Active Learning of (small) Quantile Sets

Romain Ait Abdelmalek-Lomenech[1]
joint work with Julien Bect[1], Vincent Chabridon[2] & Emmanuel Vazquez[1]

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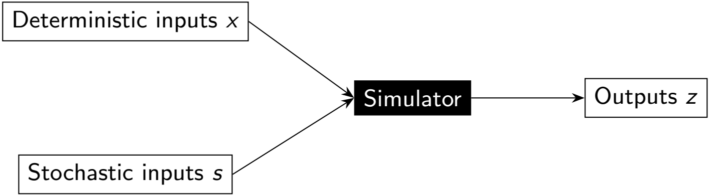
Table of Contents

Consider an **expensive-to-evaluate** numerical simulator f, with inputs in a set $\mathbb{U} = \mathbb{X} \times \mathbb{S}$:

- $x \in \mathbb{X}$ (deterministic design choices).
- $s \in \mathbb{S}$ (stochastic factors).



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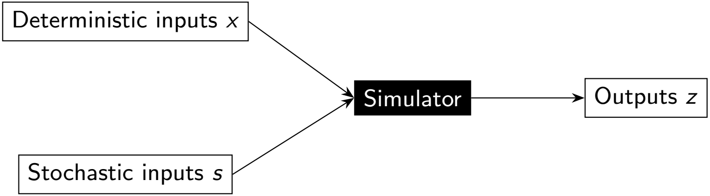

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Given:

- $C \subset \mathbb{R}^q$ a subset of the outputs space $\mathbb{R}^q$.
- $\alpha \in (0, 1)$ a threshold.
- $\mathbb{P}_S$ a known distribution on $\mathbb{S}$.

We focus on the **quantile set inversion (QSI)** problem:

Estimate the set of all $x \in \mathbb{X}$ such that

$$\mathbb{P}\left(f(x, S) \in C\right) \leq \alpha, \qquad S \sim \mathbb{P}_S.$$

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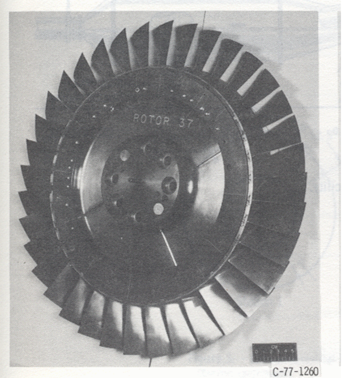
An example: the ROTOR37 compressor model

Function $f : \mathbb{X} \times \mathbb{S} \mapsto \mathbb{R}^3$ with two kind of inputs:

- $x \in \mathbb{X}$: design choice for the compressor
- $s \in \mathbb{S}$: manufacturing uncertainties, with $\mathbb{P}_S = \mathcal{U}(\mathbb{S})$.



(a) Rotor 37.

Simulator return three outputs:

- f_1: mass flow
- f_2: pressure ratio
- f_3: isentropic efficiency

We can set, for example, $\alpha = 5\%$ and

$$C = \left\{ z \in \mathbb{R}^3 : \frac{|z_1 - b_1|}{|b_1|} > 0.175 \quad \text{or} \quad \frac{|z_2 - b_2|}{|b_2|} > 0.175 \right\},$$

where b_1 and b_2 are baseline values for the mass flow and pressure ratio of the compressor.

For simplicity, we now assume $f : \mathbb{U} = \mathbb{X} \times \mathbb{S} \mapsto \mathbb{R}$, with $C = (-\infty, T]$.

The problem becomes

Estimate the quantile set:

$$\Gamma(f) = \{x \in \mathbb{X} : \mathbb{P}\left(f(x, S) \leq T\right) \leq \alpha\}.$$

Remark: With $C = (-\infty, T]$, the problem can be seen in term of quantile of $f(x, S)$. Indeed

$$x \in \Gamma(f) \quad \Longleftrightarrow \quad q_\alpha(f(x, S)) > T,$$

with $q_\alpha(f(x, S))$ the quantile of order α of $f(x, S)$ (with $S \sim \mathbb{P}_S$).

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Example of function and associated quantile set, with $T = 7.5$ and $\alpha = 5\%$.

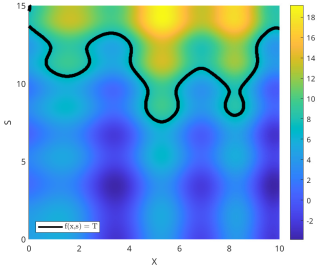

Figure: Representation of the function.

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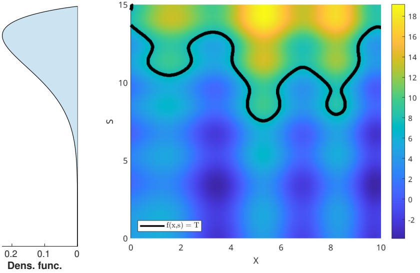

Figure: Representation of the function (right), the density of $\mathbb{P}_S$ (left)

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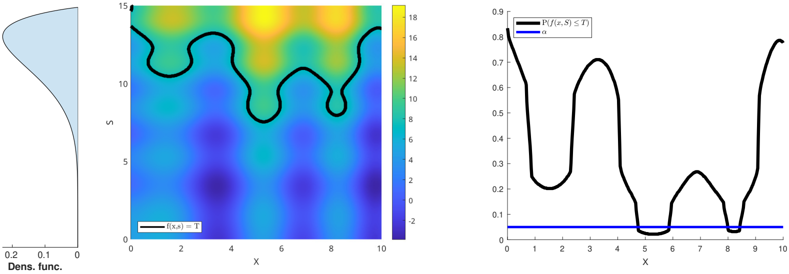

Figure: Representation of the function (middle), the density of $\mathbb{P}_S$ (left) and associated quantile set (right).

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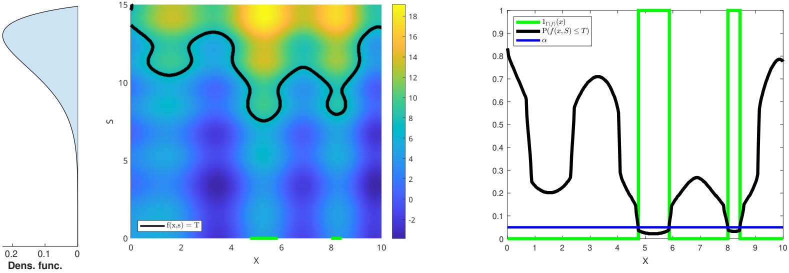

Figure: Representation of the function (middle), the density of $\mathbb{P}_S$ (left) and associated quantile set (right).

Given the expensive-to-evaluate nature of the underlying function, it is necessary to evaluate the function at points chosen with attention.

Active learning (or sequential design of experiments) approach:

Consider

- $\mathcal{I}_n = \{(u_1, f(u_1)), ..., (u_n, f(u_n))\}$ the current information,
- $a_n(u)$ a sampling criterion dependent on $\mathcal{I}_n$.

Until satisfied:

- Choose $u \in \mathbb{U}$ as the minimizer (or maximizer) of $a_n(u)$
- Evaluate f at u
- Update information $\mathcal{I}_n \mapsto \mathcal{I}_{n+1}$.

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Table of Contents

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Bayesian framework & notations:

$f \sim$ GP prior ξ on $\mathbb{U} = \mathbb{X} \times \mathbb{S}$, with constant mean μ and covariance k.

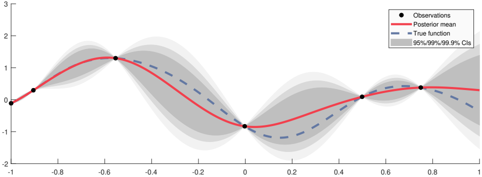

Figure: Illustration of a GP on an interval.

We denote:

- $\mathbb{P}_n$ and $\mathbb{E}_n$: conditional distribution and expectation given $\mathcal{I}_n$.
- μ_n, σ_n and k_n: posterior mean, st. deviation and covariance of ξ.
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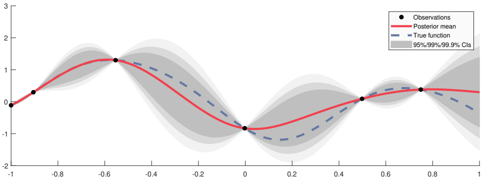

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First approach: joint-space estimation

The QSI problem is related to the **estimation of the excursion set**

$$\Lambda(f) = \{u \in \mathbb{U} \; : \; f(u) \leq T\}$$

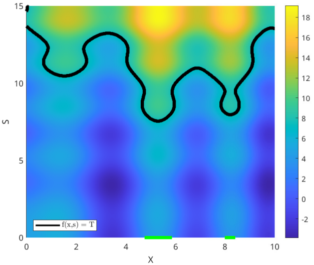

Figure: Example function. The black line delimits the set $\Lambda(f)$.

$$x \in \Gamma(f) \iff \mathbb{P}((x, S) \in \Lambda(f)) \leq \alpha,$$

Good approximation of $\Lambda(f) \implies$ good approximation of $\Gamma(f)$

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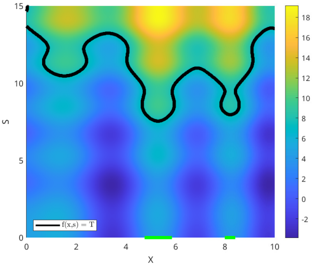

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Good approximation of $\Lambda(f)$ $\Longrightarrow$ good approximation of $\Gamma(f)$

Several Bayesian methods focus on **estimating** $\Lambda(f)$. For example:

- **Maximal uncertainty sampling methods**:
  - Maximum misclassification probability [Bryan et al. (2005)]:

$$U_{n+1} \in \underset{u \in \mathbb{U}}{\operatorname{argmax}} \min(p_n(u), 1 - p_n(u))$$

  - [Ranjan et al. (2008); Echard et al. (2011), ...]
- **Stepwise uncertainty reduction (SUR)** methods:
  - For instance [Chevalier et al. (2014)] (Joint-SUR):

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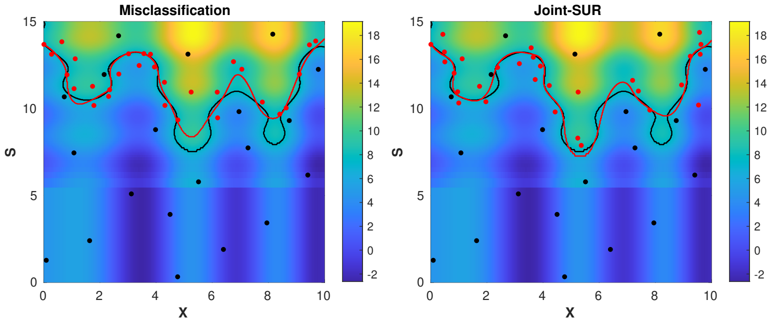

Figure: Examples of designs (red dots) obtained after $n = 30$ steps with the maximum misclassification and the 'joint-SUR' criteria.

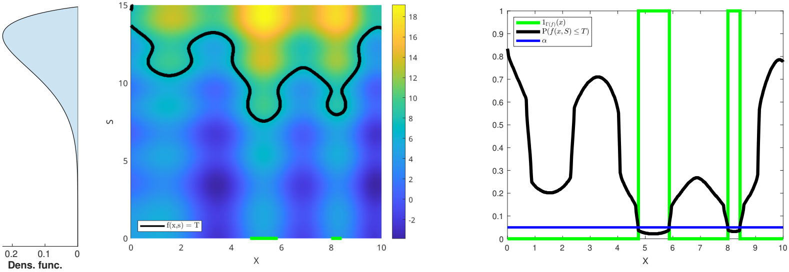

Figure: Representation of the function (middle), the density of $\mathbb{P}_S$ (left) and associated quantile set (right).

Second approach: Focusing directly on $\Gamma(f)$

To estimate $\Gamma(f)$, one only needs to focus on **'interesting parts'** of $\Lambda(f)$.

We denote:

- $\Gamma(\xi)$ the random quantile set associated to ξ.
- $\pi_n(x) = \mathbb{P}_n(x \in \Gamma(\xi))$, the posterior probability that x belongs to the (random) quantile set generated by ξ.
- $\mathcal{Q}_n = \int_{\mathbb{X}} \min(\pi_n(x), 1 - \pi_n(x)) \, \mathrm{d}x$.

QSI-SUR sampling criterion [Ait Abdelmalek-Lomenech et al. (2024)]:

$$(X_{n+1}, S_{n+1}) \in \underset{(x,s) \in \mathbb{X} \times \mathbb{S}}{\operatorname{argmin}} \mathbb{E}_n(\mathcal{Q}_{n+1} \mid (X_{n+1}, S_{n+1}) = (x, s)),$$

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The implementation proposed in [Ait Abdelmalek-Lomenech et al. (2024)] produces good results on moderately difficult examples.

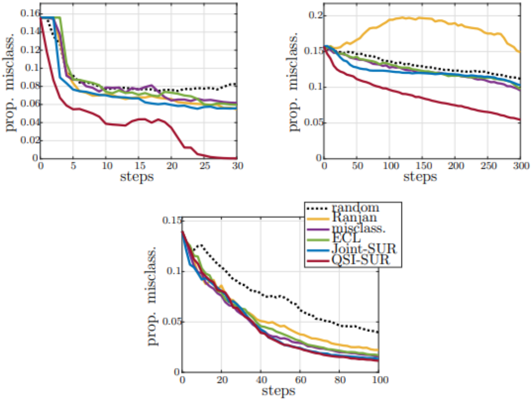

Figure: Median of the proportion of misclassified points vs. number of steps on several examples.

The QSI-SUR criterion focus on part of $\Lambda(f)$ that gives relevant information on $\Gamma(f)$.

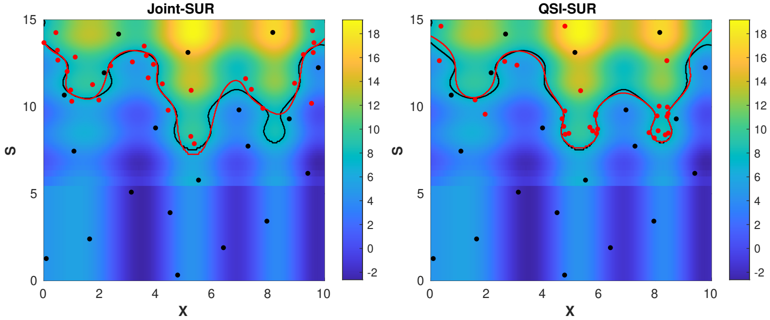

Figure: Example of design obtained with the QSI-SUR criterion and the Joint-SUR criterion.

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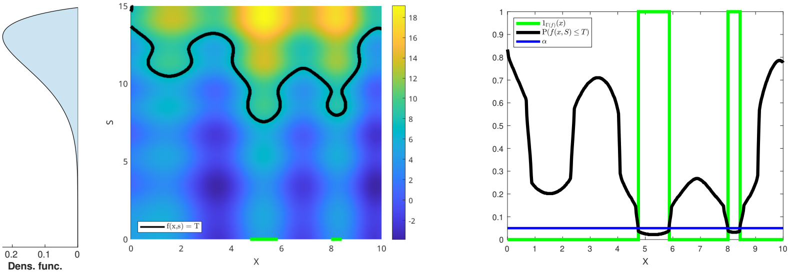

Figure: Representation of the function (middle), the density of $\mathbb{P}_S$ (left) and associated quantile set (right).

The QSI-SUR criterion is based on

$$\mathcal{Q}_n = \int_{\mathbb{X}} \min(\pi_n(x), 1 - \pi_n(x))\, \mathrm{d}x.$$

Two main issues in the implementation:

- **First issue: Computational complexity.**
  - π_n approximated using conditional sample paths of $\xi(x, \cdot)$.
  - Complexity is $O(m^3)$, where m is the number of points used for the approximation. Due to the Cholesky factorization of the covariance matrix.
  - Criterion too expensive for continouous optimization and batch design.
- **Second issue: Not adapted to "small" $\Gamma(f)$.**
  - Integral over $\mathbb{X}$ in $\mathcal{Q}_n$ is discretized.
  - Necessity of points (in $\mathbb{X}$) close to the boundary of $\Gamma(f)$
  - When $\Gamma(f)$ is small, importance sampling can prove insufficient.

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Table of Contents

To resolve the issues listed previously, we use a two part solution:

- **First issue: Computational complexity**
  - We introduce a new type of method called "Maximum Expected Estimator Modification" (MEEM).
  - We derive a MEEM criterion with complexity $O(m^2)$.
  - This criterion allows continuous optimization and batch design of experiments.
- **Second issue: Not adapted to "small" $\Gamma(f)$.**
  - We introduce a sequential Monte Carlo (SMC) framework.
  - We estimate a sequence of decreasing quantile sets, converging towards the set of interest.

Maximum Expected Estimator Modification (MEEM)

Let us consider a sequence of estimators $(\widehat{\Gamma}_n)_n$ such that

$$\widehat{\Gamma}_n : \mathcal{I}_n \mapsto \mathcal{P}(\mathbb{X}),$$

and a "distance"

$$d : \mathcal{P}(\mathbb{X})^2 \mapsto \mathbb{R}^+.$$

MEEM principle: Choose the point that maximize the expected change in the estimation, i.e.

$$U_{n+1} \in \arg\max_{u \in \mathbb{U}} \mathbb{E}_n(d(\widehat{\Gamma}_{n+1}, \widehat{\Gamma}_n) \,|\, U_{n+1} = u)$$

NB: For convenience, we assume a batch size of 1.

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"Duality" SUR / MEEM

Several SUR strategies in the litterature are equivalent to MEEM strategies.

For example:

- Optimization:
  - Expected Improvement
  - MEEM method with $d(a, b) = |a - b|$ and estimator $f_n^* = \min\{U_1, ..., U_n\}$
- Function approximation:
  - SUR method : $U_{n+1} \in \arg\min \mathbb{E}_n \left(\int_{\mathbb{U}} \sigma_n^2(u) \, \mathrm{d}u \,|\, U_{n+1} = u \right)$.
  - MEEM method with $d(h, g) = \int_{\mathbb{U}} (h(u) - g(u))^2 \, \mathrm{d}u$ and estimator $f_n = \mu_n$

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MEEM method for QSI

We choose the divergence $d(\widehat{\Gamma}_{n+1}, \widehat{\Gamma}_n) = \lambda(\widehat{\Gamma}_{n+1} \Delta \widehat{\Gamma}_n)$ we have

$$d(\widehat{\Gamma}_{n+1}, \widehat{\Gamma}_n) = \int_{\mathbb{X}} |\mathbb{1}_{\widehat{\Gamma}_{n+1}}(x) - \mathbb{1}_{\widehat{\Gamma}_n}(x)| \, \mathrm{d}x,$$

coupled with the sequence of plug-in estimators

$$\widehat{\Gamma}_n = \{x \in \mathbb{X} : \mathbb{P}(\mu_n(x, S) \leq T) \leq \alpha\},$$

We obtain the **QSI-MEEM** strategy:

$$U_{n+1} \in \underset{u \in \mathbb{U}}{\arg\max} \int_{\mathbb{X}} \mathbb{E}_n \left(|\mathbb{1}_{\widehat{\Gamma}_{n+1}}(x) - \mathbb{1}_{\widehat{\Gamma}_n}(x)| \,\middle|\, U_{n+1} = u \right) \mathrm{d}x.$$

MEEM method for QSI

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$$d(\widehat{\Gamma}_{n+1}, \widehat{\Gamma}_n) = \int_{\mathbb{X}} |\mathbb{1}_{\widehat{\Gamma}_{n+1}}(x) - \mathbb{1}_{\widehat{\Gamma}_n}(x)| \, \mathrm{d}x,$$

coupled with the sequence of plug-in estimators

$$\widehat{\Gamma}_n = \{x \in \mathbb{X} \, : \, \mathbb{P}(\mu_n(x, S) \leq T) \leq \alpha\},$$

We obtain the **QSI-MEEM** strategy:

$$U_{n+1} \in \underset{u \in \mathbb{U}}{\arg\max} \int_{\mathbb{X}} \mathbb{E}_n \left(|\mathbb{1}_{\widehat{\Gamma}_{n+1}}(x) - \mathbb{1}_{\widehat{\Gamma}_n}(x)| \, \middle| \, U_{n+1} = u \right) \mathrm{d}x.$$

Criterion does not need to be approximated using conditional sample paths of ξ.

As a consequence of the kriging update formula, we have:

Proposition

Given $\mathcal{I}_n$ and U_{n+1}, $\widehat{\Gamma}_{n+1}$ is a function of a standard Gaussian variable Z:

$$\widehat{\Gamma}_{n+1}(z) = \{x \in \mathbb{X} : P\left(\mu_n(x, S) + \kappa_n(x, S) z \leq T\right) \leq \alpha\},$$

with $\kappa_n(x, s) = k_n(U_{n+1}, (x, s))/\sigma_n(U_{n+1})$.

$\Longrightarrow$ Computational complexity of the criterion: $O(m^2)$, with m the number of points (in $\mathbb{X} \times \mathbb{S}$) used for the approximation.

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Sanity check

We observe that the QSI-MEEM method produces results similar (or better) than the QSI-SUR strategy on case with relatively large quantile sets.

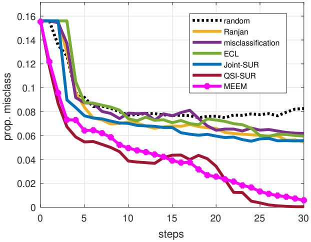

Figure: Median (left) and quantile of order 0.9 of the proportion of misclassified points vs. number of steps, for 100 repetitions of the algorithms on the introductory example.

Second issue: Estimation of small quantile sets

Idea: Multilevel splitting/**subset simulation** [Kahn and Harris (1951); Au and Beck (2001)] to efficiently sample points in $\mathbb{X}$.

- Sequentially estimate a sequence of **decreasing quantile sets**

$$\Gamma^0(f) \supset \Gamma^1(f) \supset \ ... \ \supset \Gamma^K(f) = \Gamma(f),$$

using the MEEM strategy described previously.

- Such sets can be defined by setting

$$\Gamma^k(f) = \{x \in \mathbb{X} \, : \, \mathbb{P}(f(x, S) \leq T_k) \leq \alpha\},$$

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We propose a **SMC-based** algorithm inspired by **BSS** [Li (2012); Bect et al. (2017)]

It alternates two distinct phases:

- **Estimation phase**
  - Define a new intermediary quantile set to estimate.
  - Sample points $U_n, \ldots, U_{n+r}$ using the MEEM criterion.
- **Move phase**
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Let $q_{n,k}$ a density targeting $\Gamma^k(f) = \{x \in \mathbb{X} : \mathbb{P}(f(x,S) \in C_k) \leq \alpha\}$ at step n.

Estimation phase:

- Set T_{k+1} such that

$$\mathrm{ESS}\left(\frac{\mathbb{1}_{\widehat{\Gamma}_n^{k+1}}(x)}{\mathbb{1}_{\widehat{\Gamma}_n^{k}}(x)}\right) \approx 30\%.$$

- Sample point

$$U_{n+1} \in \operatorname{argmax} J_n(u),$$

with J_n the MEEM criterion targeting $\Gamma^{k+1}(f)$.

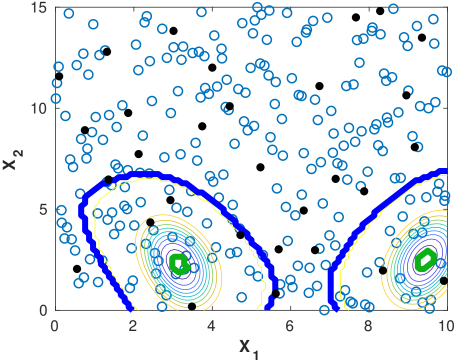

Figure: Temporary quantile set (blue line), final quantile set (green line), particles (blue dots). - $n = 0$.

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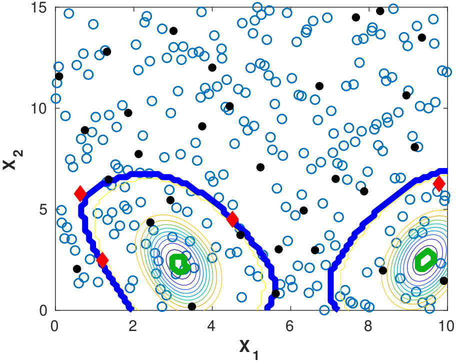

Figure: Temporary quantile set (blue line), final quantile set (green line), particles (blue dots) and projection of the sequential design (red dots). - $n = 4$.

Let $q_{n,k}$ a density targeting $\Gamma^k(f) = \{x \in \mathbb{X} : \mathbb{P}(f(x,S) \leq T_k) \leq \alpha\}$ at step n.

Move phase:

When stopping condition is met:

- Residual resampling.
- Move particles in $\Gamma^{k+1}(f)$ using MHRW with target density $q_{n,k+1}$.
- Adapt walk's variance to target acceptation rate 25%.

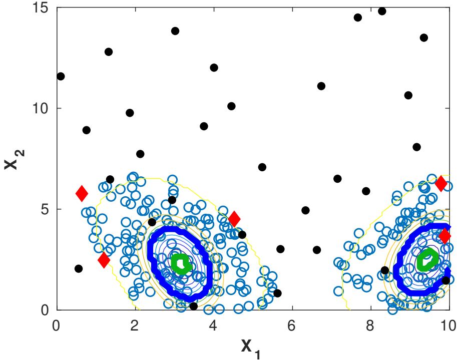

Figure: Temporary quantile set (blue line), final quantile set (green line), particles (blue dots) and projection of the sequential design (red dots). - $n = 5$.

Table of Contents

To evaluate the performances of the proposed strategy, we focus on the relative error

$$\frac{\lambda_{\mathbb{X}}(\Gamma(f)\Delta\widehat{\Gamma}_n)}{\lambda_{\mathbb{X}}(\Gamma(f))}$$

obtained at the end of the strategy, and the number of steps required to obtain these results.

The functions considered are modeled by a GP with constant mean and Matern covariance kernel (with $\nu \in \{1/2, 3/2, 5/2, +\infty\}$).

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1st example: 5-Trid function [Adorio and U.P. (2005)]

- $\mathbb{U} = \mathbb{X} \times \mathbb{S}$ with $\mathbb{X} = [-25, 25]^3$ and $\mathbb{S} = [-25, 25]^2$,
- $\mathbb{P}_S = \mathcal{U}(\mathbb{S})$
- $\alpha = 5\%$ and $C = [1098.5, +\infty)$
- Relative size of $\Gamma(f)$: $\lambda_{\mathbb{X}}(\Gamma(f)) \sim 10^{-6}$.

$$f(u) = \sum_{i=1}^{5} (u_i - 1)^2 - \sum_{i=2}^{5} u_i u_{i-1}$$

Size of the initial design: 50.

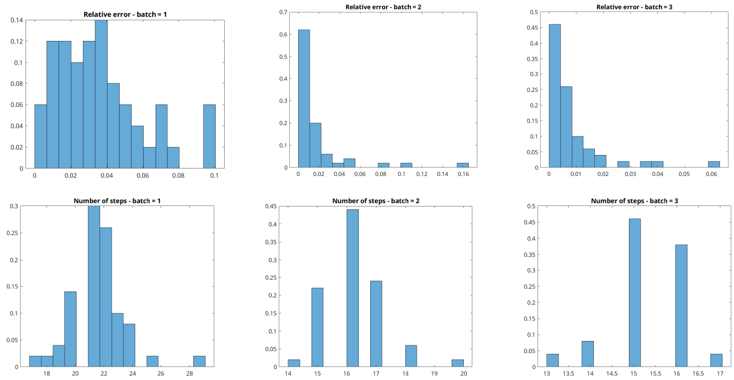


Figure: Distribution of the relative error (top) and the number of steps (bottom), for different batch size (left to right: 1, 2, 3). - (50 runs)

2nd example: OTL circuit function [E. N. and D. M. (2007)]

- $\mathbb{U} = \mathbb{X} \times \mathbb{S}$
- $\mathbb{X} = [-50, 150] \times [25, 70] \times [0.5, 3] \times [1.2, 2.5] \times [0.25, 1.2]$
- $\mathbb{S} = [-50, 300]$,
- $\mathbb{P}_S = trunc\mathcal{N}(175, 50)$
- $\alpha = 5\%$ and $C = [2.65, +\infty)$
- Relative size of $\Gamma(f)$: $\lambda_{\mathbb{X}}(\Gamma(f)) \sim 10^{-7}$.

$f(x, s)$ represents the midpoint voltage of a circuit given the choice of resistances designs x and the current gain s.

Size of the initial design: 60.

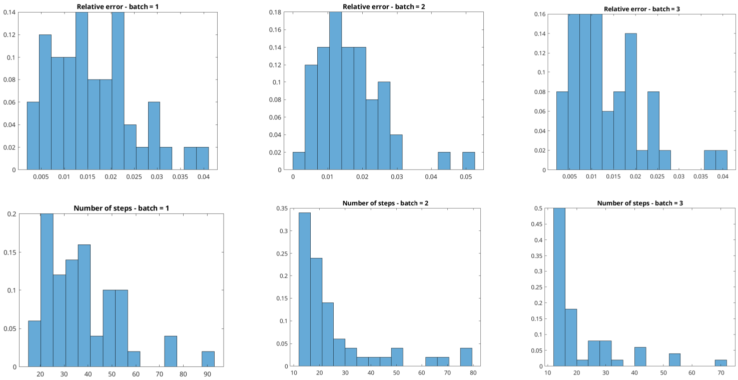


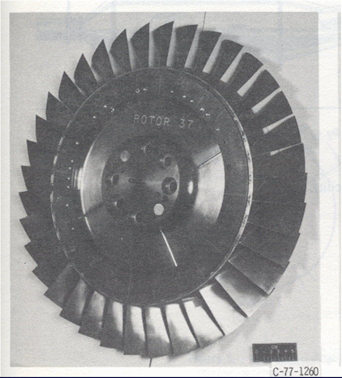
Figure: Distribution of the relative error (top) and the number of steps (bottom), for different batch size (left to right: 1, 2, 3). - (50 runs).

3rd example: ROTOR37 model [Reid and Moore (1978)]

Gaussian metamodel (provided by S. Da Veiga and SafranTech) of the ROTOR37 compressor model.

The function $f : \mathbb{X} \times \mathbb{S} \mapsto \mathbb{R}^3$ takes two kind of inputs:

- $x \in \mathbb{X} = [0, 1]^{13}$: design choice for the compressor
- $s \in \mathbb{S} = [0, 1]^5$: manufacturing uncertainties ($\mathbb{P}_S = \mathcal{U}(\mathbb{S})$)



Simulator returns three outputs:

- f_1: the mass flow
- f_2: the pressure ratio
- f_3: the isentropic efficiency

Goal: finding the set of determinisitic design choice leading to values of the mass flow and pressure ratio being close to baselines values (b_1, b_2) with sufficiently high probability.

We consider:

- $C = \left\{ z \in \mathbb{R}^3 : \frac{|z_1 - b_1|}{|b_1|} > 0.175 \quad \text{or} \quad \frac{|z_2 - b_2|}{|b_2|} > 0.175 \right\}$
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Relative size of $\Gamma(f)$: $\lambda_{\mathbb{X}}(\Gamma(f)) \sim 10^{-8}$

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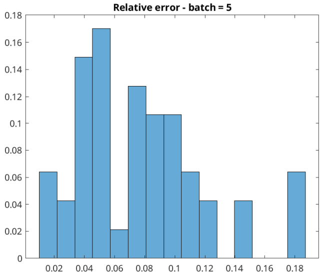
We start the strategy from an initial design of size 90. A batch size of 5 is used.



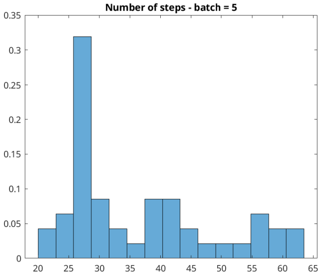


Figure: Distribution of the relative error (left) and the number of steps (right), for a batch size of 5. - (50 runs).

Conclusion:

- Introducing the concept of MEEM allows to reproduce (or improve) the results obtained by using the QSI-SUR criterion on moderately difficult examples.
- The MEEM criterion permits a welcomed gain regarding the computational complexity, due to the absence of conditional Gaussian sample paths
- Coupled with a SMC framework, the criterion allows to accurately estimate small quantile sets (size of order $10^{-6} - 10^{-8}$).

Future research might be dedicated to treating cases where $\alpha \sim 0$.

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Thank you for your attention!

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Choice of the target densities:

Natural idea (in the spirit of [Dubourg et al. (2013); Bect et al. (2017)]):

$$q_{n,k}(x) \propto \pi_n^k(x) = \mathbb{P}_n(x \in \Gamma^k(\xi))$$

- Does not admit a closed-form expression.
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Idea: Replace $\pi_n^k(x)$ by $\mathbb{1}(x \in \Gamma_{n,k}^+)$. How to define $\Gamma_{n,k}^+$?

Given $x_0 \in \mathbb{X}$, μ_n and σ_n the posterior mean and standard deviation of ξ and $\beta \in (1/2, 1)$, consider the **quantile function**:

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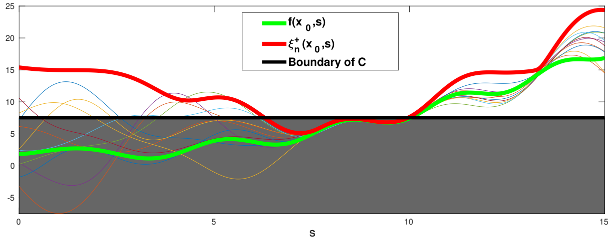

Figure: Example of quantile function $\xi_n^+(x_0, \cdot)$, with a fixed x_0.

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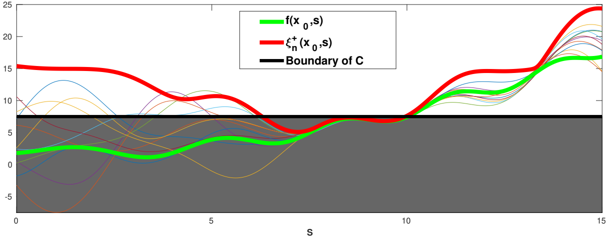

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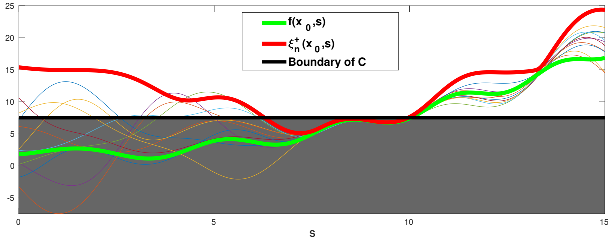

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