A SUR version of the Bichon criterion for excursion set estimation

Duhamel Clément, Prieur Clémentine, Helbert Céline, Munoz Zuniga Miguel, Sinoquet Delphine

Université Grenoble Alpes, INRIA, IFP Energies Nouvelles, École Centrale de Lyon

Introduction to the inversion framework

Motivation: many inversion issues are present in industry [El Amri, 2019].
Goal: find all sets of parameters such that a quantity of interest remains below a threshold.
Mathematical Formulation: estimation of the following $\Gamma^\star$ set while limiting the number of g black-box evaluations:

$$\Gamma^\star := \left\{ \mathbf{x} \in \mathbb{X},\ g(\mathbf{x}) \leq T \right\} \tag{1}$$

with $\mathbb{X} \subset \mathbb{R}^d$ design space (compact) and T threshold.
Application (floating wind turbine): pre-calibration step consists in estimating model parameters that fit the measured data.

1) Surrogate models and GP Regression

Aim: approximation of the original model
Advantages: defined from a limited number of true evaluation and faster to evaluate.

One type of surrogate model: **Gaussian Process Regression**:

Hypothesis: model g is a realisation of a Gaussian Process.
Construction: with a Design of Experiment (DoE), sequentially enriched by an inversion-adapted acquisition criterion [Picheny et al., 2010].

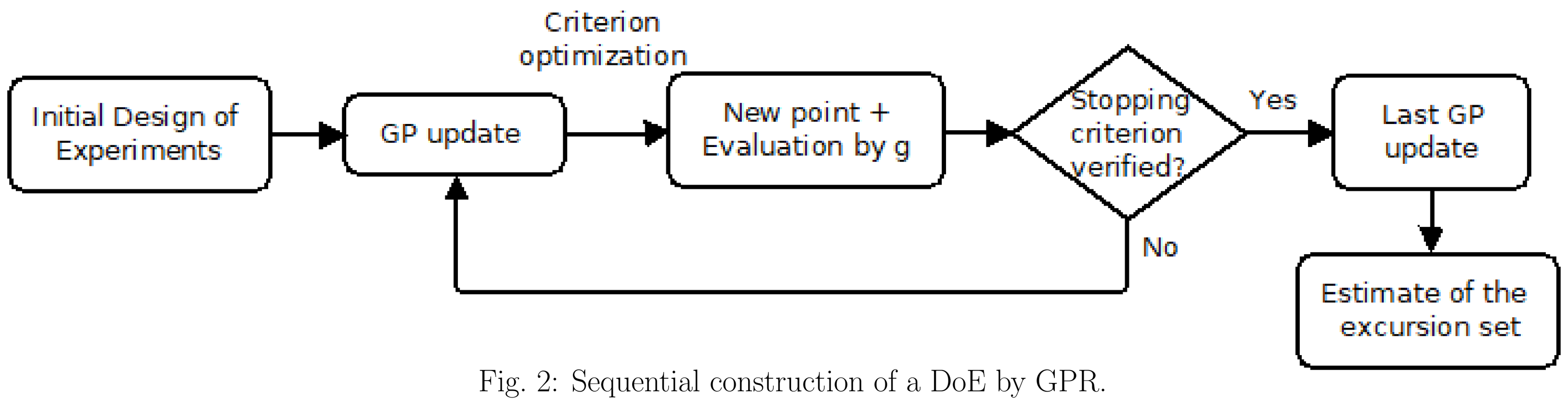


Fig. 2: Sequential construction of a DoE by GPR.

2) Bichon criterion [Bichon et al., 2008]

Bichon criterion: inversion-adapted acquisition criterion
Goal: find a compromise between finding a point:
-close enough to the border to be estimated,
-with a sufficiently high prediction standard deviation.
Notations: $\mathbf{x}_{n+1}$ new added point, ξ Gaussian process representing the model, $\mathscr{E}_n$ event given by evaluations on the DoE $(\mathscr{X}_n)$: $\xi(\mathscr{X}_n) = g(\mathscr{X}_n)$ and σ_n prediction standard deviation.
Formulation:

$$\mathbf{x}_{n+1} := \underset{\mathbf{x}\in\mathbb{X}}{\operatorname{argmax}}\, \mathrm{EFF}(\mathbf{x}) \quad \text{with} \quad \mathrm{EFF}(\mathbf{x}) := \mathbb{E}\left[\left(\alpha\sigma_n(\mathbf{x}) - |T - \xi(\mathbf{x})|\right)^+ \,\middle|\, \mathscr{E}_n \right] \tag{4}$$

3) SUR Strategies [Bect et al., 2012]

Stepwise Uncertainty Reduction (SUR) strategies:

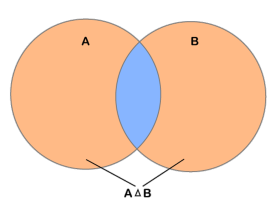
Quantify uncertainty reduction that can be achieved by the add of new point.
Notation: $\mathscr{H}_n$ uncertainty measure conditionnally to the event $\mathscr{E}_n$.
Formulation:

$$\mathbf{x}_{n+1} \in \underset{\mathbf{x}\in\mathbb{X}}{\arg\min}\, \mathscr{J}_n(\mathbf{x}) \quad \text{and} \quad \mathscr{J}_n(\mathbf{x}) := \mathbb{E}\left[\mathscr{H}_{n+1}(\mathbf{x})\right] \tag{2}$$

with $\mathscr{H}_{n+1}(\mathbf{x})$ expected uncertainty measure conditionnaly to $\mathscr{E}_n$ and to adding $\mathbf{x}$ to the DoE $\mathscr{X}_n$.

Example: SUR Vorob'ev strategy [Chevalier, 2013]:

$$\mathscr{H}_n^V := \mathbb{E}\left[\mathbb{P}_\mathbb{X}\left(\Gamma \Delta Q_{n,\alpha_n^\star}\right) \,\middle|\, \mathscr{E}_n \right] \tag{3}$$



with $\mathbb{P}_\mathbb{X}$ probability measure on $\mathbb{X}$, $\Gamma := \{\mathbf{z} \in \mathbb{X},\ \xi(\mathbf{z}) \leq T\}$, $Q_{\alpha_n^\star}$ Vorob'ev expectation (generalization of expectation for random sets) [Molchanov and Molchanov, 2005] and Δ symetric difference for random sets.

4) SUR Bichon criterion (Formulations)

Motivations: Find a more robust and easier to implement criterion than SUR Vorob'ev one and with better performances than direct strategies

SUR Bichon criterion: defined by integrating Bichon criterion on the design space:

$$\mathscr{H}_n^{\mathrm{B}} := \int_\mathbb{X} \mathrm{EFF}(\mathbf{z})\, \mathrm{d}\mathbb{P}_\mathbb{X}(\mathbf{z}), \quad \mathscr{J}_n^{\mathrm{B}}(\mathbf{x}) := \mathbb{E}\left[\mathscr{H}_{n+1}(\mathbf{x})\right] \tag{5}$$

$$\mathscr{H}_{n+1}^{\mathrm{B}}(\mathbf{x}) := \int_\mathbb{X} \mathbb{E}\left[\left(\alpha\sigma_{n+1}(\mathbf{z}) - |T - \xi(\mathbf{z})|\right)^+ \,\middle|\, \xi(\mathbf{x}), \mathscr{E}_n \right] \mathrm{d}\mathbb{P}_\mathbb{X}(\mathbf{z}) \tag{6}$$

with σ_{n+1} prediction standard deviation with the add of $\mathbf{x}$ to DoE (independent of the evaluation).

Simplified formulation:

$$\mathscr{J}_n^{\mathrm{B}}(\mathbf{x}) = \int_\mathbb{X} \mathrm{EFF}_\mathbf{x}(\mathbf{z})\, \mathrm{d}\mathbb{P}_\mathbb{X}(\mathbf{z}) \tag{7}$$

$$\begin{aligned} \text{with } \mathrm{EFF}_\mathbf{x}(\mathbf{z}) = (m_n(\mathbf{z}) - T) & \left[2\,\phi\left(\frac{T - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})}\right) - \phi\left(\frac{T^- - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})}\right) - \phi\left(\frac{T^+ - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})}\right) \right] \\ - \sigma_n(\mathbf{z}) & \left[2\,\varphi\left(\frac{T - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})}\right) - \varphi\left(\frac{T^- - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})}\right) - \varphi\left(\frac{T^+ - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})}\right) \right] \\ + \epsilon(\mathbf{z}) & \left[\phi\left(\frac{T^+ - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})}\right) - \phi\left(\frac{T^- - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})}\right) \right] \end{aligned} \tag{8}$$

φ and ϕ respectively pdf and cdf of $\mathscr{N}(0,1)$ and m_n prediction mean. $T^\pm := T \pm \varepsilon(\mathbf{z})$ and $\varepsilon(\mathbf{z}) := \alpha\sigma_{n+1}(\mathbf{z})$.

5) SUR Bichon criterion (Numerical Performances)

Implementation choice:
-performance comparison measure: $\mathbb{P}_\mathbb{X}(\hat{\Gamma}_n \Delta \Gamma^\star)$ with $\hat{\Gamma}_n$ estimator of set $\Gamma^\star$ after n obs.
-test function is the Branin-rescaled function on $\mathbb{X} := [0,1]^2$ with $T = 10$.
-SUR optimisation with Genoud algorithm.
-SUR Integration MC Sobol with $n.points = 10\,000$; $\alpha = 1$.

Encouraging results for non-connex sets: Fig. 4

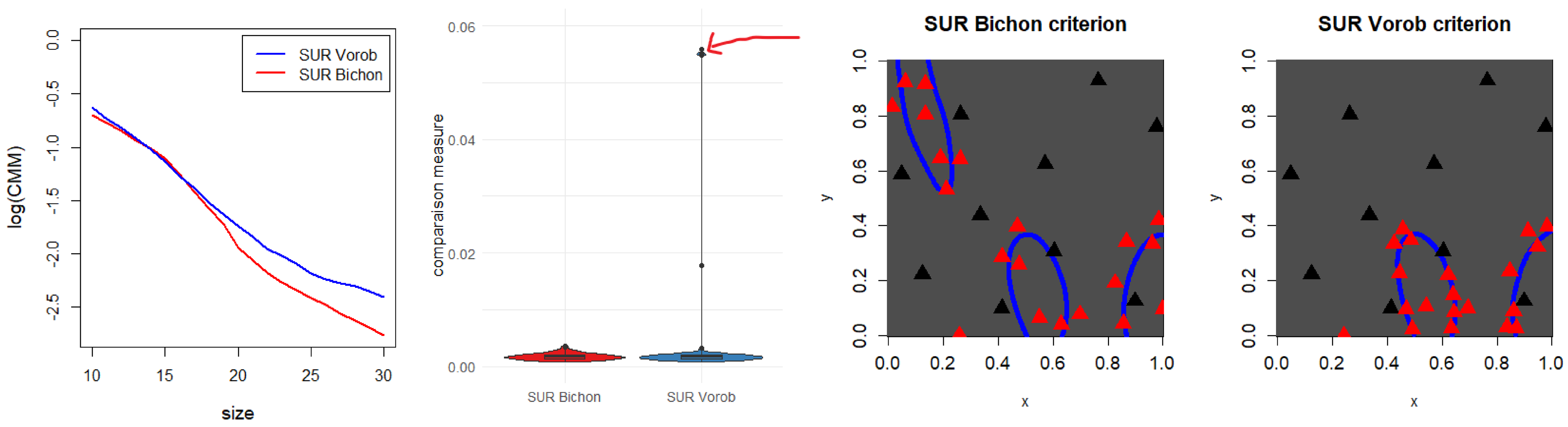


Fig. 4: On the left, representation of the log comparaison measure mean throught iterations, for the inversion of the Branin-rescaled function with $T = 10$, for 100 different initial DoE of size 10 and type LHS Maximin. In the middle, violinplot of the performance comparaison measure after 20 iterations. On the right, representation of the respectively $\Gamma^\star$ estimator for one of the red arrow pointed cases. At right, representation of the respectively $\Gamma^\star$ estimator for one of the red arrow pointed cases.

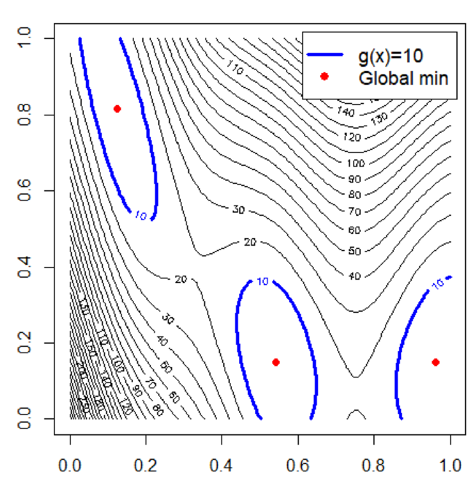


Fig. 5: Representation of the Branin-rescaled function on $\mathbb{X}$.

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