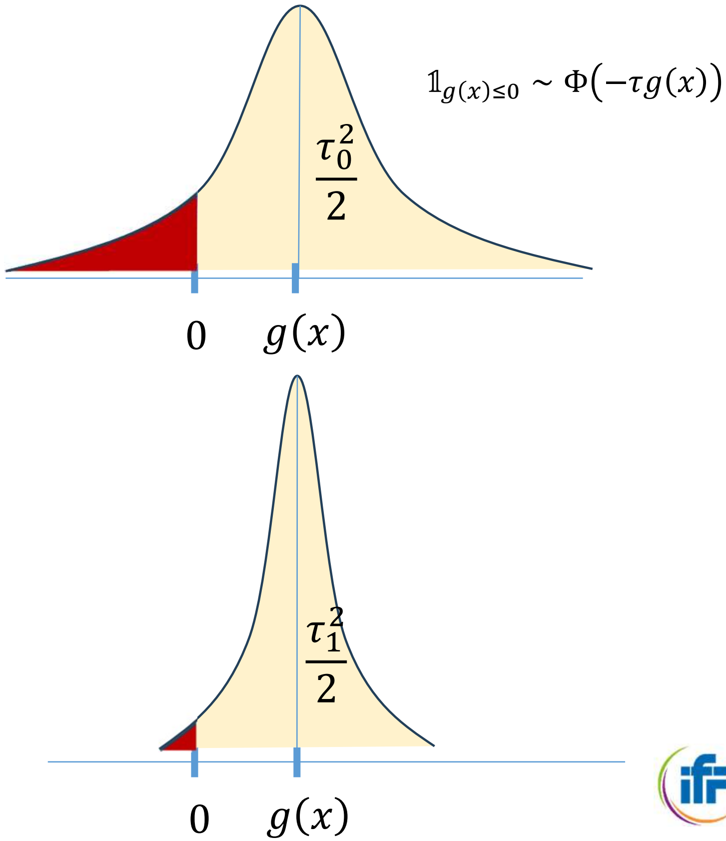


COMINED CRITERION FROM WITHIN

$0 < \tau_0 < \cdots < \tau_T$

$$x_{m+1}^t = \underset{x \in C^t \setminus \{x_l\}_{l=1}^m}{\operatorname{argmax}} \Phi(-\tau_t g(x)) \left[\min_{i=1,\ldots,m} \Phi(-\tau_t g(x_i)) \|x_i - x\|_s^{2p} \right]$$





APPLICATION WITH HIDDEN CONSTRAINTS

In **hidden** constraints context: one **binary** constraint $y(x) \in \{0,1\}$

- $y(x)$ result of **expensive simulations**
- $y(x)$ **non-continuous constraint**: untractable with usual constrained space-filling construction techniques

Consider a conditioned **Gaussian Process Classifier [Bachoc et al. 2020]** model $Y_n(x) = Y(x)|x_n, y_n$ of the hidden constraint $y(x)$. It predicts: $p_n(x) = \mathbb{P}[Y_n(x) = 1]$

CoMinED can be applied with :

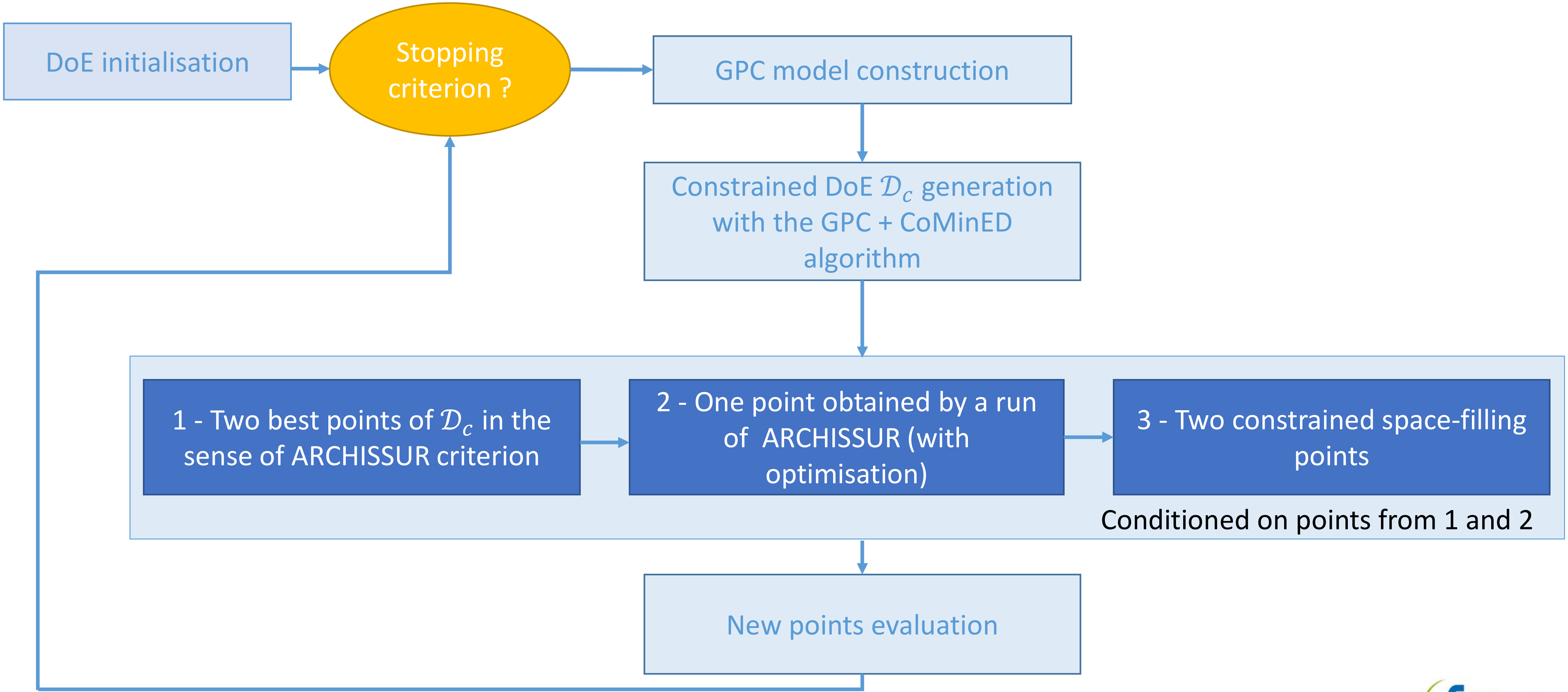
$$g(x) = \alpha^* - p_n(x)$$

$$x_{m+1}^t = \underset{x \in \mathrm{C}^t \backslash \{x_l\}_{l=1}^m}{\operatorname{argmax}} \Phi(-\tau_t g(x)) \left[\min_{i=1,\ldots,m} \Phi(-\tau_t g(x_i)) \|x_i - x\|_s^{2p} \right]$$

α^* estimated within the Vorob'ev expectation of $\Gamma = \{x \in \Omega | Y_n(x) = 1\}$ estimation

$$\hat{\boldsymbol{\Gamma}}_{\boldsymbol{n}} = \{\boldsymbol{x} \in \boldsymbol{\Omega}, \boldsymbol{p_n}(\boldsymbol{x}) \geq \boldsymbol{\alpha}^*\}$$

PROPOSED ADAPTIVE SPACE-FILLING STRATEGY



STOPPING CRITERION OF THE ADAPTIVE ALGORITHM

1st scenario: **reaching a total number of simulations or "convergence"**

At iteration i stop if:

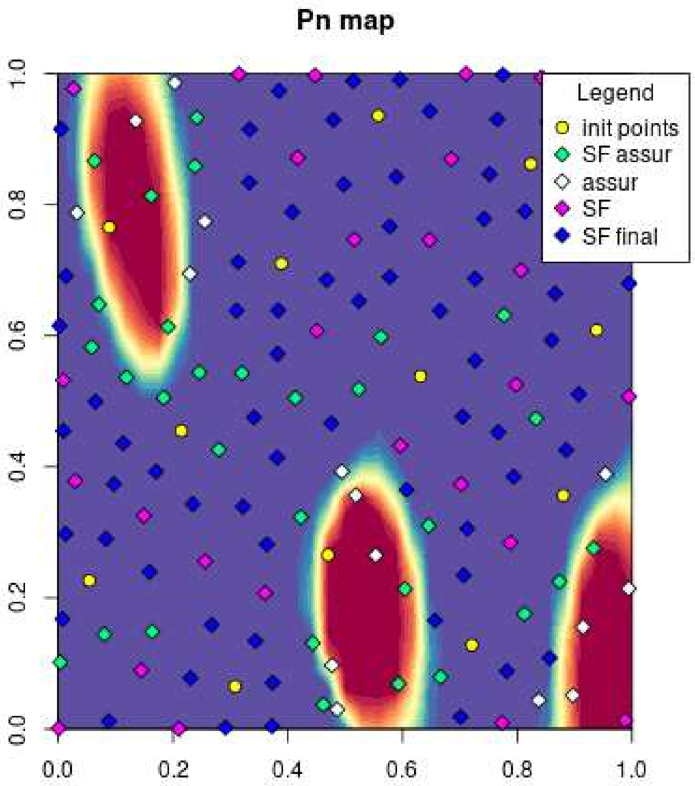
$$n_{sim}^{i} > n_{sim}^{adapt} \quad or \quad \frac{|Var_j(\Gamma) - Var_{j-1}(\Gamma)|}{\mathbb{E}_j[\mu(\Gamma)]} < \epsilon \quad \forall j \in \{i - l. \dots . i\}$$

$$n_{sim}^{adapt} = \lfloor C n_{sim} \rfloor$$

With the remaining simulation budget: Constrained space-filling with current GPC model

2nd scenario: **reaching a number of successful simulations**

ILLUSTRATION ON BRANIN EXAMPLE



Inputs:

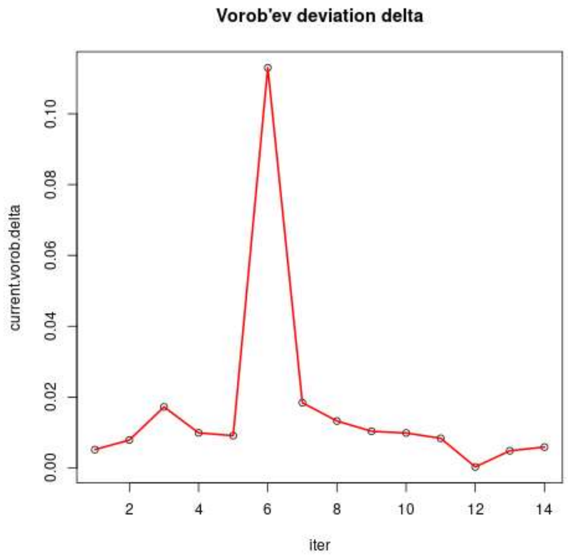
$n_{init} = 12$

$n_{sim}^{max} = 12 + 30 * 5$

$n_{sim}^{adapt} = 24 * 5$

$l = 4$

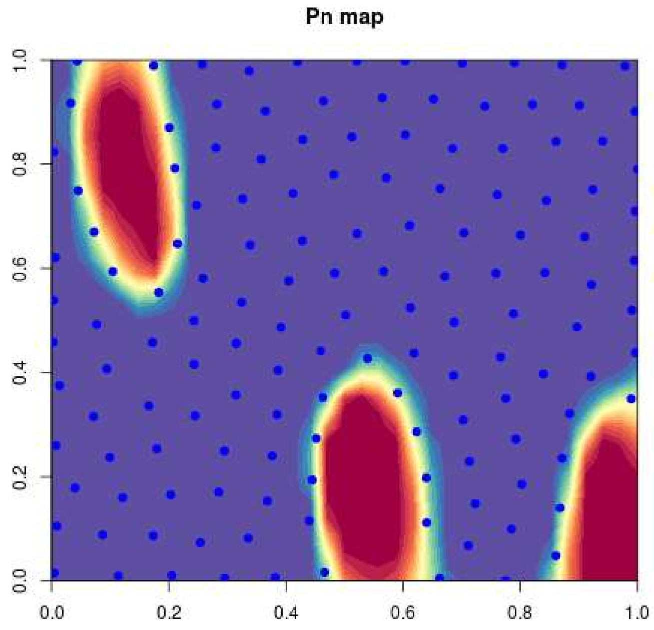
$\epsilon = 10^{-2}$



COMPARAISON OF RESULTS

- Comparison with **optimal** constrained DoE
  → In practice : obtained with simulated annealing [Auffray. 2012] adapted to non-connex domains [internal IFPEN report] on the final DoE of the adaptive procedure

- Comparison with a **crude rejection** method

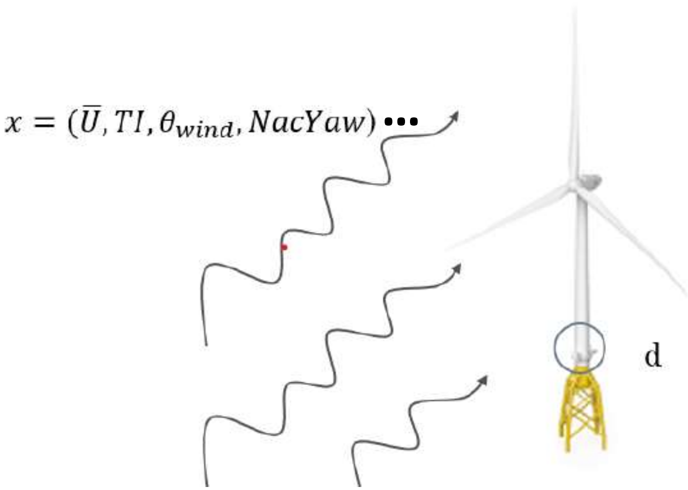


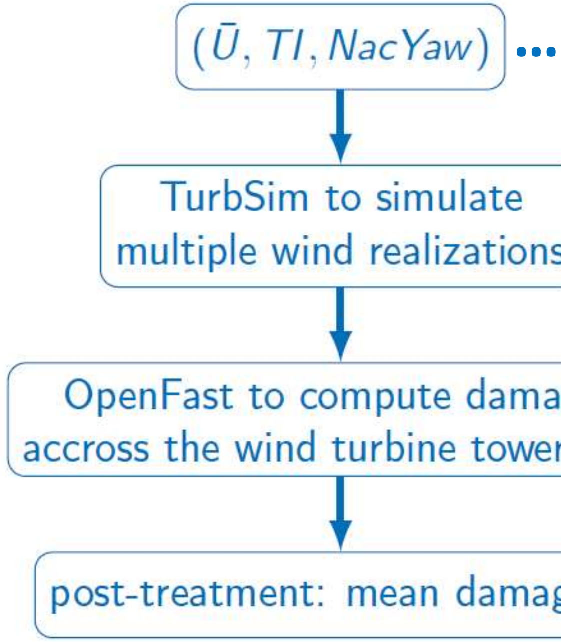
DAMAGE PREDICTION OF A WIND TURBINE

Wind loads are described by 13 parameters:

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

…





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COMPARAISON OF RESULTS – WIND TURBINE

Initial doe size: 100
total simulation points: 1000
dimension: 13

$$Q_{\alpha^*} = \{x \in \Omega : p_n(x) \geq \alpha^*\}$$

	MINMAX	MAXMIN	EFFICIENCY
LHS MAXIMIN + REJECTION	2.12	1.25	0.42
Initial GPC + COMINED	1.68	0.85	**0.93**
ASUR SF	1.66	0.98	0.75
ASUR SF + COMINED (Greedy) (80% + 20%)	**1.63**	**0.94**	**0.79**

Robustesse ?
More conservative ?
Points on frontier more
Spread on the feasable area

$$\text{Efficiency} = \frac{n_{success}}{n_{sim}}$$

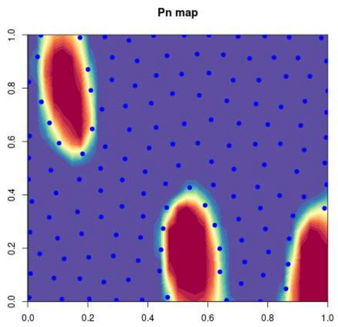
COMPARAISON OF RESULTS – WIND TURBINE

Initial doe size: 100
total simulation points: 1000
dimension: 13

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

Q2 ->	Proba 0.2	Proba 0.4	Proba 0.5	Proba 0.6	Proba 0.8	Proba0.95
REJECTION (0.067)	NA	NA	NA	NA	NA	NA
Initial GPC + COMINED	**0.57**	**0.61**	0.61	0.63	0.64	0.76
ASUR SF	0.08	0.45	0.77	**0.86**	**0.92**	0.97
ASUR SF + COMINED (80% + 20%)	-0.002	**0.61**	**0.81**	0.85	0.91	**0.98**

$$\text{Efficiency} = \frac{n_{success}}{n_{sim}}$$



Work in progress

A PROCESS OF SUR-IFICATION

Stepwise Uncertainty Reduction (SUR) and assimilated one-step-lookahead strategies

criteria

- Variance
- Expected Improvement
- Integrated Bernouilli Variance
- Vorob'ev deviation
- **Bichon**
- Ranjan

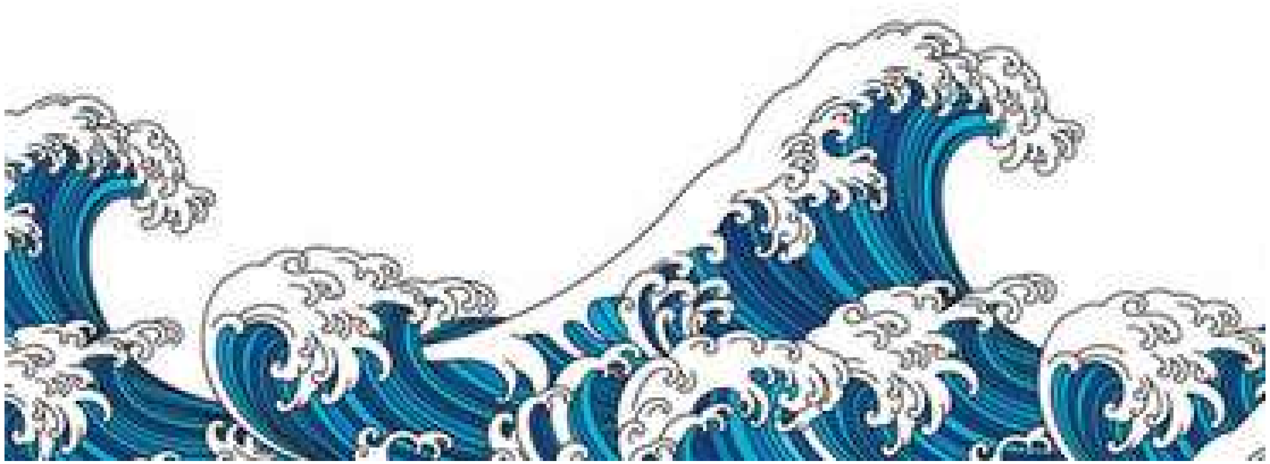
…

A PROCESS OF SUR-IFICATION

Stepwise Uncertainty Reduction (SUR) and assimilated one-step-lookahead strategies

Proofs of convergence
of the SUR based estimator

SUR-ification of criteria



criteria

A SAMPLE FROM THE PROCESS OF SUR-IFICATION

Stepwise Uncertainty Reduction (SUR) and assimilated one-step-lookahead strategies

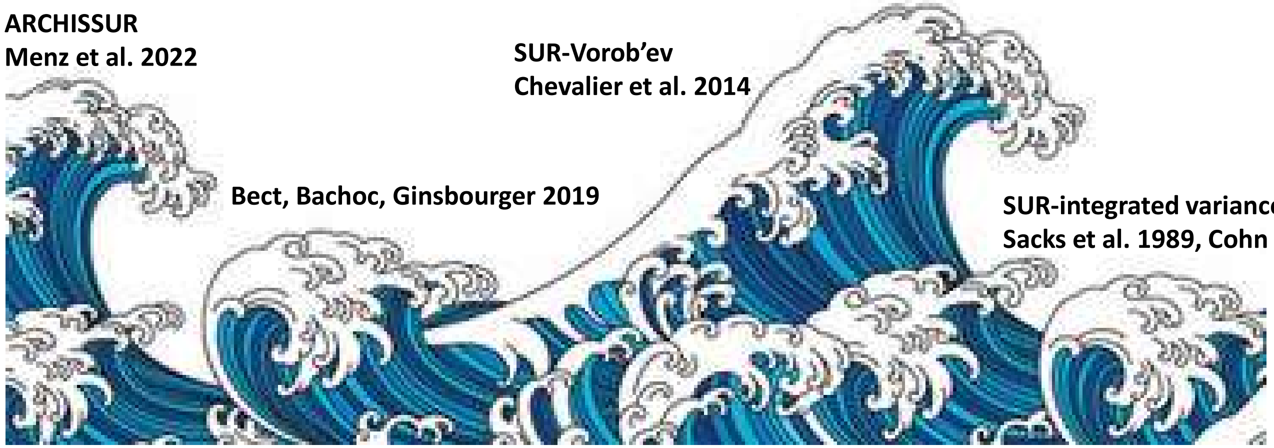
Proofs of convergence
of the SUR based estimator

SUR-ification of criteria

SUR-EER
Roy et al. 2001

ARCHISSUR
Menz et al. 2022

SUR-Vorob'ev
Chevalier et al. 2014



Bect, Bachoc, Ginsbourger 2019

SUR-integrated variance
Sacks et al. 1989, Cohn et al. 1996

SUR-Bichon
Duhamel et al. 2024

criteria

SUR-Integrated Bernouilli
Bect et al. 2012

Bect Vazquez 2010
Bull 11
Srinivas et al 2012

PROCESS OF SUR-IFICATION

Stepwise Uncertainty Reduction - SUR

Proofs of convergence
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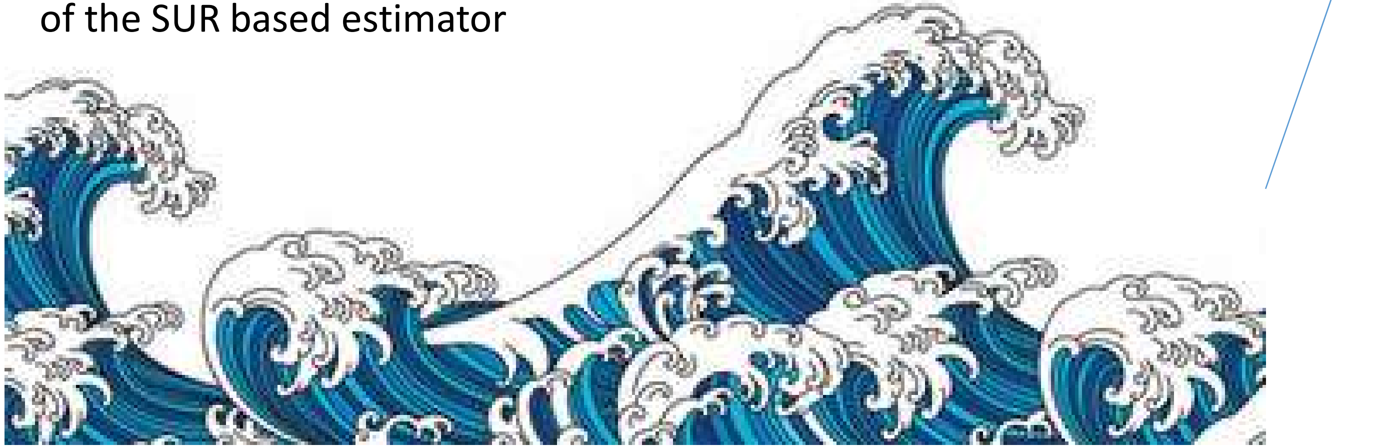
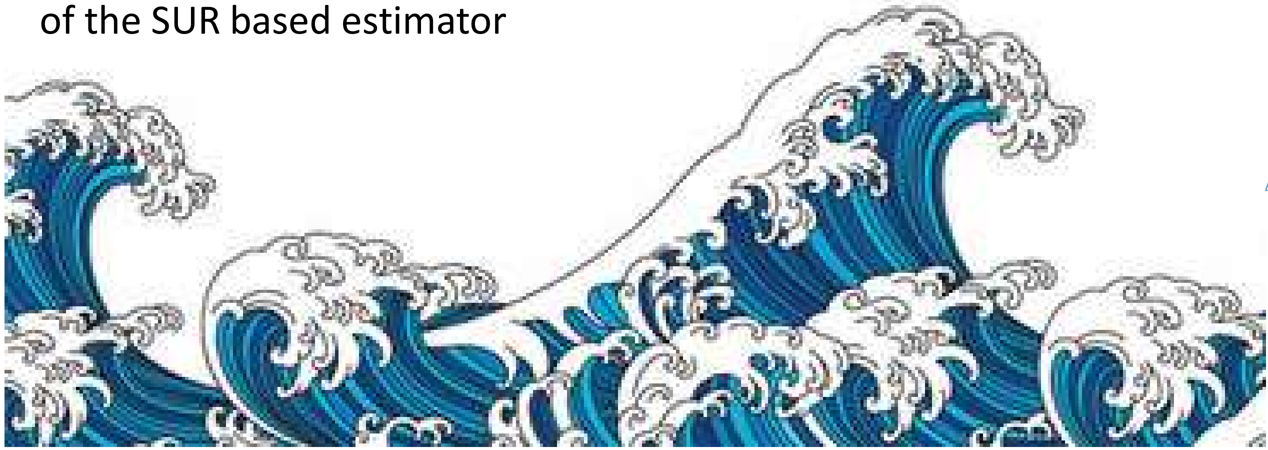
SUR-ification of criteria



PROCESS OF SUR-IFICATION

Stepwise Uncertainty Reduction - SUR



Proofs of convergence
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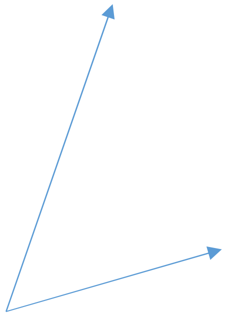

PROCESS OF SUR-IFICATION

Stepwise Uncertainty Reduction - SUR

Proofs of convergence
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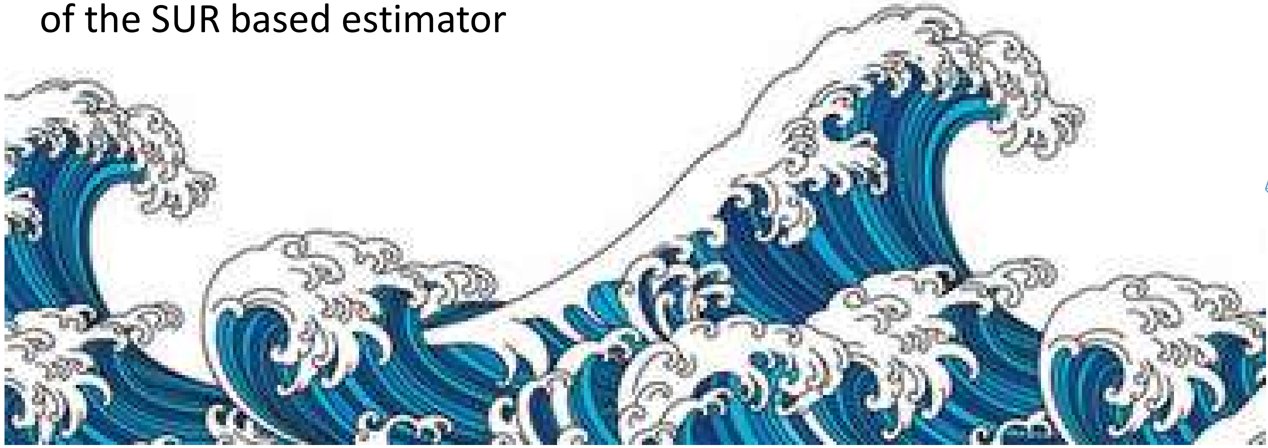


1. VANILLA ONE-STEP-LOOKAHEAD

$$g_{t,m+1}(x) = \alpha_m^* - p_{t,m+1}(x)$$

$$\alpha_m^* \sim 1/2$$

$$\underset{x_{m+1}\in C^t \backslash \{x_l\}_{l=1}^m}{argmax} \mathbb{E}_{Y_{m+1}}[U_{t,m+1}]$$

$$U_{t,m+1} = \min_{i=1,\dots,m} \frac{1}{2p} \log\Big(\Phi\big(-\tau_t g_{t,m+1}(x_{m+1})\big)\Big) + \frac{1}{2p} \log\Big(\Phi\big(-\tau_t g_{t,m}(x_i)\big)\Big) + \log(\|x_i - x_{m+1}\|_s)$$

$$\underset{x_{m+1}}{argmax}\, \mathbb{E}_{Y_{m+1}}\big[\Phi\big(-\tau_t g_{t,m+1}(x_{m+1})\big)\big] \min_{i=1,\dots,m} \Phi\big(-\tau_t g_{t,m}(x_i)\big)\|x_i - x_{m+1}\|_s^{2p}$$

$$\mathbb{E}_{Y_{m+1}}\big[\Phi\big(-\tau_t g_{t,m+1}(x_{m+1})\big)\big] = p_{t,m}(x_{m+1})\Phi\big(-\tau_t(\alpha_m^* - 1)\big) + \big(1 - p_{t,m}(x_{m+1})\big)\Phi(-\tau_t \alpha_m^*)$$

2. A STEP BACK

$$g_{t,m}(x) = \alpha_m^* - p_{t,m}(x)$$

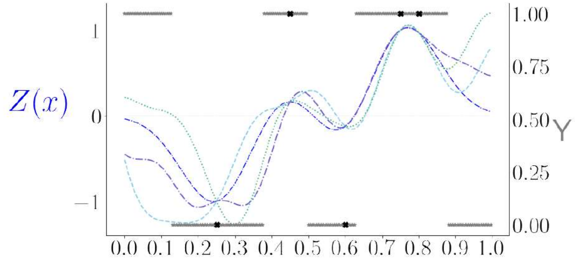
$$\underset{x_{m+1}}{argmax} \left[\Phi\left(-\tau_t g_{t,m}(x_{m+1})\right) \min_{i=1,\dots,m} \Phi\left(-\tau_t g_{t,m}(x_i)\right) \|x_i - x_{m+1}\|_s \right]$$

$$\prod_{i=1}^{N} \Phi\left(\tau_t\left(\mu_{t,m}^i(x_{m+1}) - \sigma_{t,m}(x_{m+1})\Phi^{-1}(\alpha_m^*)\right)\right)$$

$$\prod_{i=1}^{N} \Phi\left(\tau_t\left(\mu_{t,m}^i(x_{m+1}) + k\,\sigma_{t,m}(x_{m+1})\right)\right)$$

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

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



$$\underset{x_{m+1}}{argmax} \left[\prod_{i=1}^{N} \Phi\left(\tau_t\left(\mu_{t,m}^i(x_{m+1}) + k\,\sigma_{t,m}(x_{m+1})\right)\right) \min_{i=1,\dots,m} \Phi\left(-\tau_t g_{t,m}(x_i)\right) \|x_i - x_{m+1}\|_s^{2p} \right]$$

One-step-lookahead

$$\underset{x_{m+1}}{argmax}\, \mathbb{E}_{Y_{m+1}} \left[\prod_{i=1}^{N} \Phi\left(\tau_t \mu_{t,m+1}^i(x_{m+1})\right) \right] \min_{i=1,\dots,m} \Phi\left(-\tau_t g_{t,m}(x_i)\right) \|x_i - x_{m+1}\|_s^{2p}$$

3. ONE-STEP-LOOKAHEAD MIXED

$$\underset{x_{m+1}}{argmax}\, \mathbb{E}_{Y_{m+1}}\left[\Phi\left(-\tau_t g_{t,m+1}(x_{m+1})\right)\right] \min_{i=1,\dots,m} \Phi\left(-\tau_t g_{t,m}(x_i)\right) \|x_i - x_{m+1}\|_s^{2p}$$

$$\underset{x_{m+1}}{argmax}\, \mathbb{E}_{Y_{m+1}}\left[\left(1 - \mathrm{Var}_{\mathrm{t,m+1}}^{\Gamma}\right) \times \Phi\left(-\tau_t g_{t,m+1}(x_{m+1})\right)\right] \min_{i=1,\dots,m} \Phi\left(-\tau_t g_{t,m}(x_i)\right) \|x_i - x_{m+1}\|_s^{2p}$$

Good order of magnitude ?

PUBLICATIONS

- *Estimation of simulation failure set with active learning based on Gaussian process classifiers and random set theory.*
  Submitted to Structural Safety, Oct. 2024.
  Menz, M., Munoz Zuniga, M., Sinoquet, D.

- *Learning and space-filling the hidden design space associated to failure of computer experiments*
  To be submitted beginning 2024*.*
  Menz, M., Munoz Zuniga, M., Sinoquet, D.

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  provide rates of convergence for expected improvement. Here the function f to optimize is deterministic and belongs to the RKHS of k However in general $P(\xi \in RKHS(k)) = 0 \Longrightarrow$ problematic from a Bayesian point of view
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  prove the consistency of Expected Global Improvement. They work with covariance functions which are not too smooth and not degenerate (we will improve this point here)
- Julien Bect, François Bachoc, David Ginsbourger. "A supermartingale approach to Gaussian process based sequential design of experiments." Bernoulli, 25(4A) 2883-2919 November 2019.

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