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A SUR version of the Bichon criterion for excursion set estimation

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Abstract

Many model inversion problems occur in industry. These problems consist in finding the set of parameter values such that a certain quantity of interest respects a constraint, for example remains below a threshold. In general, the quantity of interest is the output of a simulator, costly in computation time.

An effective way to solve this problem is to replace the simulator by a Gaussian process regression, with an experimental design enriched sequentially by a well chosen acquisition criterion. Different inversion-adapted criteria exist such as the Bichon criterion (also known as Expected Feasibility Function) and deviation number. There also exist a class of enrichment strategies (Stepwise Uncertainty Reduction - SUR) which select the next point by measuring the expected uncertainty reduction induced by its selection.

In this paper we propose a SUR version of the Bichon criterion. An explicit formulation of the criterion is given and test comparisons show good performances on classical test functions.

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1 Introduction

Nowadays, many industrial issues are related to a problem of excursion set estimation for instance, to find feasible solutions of complex optimal design problems. This problem consists in finding, the set of input parameter values such that a quantity of interest defined from its outputs respects a constraint, for example remains below a threshold. In general, the quantity of interest is an output of a numerical model, computationally expensive, which is often a black-box function, representing the complex physical phenomenon. The problem is also known as an inversion problem (Chevalier [2013]). For example, the application to a vehicle pollution control system, allowing compliance with pollutant emission norms was studied in El Amri et al. [2020].

An effective way to solve this kind of problems is to replace the costly black-box function of interest by a surrogate model based on Gaussian processes. The advantage of a Gaussian process is that it is entirely determined by its two first moments: mean and covariance functions. Also, the formulas for updating mean and covariance functions conditionally on observations are easily tractable. The set of evaluation points and the corresponding evaluations of the black-box function is called Design of Experiments (DoE) and the choice of new evaluation points is made sequentially by the optimization of an acquisition criterion that depends on the Gaussian process (see for example Bect et al. [2012] and Moustapha et al. [2021]). Acquisition criteria are useful to select the runs which provide the best information considering a given objective: improvement of the predictive quality of the whole response surface, optimizing a quantity of interest, quantification of a failure probability, estimating an excursion set (inversion), etc. Acquisition criteria suitable for inversion include: the deviation number denoted U (Echard et al. [2011]), the Bichon criterion also known as Expected Feasibility Function (Bichon et al. [2008]), and the Ranjan criterion (Ranjan et al. [2008]). The two last criteria are adaptations of the classical optimization-oriented Expected Improvement criterion (Jones et al. [1998]) for excursion set estimation. The U criterion is the ratio of the absolute deviation of the prediction mean from the threshold defining the excursion set, to the value of the prediction standard deviation. All these criteria are based on an exploration targeted to a better knowledge of the boundary of the excursion set.

In addition, there is a more elaborate and in general more efficient class of criteria that anticipate the impact of adding new points to the DoE: the Stepwise Uncertainty Reduction (SUR) strategies (Bect et al. [2012]). For example, SUR strategies based on the volume of the excursion set can be cited as particularly suitable for the inversion framework. It is shown in Bect et al. [2012] that those SUR criteria provide better performances compared to other criteria.

Chevalier [2013] introduced a SUR strategy based on Vorob'ev random set theory (Molchanov [2005]), that goes beyond taking into account the volume of excursion sets like other SUR strategies. However, we have noticed that SUR Vorob'ev criterion (SUR Vorob'ev) is not robust enough in the sense that it lacks exploration such that with a reasonable number of simulations it sometimes misses some of connected components of the set. Moreover, SUR Vorob'ev requires some approximations about the Vorob'ev threshold. Therefore we propose to tackle these issues by a SUR version of the Bichon criterion (SUR Bichon), which is easier to set up and more robust than SUR Vorob'ev. It should be noted that a SUR version of the U criterion could have been envisaged but this would require simulation of the observations for the estimation of the associated criterion and therefore a higher computational cost.

This article is divided into three main sections. In section 2, the framework of excursion set estimation is recalled. Details on the construction of the sequential DoE based on Gaussian process regression are given as well as details on the Bichon acquisition criterion. Section 3 is dedicated to the new SUR Bichon criterion, with some reminders on SUR strategies beforehand, and a simplified and easy-to-implement formulation of this new criterion. Numerical aspects are discussed in section 4 with tests of SUR Bichon performances, compared to those of SUR Vorob'ev and Bichon for several analytical examples. Appendices present technical proofs, theoretical results on kriging and

bases of Vorob'ev theory.

2 The framework for estimating excursion sets

2.1 Some reminders on Gaussian process regression

Let \mathbb{X} be a compact set of \mathbb{R}^d ($d \in \mathbb{N}^*$) and $g : \mathbb{X} \rightarrow \mathbb{R}$ a black-box function, whose analytical expression is unknown but which can be evaluated at any point of \mathbb{X} at a heavy computational cost. The objective of an excursion set estimation problem is to estimate the domain defined by

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

with T a fixed threshold, while limiting the number of costly evaluations of g .

Surrogate models, also known as meta-models, are approximations of the output of the simulator built from a sample of simulations and that are not expensive to evaluate. Therefore they can replace the original expensive simulator in a time-saving manner. Among surrogate models, Gaussian Process Regression (GPR) is very popular: g is considered as a realization of a Gaussian process (GP) ξ defined on a probabilistic space $(\Omega, \mathcal{F}, \mathbb{P})$, i.e. $g(\mathbf{x}) = \xi(\mathbf{x}, \omega)$ for a given ω in Ω . This type of surrogate models gives, in addition to a prediction, an associated prediction error estimate.

More precisely, the process is written as the sum of a deterministic part and a stochastic part:

$$\xi(\mathbf{x}) := m(\mathbf{x}) + \mathbf{Z}(\mathbf{x}), \quad \forall \mathbf{x} \in \mathbb{X} \quad (2)$$

with m the trend of ξ (deterministic part) and \mathbf{Z} a stationary GP, of zero mean, known covariance kernel $k : \mathbb{X}^2 \rightarrow \mathbb{R}$ and in particular variance function $\sigma^2(\mathbf{x}) := k(\mathbf{x}, \mathbf{x})$ for any \mathbf{x} in \mathbb{X} (stochastic part). To limit the complexity of estimating the trend function m , the choice of this latter is often parametrized as a linear combination of known basis functions $(f_i)_{i=1}^l$ with coefficients $\boldsymbol{\beta} := \{\beta_i\}_{i=1}^l$ to be estimated. The choice of the covariance kernel associated with the GP \mathbf{Z} is crucial since it determines the predictor regularity. Different implementation choices are detailed in Section 4.1.

Let's denote $g(\chi_n) := (g(\mathbf{x}^{(1)}), \dots, g(\mathbf{x}^{(n)}))^\top$ the evaluations of g on an initial design of experiments $\chi_n := (\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)})$ belonging to \mathbb{X}^n . The random vector $\xi(\chi_n)$ then corresponds to the finite-dimensional distribution of the process $(\xi(\mathbf{x}), \mathbf{x} \in \mathbb{X})$ on χ_n and we define \mathcal{E}_n as the event $\xi(\chi_n) = g(\chi_n)$. $K := (k(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}))_{1 \leq i, j \leq n}$ is the covariance matrix on χ_n and $\mathbf{k}(\mathbf{x})$ the covariance vector between \mathbf{x} and χ_n defined by $\mathbf{k}(\mathbf{x}) := (k(\mathbf{x}, \mathbf{x}^{(1)}), \dots, k(\mathbf{x}, \mathbf{x}^{(n)}))^\top$ for any \mathbf{x} in \mathbb{X} . We denote $\mathbf{f}(\mathbf{x}) := (f_1(\mathbf{x}), \dots, f_l(\mathbf{x}))^\top$ the evaluation vector of \mathbf{f} on \mathbf{x} defining the trend and $\mathbb{F} \in \mathbb{R}^{n \times l}$ the matrix with $\mathbf{f}(\mathbf{x}^{(i)})^\top$ as i^{th} row. When $\boldsymbol{\beta}$ is known, the process ξ conditioned on the event \mathcal{E}_n is still Gaussian (O'Hagan [1978]) with mean, variance and covariance respectively denoted m_n , σ_n^2 , and k_n given by

$$m_n(\mathbf{x}) = \mathbf{f}(\mathbf{x})^\top \boldsymbol{\beta} + \mathbf{k}(\mathbf{x})^\top K^{-1} (g(\chi_n) - \mathbb{F} \boldsymbol{\beta}), \quad (3)$$

$$\sigma_n^2(\mathbf{x}) = \sigma^2(\mathbf{x}) - \mathbf{k}(\mathbf{x})^\top K^{-1} \mathbf{k}(\mathbf{x}), \quad (4)$$

$$k_n(\mathbf{x}, \mathbf{x}') = k(\mathbf{x}, \mathbf{x}') - \mathbf{k}(\mathbf{x})^\top K^{-1} \mathbf{k}(\mathbf{x}'). \quad (5)$$

We notice that the best linear unbiased predictor (BLUP) (with respect to mean quadratic error) is given by (3) with variance (4) and covariance (5).

When $\boldsymbol{\beta}$ is unknown and estimated by the maximum likelihood estimator (MLE)

$$\hat{\boldsymbol{\beta}} := (\mathbb{F}^\top K^{-1} \mathbb{F})^{-1} \mathbb{F}^\top K^{-1} g(\chi_n), \quad (6)$$

formulas (3), (4) and (5) become

$$m_n(\mathbf{x}) = \mathbf{f}(\mathbf{x})^\top \hat{\boldsymbol{\beta}} + \mathbf{k}(\mathbf{x})^\top K^{-1} (g(\chi_n) - \mathbb{F} \hat{\boldsymbol{\beta}}), \quad (7)$$

$$\sigma_n^2(\mathbf{x}) = \sigma^2(\mathbf{x}) - \mathbf{k}(\mathbf{x})^\top K^{-1} \mathbf{k}(\mathbf{x}) + (\mathbf{f}(\mathbf{x})^\top - \mathbf{k}(\mathbf{x})^\top K^{-1} \mathbb{F}) (\mathbb{F}^\top K^{-1} \mathbb{F})^{-1} (\mathbf{f}(\mathbf{x})^\top - \mathbf{k}(\mathbf{x})^\top K^{-1} \mathbb{F})^\top, \quad (8)$$

$$k_n(\mathbf{x}, \mathbf{x}') = k(\mathbf{x}, \mathbf{x}') - \mathbf{k}(\mathbf{x})^\top K^{-1} \mathbf{k}(\mathbf{x}') + (\mathbf{f}(\mathbf{x})^\top - \mathbf{k}(\mathbf{x})^\top K^{-1} \mathbb{F}) (\mathbb{F}^\top K^{-1} \mathbb{F})^{-1} (\mathbf{f}(\mathbf{x}')^\top - \mathbf{k}(\mathbf{x}')^\top K^{-1} \mathbb{F})^\top. \quad (9)$$

Their interpretation as conditional expectation, covariance and variance is still possible in a Bayesian context with a non informative prior distribution on the parameter β (Helbert et al. [2009]).

In order to save costly evaluations of function g , a sequential strategy of enrichment of the DoE is classically used (see e.g. Ginsbourger [2017]). Figure 1 provides a generic scheme of a sequential strategy. The stopping criteria can be a budget of simulations or a threshold on the remaining uncertainty on the estimation of the excursion set.

Sequential construction of a DoE (by GPR)

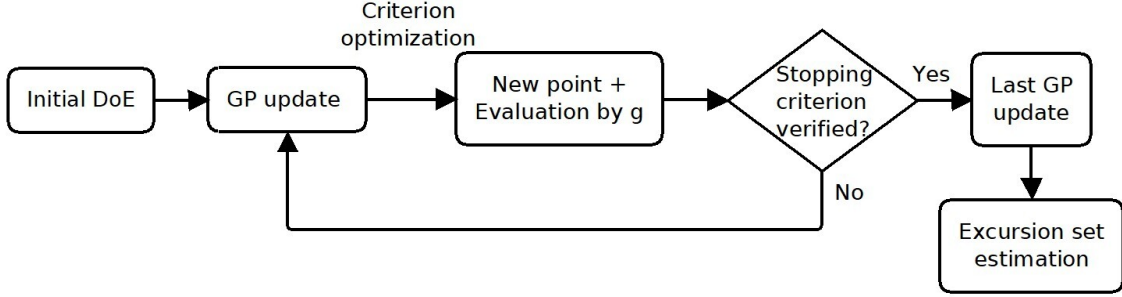


Figure 1: Diagram of the sequential DoE construction, coupled with GPR.

Among enrichment criteria, one can distinguish criteria that lead to an overall improvement of the model from goal-oriented criteria, which are adapted to particular frameworks such as optimization or inversion. The classical Mean Squared Error (MSE) criterion (Jin et al. [2002]), aims to select the point which has the highest prediction variance, as well as its integral versions IMSE and MMSE (Picheny et al. [2010]) standing for Maximum Mean Squared Error. Among goal oriented criteria, classical Expected Improvement (EI) from Jones et al. [1998], allows for global optimization. Several inversion-adapted criteria can be cited: deviation number (Echard et al. [2011]), ratio of the distance of the prediction mean to the threshold to the kriging standard deviation; Bichon criterion also known as Expected Feasibility Function (EFF) (Bichon et al. [2008]), and Ranjan criterion (Ranjan et al. [2008]).

2.2 Towards more exploration: the Bichon criterion

The Bichon criterion (Bichon), originally presented in Bichon et al. [2008] is a goal-oriented criterion for the DoE enrichment. This criterion is an adaptation of EI from Jones et al. [1998], introduced in the context of global optimization, to the inversion framework.

As a reminder, the original idea of EI is to select a point \mathbf{x} that allows an improvement of $g_{\min} - \xi(\mathbf{x})$ with g_{\min} the current minimum observed on the DoE, while taking into account the uncertainty of the surrogate model. The idea behind Bichon is to adapt this strategy to the excursion set estimation framework by considering both the variability of the surrogate model and the potential improvement in the knowledge of the excursion set boundary. This is the exploration-exploitation compromise.

To introduce Bichon, it is necessary to define, for a fixed \mathbf{x} belonging to \mathbb{X} , a random variable $\text{FF}(\mathbf{x})$ (Feasibility Function) defined by

$$\begin{aligned} \text{FF}(\mathbf{x}) &:= \varepsilon(\mathbf{x}) - \min \{ |T - \xi(\mathbf{x})|, \varepsilon(\mathbf{x}) \} \\ &= (\varepsilon(\mathbf{x}) - |T - \xi(\mathbf{x})|)^+, \end{aligned} \quad (10)$$

with $(\cdot)^+ := \max(\cdot, 0)$. This function represents the distance of the surrogate model to the bounds of the interval $[T - \varepsilon(\mathbf{x}), T + \varepsilon(\mathbf{x})]$ only if the surrogate model belongs to this interval and is 0 otherwise. In practice, the interval width $\varepsilon(\mathbf{x})$ is chosen proportional to the kriging standard deviation $\sigma_n(\mathbf{x})$, leading in particular to a null value of the criterion for the points already present in the DoE. An example is given in Figure 2. The feasibility function is drawn for one sample path of $\xi | \mathcal{E}_n$. Its maximization aims to select points close to the boundary of the excursion set estimate or points associated to high values of $\varepsilon(\mathbf{x})$. Then, the average of FF over all sample paths, gives

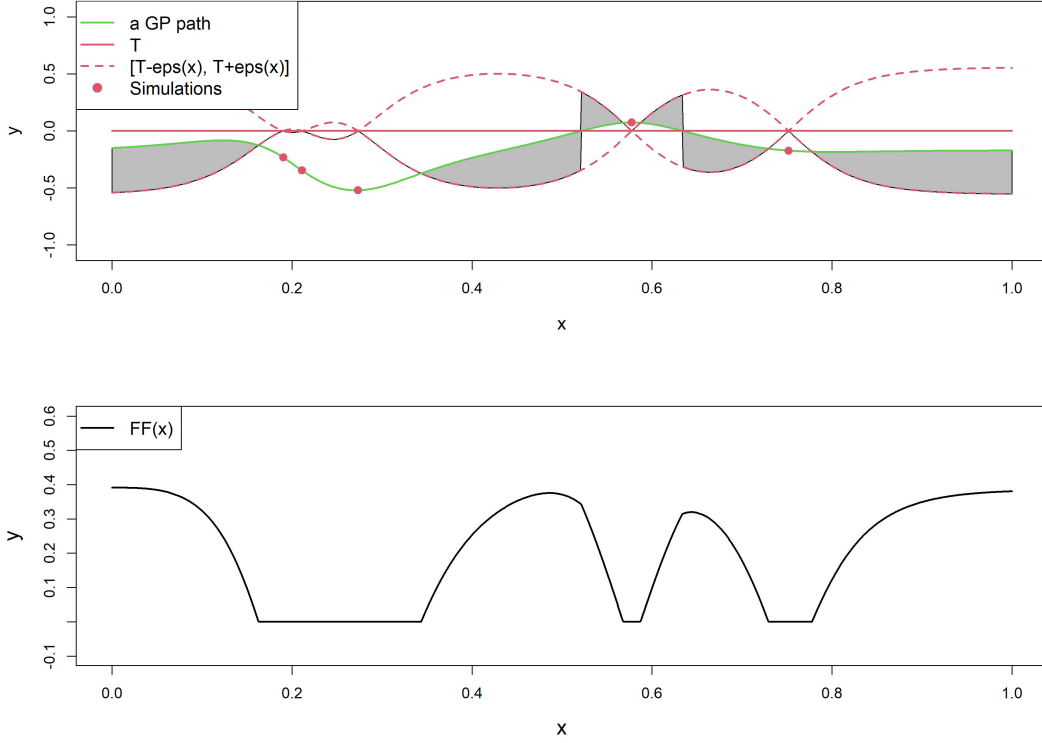


Figure 2: Representation of Feasibility Function (bottom) for a given example of a GP sample path conditioned on 5 evaluations of the g function, a threshold T set to 0 and $\varepsilon(x) := \sigma_n(\mathbf{x})$ (top).

the Expected Feasibility Function (EFF)

$$\text{EFF}(\mathbf{x}) := \mathbb{E} \left[(\varepsilon(\mathbf{x}) - |T - \xi(\mathbf{x})|)^+ \mid \mathcal{E}_n \right]. \quad (11)$$

The new selected points according Bichon are

$$\mathbf{x}^{(n+1)} \in \underset{\mathbf{x} \in \mathbb{X}}{\text{argmax}} \text{EFF}(\mathbf{x}). \quad (12)$$

To interpret (11), it is possible to make an heuristic analogy with the theory of statistical tests (Dagnelie [1992]). Let \mathbf{x} be fixed, suppose that $\xi(\mathbf{x}) | \mathcal{E}_n \sim \mathcal{N}(m_n(\mathbf{x}), \sigma_n(\mathbf{x}))$ with $m_n(\mathbf{x})$ unknown and $\sigma_n(\mathbf{x}) > 0$ known and let us define the following statistical test

$$H_0 : m_n(\mathbf{x}) = T \quad \text{against} \quad H_1 : m_n(\mathbf{x}) \neq T \quad (13)$$

We choose $v_{\mathbf{x}} := \frac{\xi(\mathbf{x}) - T}{\sigma_n(\mathbf{x})} \mid \mathcal{E}_n$ as the test statistic which follows standard normal distribution under H_0 . Consequently, if we want to refute Hypothesis H_0 at order α it is necessary that

$$|v_{\mathbf{x}}| > \kappa \quad (14)$$

with $\kappa := q_{1-\frac{\alpha}{2}}$ the quantile of order $1 - \frac{\alpha}{2}$ of the standard normal distribution.

However, what we wish to do is not to refute the hypothesis that $m_n(\mathbf{x}) = T$ but rather to select, among the \mathbf{x} for which the hypothesis H_0 is plausible i.e. $\kappa - |v_{\mathbf{x}}| > 0$, the \mathbf{x} for which the quantity $\kappa - |v_{\mathbf{x}}|$ is the largest in average. Multiplying $(\kappa - |v_{\mathbf{x}}|)^+$ by $\sigma_n(\mathbf{x})$ leads to Bichon criterion with $\varepsilon(\mathbf{x}) := \kappa\sigma_n(\mathbf{x})$, and has the effect to increase the exploration ability of the criterion.

Finally, an explicit formulation of Bichon (see Bect et al. [2012] for a proof) can be calculated based on the posterior kriging trend and variance, the threshold T and the width $\varepsilon(\mathbf{x})$

$$\begin{aligned} \text{EFF}(\mathbf{x}) = & (m_n(\mathbf{x}) - T) \left[2\phi\left(\frac{T - m_n(\mathbf{x})}{\sigma_n(\mathbf{x})}\right) - \phi\left(\frac{T^- - m_n(\mathbf{x})}{\sigma_n(\mathbf{x})}\right) - \phi\left(\frac{T^+ - m_n(\mathbf{x})}{\sigma_n(\mathbf{x})}\right) \right] \\ & - \sigma_n(\mathbf{x}) \left[2\varphi\left(\frac{T - m_n(\mathbf{x})}{\sigma_n(\mathbf{x})}\right) - \varphi\left(\frac{T^- - m_n(\mathbf{x})}{\sigma_n(\mathbf{x})}\right) - \varphi\left(\frac{T^+ - m_n(\mathbf{x})}{\sigma_n(\mathbf{x})}\right) \right] \\ & + \varepsilon(\mathbf{x}) \left[\phi\left(\frac{T^+ - m_n(\mathbf{x})}{\sigma_n(\mathbf{x})}\right) - \phi\left(\frac{T^- - m_n(\mathbf{x})}{\sigma_n(\mathbf{x})}\right) \right], \end{aligned} \quad (15)$$

with $T^\pm := T \pm \varepsilon(\mathbf{x})$, φ and ϕ represent respectively the probability density and cumulative distribution functions of the standard normal distribution. In practice, the enrichment of the DoE is done by maximizing the criterion given by Equation (15). The main objective of this work is to propose a SUR version of this goal-oriented criterion, in order to obtain a SUR method that is simpler to set up and more robust than SUR Vorob'ev.

3 SUR Bichon criterion

This section focuses on an adaptation of the Bichon criterion to a SUR strategy. The new SUR criterion we introduce can be implemented in the framework of GPR without any approximation unlike SUR Vorob'ev (see Appendix A and Chevalier [2013]). Moreover, SUR Bichon performs better than Bichon criterion and corrects the lack of robustness observed when applying SUR Vorob'ev, at least on test cases studied in Section 4.

3.1 Reminders on SUR strategies

SUR strategies aim at maximizing the mean uncertainty reduction induced by new evaluations. Let us introduce a residual uncertainty \mathcal{H}_n , computed with the GP model conditioned on \mathcal{E}_n . From this residual uncertainty, the conditional residual uncertainty $\mathcal{H}_{n+1}(\mathbf{x})$ is defined as the updated uncertainty when adding \mathbf{x} to DoE χ_n . This conditional uncertainty is then a measurable function of the random variable $\xi(\mathbf{x})|\mathcal{E}_n$. The associated SUR strategy is then defined by

$$\mathbf{x}^{(n+1)} \in \underset{\mathbf{x} \in \mathbb{X}}{\text{argmin}} \mathcal{J}_n(\mathbf{x}) \quad \text{with} \quad \mathcal{J}_n(\mathbf{x}) := \mathbb{E}[\mathcal{H}_{n+1}(\mathbf{x})]. \quad (16)$$

Note that the expectation in $\mathcal{J}_n(\mathbf{x})$ is relative to the distribution of $\xi(\mathbf{x})|\mathcal{E}_n$. Eq. (16) means that evaluating the surrogate model at $\mathbf{x}^{(n+1)}$ will decrease at most, the expected residual uncertainty.

More details on SUR strategies and their origin from k -step lookahead strategies can be found in Bect et al. [2012]. Among classical SUR strategies based on GPR, we can quote for example different criteria using the excursion set volume, presented in Bect et al. [2012]. A more complex criterion requiring notions about the random set theory of Vorob'ev (Molchanov [2005]) introduced in Chevalier [2013], can also be cited. We refer to Appendix A for more details on Vorob'ev theory and the associated SUR Vorob'ev strategy.

SUR strategies are numerically more complex to implement, but are generally more efficient than other goal oriented strategies (Bect et al. [2012] and Chevalier [2013]), for the same number of

evaluations. A reduction in the numerical complexity of SUR strategies is frequently used through the use of kriging update formulas introduced in Chevalier [2013] (see Appendix B).

3.2 Formulation of the SUR Bichon criterion

Let $\mathbb{P}_{\mathbb{X}}$ a probability measure on \mathbb{X} . Following the formalism of SUR strategies given in section 3.1, we first define a residual uncertainty \mathcal{H}_n by

$$\begin{aligned}\mathcal{H}_n &:= \int_{\mathbb{X}} \text{EFF}(\mathbf{z}) \, d\mathbb{P}_{\mathbb{X}}(\mathbf{z}) \\ &= \int_{\mathbb{X}} \mathbb{E} \left[(\kappa\sigma_n(\mathbf{z}) - |T - \xi(\mathbf{z})|)^+ \mid \mathcal{E}_n \right] d\mathbb{P}_{\mathbb{X}}(\mathbf{z}), \quad \text{with } \kappa > 0.\end{aligned}\tag{17}$$

The corresponding conditional residual uncertainty is then defined by

$$\mathcal{H}_{n+1}(\mathbf{x}) := \int_{\mathbb{X}} \mathbb{E} \left[(\kappa\sigma_{n+1}(\mathbf{z}) - |T - \xi(\mathbf{z})|)^+ \mid \xi(\mathbf{x}), \mathcal{E}_n \right] d\mathbb{P}_{\mathbb{X}}(\mathbf{z}), \quad \text{with } \kappa > 0,\tag{18}$$

with $\sigma_{n+1}(\mathbf{z})$ the kriging standard deviation computed from Equation (34) in Appendix B and \mathbf{x} being the $n + 1^{\text{th}}$ observation point. In practice, the chosen probability measure $\mathbb{P}_{\mathbb{X}}$ is the Lebesgue measure restricted and normalized on \mathbb{X} and the coefficient κ is usually set to 1 like in Bichon (Bect et al. [2012]). The residual uncertainty \mathcal{H}_n represents the average (with respect to $\mathbb{P}_{\mathbb{X}}$) of mean distances (in positive values) of $\xi(\mathbf{z})$ to the bounds of the interval $[T - \kappa\sigma_n(\mathbf{z}), T + \kappa\sigma_n(\mathbf{z})]$, conditioned on \mathcal{E}_n . An overall reduction in σ_n leads to a decrease in the uncertainty \mathcal{H}_n . The same applies to the addition of a new point close to the boundary defined by the threshold T .

The problem is to find

$$\mathbf{x}^{(n+1)} \in \underset{\mathbf{x} \in \mathbb{X}}{\text{argmin}} \mathcal{J}_n(\mathbf{x}) \quad \text{with} \quad \mathcal{J}_n(\mathbf{x}) := \mathbb{E} \left[\int_{\mathbb{X}} \mathbb{E} \left[(\kappa\sigma_{n+1}(\mathbf{z}) - |T - \xi(\mathbf{z})|)^+ \mid \xi(\mathbf{x}), \mathcal{E}_n \right] d\mathbb{P}_{\mathbb{X}}(\mathbf{z}) \right],\tag{19}$$

with $\kappa > 0$. The first expectation is relative to $\xi(\mathbf{x}) \mid \mathcal{E}_n$ and the second one is relative to $\xi(\mathbf{z})$ knowing $\xi(\mathbf{x}), \mathcal{E}_n$.

Lemma 1.

$$\mathcal{J}_n(\mathbf{x}) = \int_{\mathbb{X}} \mathbb{E} \left[(\kappa\sigma_{n+1}(\mathbf{z}) - |T - \xi(\mathbf{z})|)^+ \mid \mathcal{E}_n \right] d\mathbb{P}_{\mathbb{X}}(\mathbf{z}).\tag{20}$$

Proof.

The integrand of the chosen residual uncertainty in (18) is a positive quantity, by positivity of the expectation. So, by re-injecting the expression of uncertainty (18) into (16), then applying Fubini–Tonelli theorem (thanks to σ -finite measures and positive integrand), we obtain

$$\mathcal{J}_n(\mathbf{x}) = \int_{\mathbb{X}} \mathbb{E} \left[\mathbb{E} \left[(\kappa\sigma_{n+1}(\mathbf{z}) - |T - \xi(\mathbf{z})|)^+ \mid \xi(\mathbf{x}), \mathcal{E}_n \right] \right] d\mathbb{P}_{\mathbb{X}}(\mathbf{z}),\tag{21}$$

Then, in (21) the two expectations are reduced in one to obtain (20). \square

Finally, Proposition 1 below provides an explicit formula for the integrand of (20).

Proposition 1. For all \mathbf{x}, \mathbf{z} belonging to \mathbb{X}^2 , we have

$$\begin{aligned} & \mathbb{E} \left[\left(\kappa \sigma_{n+1}(\mathbf{z}) - |T - \xi(\mathbf{z})| \right)^+ \middle| \mathcal{E}_n \right] \\ &= (m_n(\mathbf{z}) - T) \left[2 \phi \left(\frac{T - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})} \right) - \phi \left(\frac{T^- - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})} \right) - \phi \left(\frac{T^+ - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})} \right) \right] \\ & \quad - \sigma_n(\mathbf{z}) \left[2 \varphi \left(\frac{T - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})} \right) - \varphi \left(\frac{T^- - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})} \right) - \varphi \left(\frac{T^+ - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})} \right) \right] \\ & \quad + \varepsilon_{\mathbf{x}}(\mathbf{z}) \left[\phi \left(\frac{T^+ - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})} \right) - \phi \left(\frac{T^- - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})} \right) \right] \end{aligned} \quad (22)$$

where $\varepsilon_{\mathbf{x}}(\mathbf{z}) := \kappa \sigma_{n+1}(\mathbf{z})$, $T^\pm := T \pm \varepsilon_{\mathbf{x}}(\mathbf{z})$, φ and ϕ denote the probability density and cumulative distribution functions of the standard normal distribution, respectively.

The dependency in \mathbf{x} in Equation (22) is only given via $\varepsilon_{\mathbf{x}}(\mathbf{z}) = \kappa \sigma_{n+1}(\mathbf{z})$, therefore only via $\sigma_{n+1}(\mathbf{z})$, which is independent of the model evaluation on \mathbf{x} according to the kriging formulas. In practice, kriging update formulas (see Equation (34) Appendix B) will be used to get a fast evaluation of $\varepsilon_{\mathbf{x}}(\mathbf{z})$. The proof of Proposition 1 is postponed to Appendix C.

4 Numerical experiments

The performances of SUR Bichon are illustrated on two analytical examples, and compared to SUR Vorob'ev and standard Bichon performances. The chosen test functions are the rescaled Branin function in dimension 2 and rescaled Hartmann function in dimension 6 (Picheny et al. [2013]). The choice of the threshold T for each of these functions is discussed later.

Several DoE enrichment strategies can be considered: an enrichment by Bichon $\chi_{0,n}$, one using SUR Bichon $\chi_{1,n}$ and one using SUR Vorob'ev $\chi_{2,n}$, all three after n iterations. The criteria performance is evaluated through two different estimators: naive estimator $\hat{\Gamma}_1 := m_n^{-1}(\cdot - \infty, T]$ and Vorob'ev estimator noted $\hat{\Gamma}_2$, which corresponds to the Vorob'ev expectation (Appendix A). The performances of the different criteria are then compared after n iterations with the approximation error $\text{Err}(\hat{\Gamma}_i(\chi_{j,n})) := \mathbb{P}_{\mathbb{X}}(\hat{\Gamma}_i(\chi_{j,n}) \Delta \Gamma^*) / \mathbb{P}_{\mathbb{X}}(\Gamma^*)$, for $(i, j) \in \{1, 2\}^2$. This error measures the relative volume of the symmetric difference between estimator $\hat{\Gamma}_i(\chi_{j,n})$ and true excursion set Γ^* defined in (1).

4.1 Implementation choices

As mentioned earlier, the choices of trend m and covariance kernel k are fundamental. In the following, the trend is chosen as a single constant term m , see Roustant et al. [2012] for more details. A classical kernel product of type Matérn 5/2 is chosen:

$$k(\mathbf{x}, \mathbf{x}') := \text{Cov}(\mathbf{Z}(\mathbf{x}), \mathbf{Z}(\mathbf{x}')) = \sigma_c^2 \prod_{i=1}^d R_{\text{Matérn } 5/2}(h_i, \theta_i), \quad \forall (\mathbf{x}, \mathbf{x}') \in \mathbb{X}^2, \quad (23)$$

with a vector of parameters θ belonging to \mathbb{R}_+^{*d} , estimated by maximizing the likelihood at each iteration, $h_i = |\mathbf{x}_i - \mathbf{x}'_i|$, σ_c a fixed parameter and

$$R_{\text{Matérn } 5/2}(h_i, \theta_i) := \left(1 + \frac{\sqrt{5}|h_i|}{\theta_i} + \frac{5h_i^2}{3\theta_i^2} \right) \exp \left(-\frac{\sqrt{5}|h_i|}{\theta_i} \right). \quad (24)$$

This choice leads to trajectories of class C^2 (Paciorek [2003]).

The implementation of SUR Bichon from formulas (20) and (22), is greatly inspired by the implementation of various SUR criteria in the package *KrigInv* (Chevalier et al. [2014]). In addition, the chosen measure $\mathbb{P}_{\mathbb{X}}$ is the renormalized Lebesgue measure restricted to \mathbb{X} , which is possible because \mathbb{X} is compact. In (20), the integration is performed using a Sobol' sequence with *n.points* integration points (package *randtoolbox* Dutang and Savicky [2013]). The criterion is optimized with the genetic algorithm Genoud (with *pop.size* = 50d) (package *rgenoud*, Mebane Jr and Sekhon [2011]). Unless explicitly stated, κ in (22) is set to 1, initial DoEs are obtained by LHS optimized by maximizing minimal distances between the points (Latin Hypercube Sampling, Dupuy et al. [2015]) with size to be specified in the following, and *n.points* defined above is set to 10^4 .

The volume of Γ^* and $\hat{\Gamma}_i(\chi_{j,n})\Delta\Gamma^*$ are approached using a quasi-Monte Carlo methods (Lemieux [2009]) with a Sobol' sequence of size 10^4 .

4.2 Performance tests on Branin-rescaled 2D function

The Branin-rescaled function, defined in Picheny et al. [2013] on $\mathbb{X} := [0, 1]^2$, is represented in Figure 3. The Γ^* excursion set is defined by the upper bound $T = 10$ on the function values, which leads to 3 disconnected areas and the volume of Γ^* represents 15.74% of the total volume of \mathbb{X} . The tests are performed on 100 different initial DoEs of size 10. 20 iterations (1 simulation per iteration) are run for SUR Bichon, SUR Vorob'ev and Bichon.

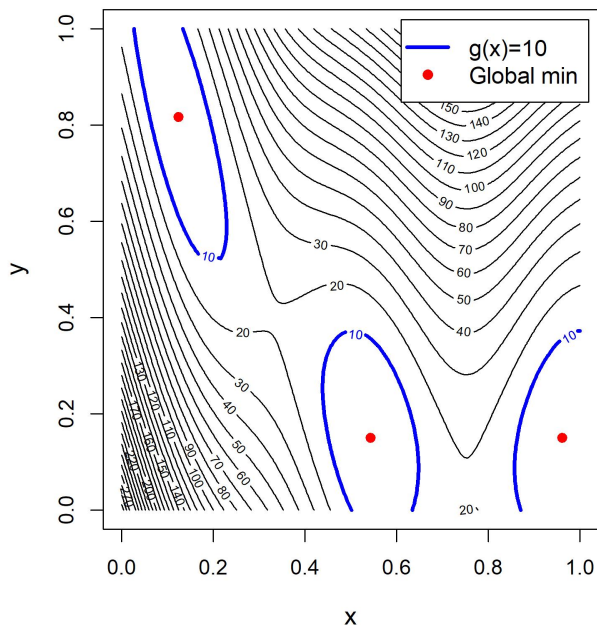


Figure 3: Representation of the Branin-rescaled function on \mathbb{X} .

Black solid lines (line plot) of Figure 4 represent the approximation error for each of the 100 initial DoEs of size 10. This makes it possible to visualize the enrichment performances throughout the iterations. Bichon seems to perform less well than the other two SUR criteria: the median is higher. SUR Bichon appears more robust than SUR Vorob'ev throughout the enrichment, no matter which estimator is chosen. Indeed, in the case of SUR Vorob'ev, several extreme cases present stagnation of the approximation error. These rare stagnations are due to the late discovery of one of the three components of the excursion set as illustrated below. The logarithmic scale of the graph seems to show a stagnation of the curve for these few cases, but it is in fact a faster progression towards a threshold value, due to the simplification of the problem to the two remaining

components. Also, the approximation error with $\hat{\Gamma}_1$ seems more robust than with $\hat{\Gamma}_2$ (see Appendix D for more details), and this can be explained by the fact that estimators $\hat{\Gamma}_1$ and $\hat{\Gamma}_2$ are respectively based on an extension of median and mean concepts to sets (Appendix A).

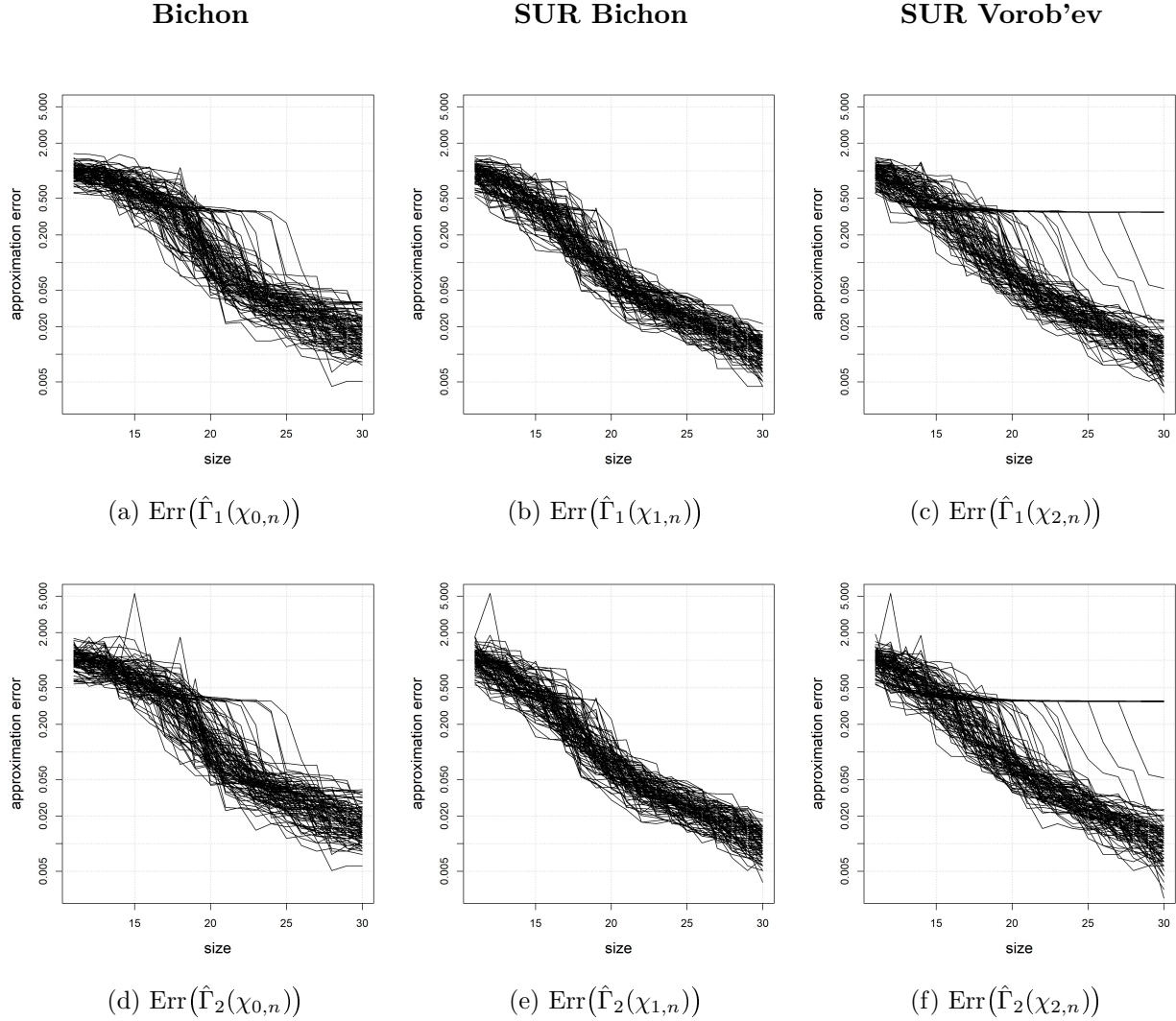


Figure 4: Line plots (with logarithmic scale) of the approximation error $\text{Err}(\hat{\Gamma}_i(\chi_{j,n}))$ for the different criteria during 20 iterations, for Branin-rescaled function inversion ($d = 2$) with $T = 10$, for 100 different initial DoEs of size 10 of type LHS Maximin, for $\kappa = 1$ and with $\text{n.points} = 10^4$. Left column: Bichon with naive estimator (a) and Vorob'ev estimator (d). Middle column: SUR Vorob'ev with naive estimator (b) and Vorob'ev estimator (e). Right column: SUR Bichon with naive estimator (c) and Vorob'ev estimator (f).

We focus on one run of the enrichment with SUR Vorob'ev associated with one of the outliers of Figure 4. The associated $\hat{\Gamma}_1$ (resp. $\hat{\Gamma}_2$) estimators are represented as green full (resp. dotted) line on Figure 5, after 20 iterations. This figure shows that SUR Vorob'ev misses one of the three areas of the exact excursion set Γ^* presented in Figure 3. The use of SUR Bichon allows a better exploration of the design space, which here allows to detect the three areas of $\hat{\Gamma}^*$. We notice that there is very few differences between the two types of estimators and given the robustness of naive estimator $\hat{\Gamma}_1$ compared to $\hat{\Gamma}_2$ (Appendix D), naive estimator is kept for the remaining tests in dimension 2.

The characteristic statistical values of the empirical distribution for the error approximation with naïve $\hat{\Gamma}_1$ estimator are given in Table 1 for SUR Bichon, SUR Vorob'ev and Bichon. This table confirms the poor performance of Bichon in relation to the two SUR criteria. In the following, Bichon is set aside to focus on the comparison of the two SUR Bichon and SUR Vorob'ev. It can

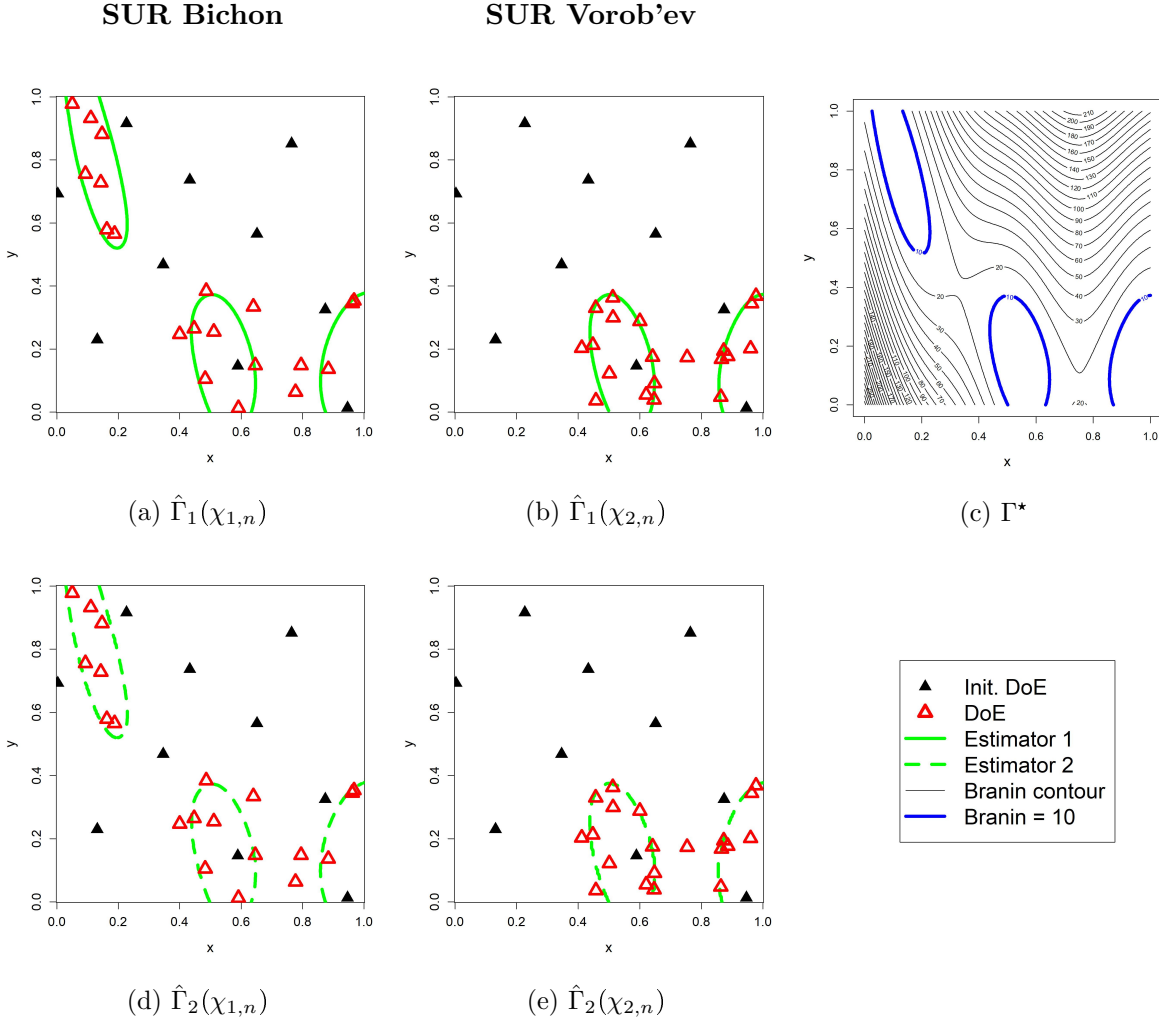


Figure 5: Representation of two $\hat{\Gamma}$ estimators for each of the two criteria after 20 iterations, in comparison with the true excursion set (top right), for Branin-rescaled function inversion ($d = 2$) with $T = 10$, for a particular initial DoE of size 10 where SUR Bichon outperforms SUR Vorob'ev. Left column: SUR Bichon with naive estimator (a) and Vorob'ev estimator (d). Middle column: SUR Vorob'ev with naive estimator (b) and Vorob'ev estimator (e). Right column: true Γ^* excursion set and Branin-rescaled contour lines (c).

be also seen that only for the quantile 5%, the results are slightly better for SUR Vorob'ev. All others results show SUR Bichon is more efficient than SUR Vorob'ev: the outliers of SUR Vorob'ev deteriorate the characteristic values especially mean or standard deviation.

To summarize, the study of the performances of SUR Bichon on Branin-rescaled function, showed that for $T = 10$ the sought excursion set with three connected components is better detected when using SUR Bichon. Indeed, the latter, unlike SUR Vorob'ev, makes it possible to avoid extreme cases for which one of the three connected components is completely missed.

4.3 Performance tests on Hartmann-rescaled 6D function

In this section the inversion results for the Hartmann-rescaled function from Picheny et al. [2013] on $\mathbb{X} := [0, 1]^6$ are presented. The excursion set Γ^* is defined by the upper bound $T = -1.6$, with a volume that represents 15.45% of the total volume of \mathbb{X} . Results of clustering methods (not presented here) suggest that Γ^* is composed of only one large connected component. The tests are performed on 50 different initial DoEs of size 30 and 600 iterations of DoE enrichment are run for both SUR Bichon and SUR Vorob'ev.

Crit. ($\times 100$)	ite = 10			ite = 20		
	SUR B.	SUR V.	B.	SUR B.	SUR V.	B.
Mean	7.82	12.35	15.07	1.09	3.18	1.71
Median	7.24	7.78	11.94	1.08	1.08	1.59
Quantile 5%	4.36	4.24	5.53	0.57	0.51	0.89
Quantile 95%	12.94	36.42	37.87	1.59	35.13	3.25
Standard Deviation	3.21	10.79	9.97	0.34	8.17	0.73
Interquartile Range	3.80	5.38	9.24	0.52	0.64	0.89

Table 1: Summary of empirical distributions of the $\text{Err}(\hat{\Gamma}_i(\chi_{j,n}))$ for the different criteria after 10 and 20 iterations, for Branin-rescaled function inversion ($d = 2$) with $T = 10$, for 100 different initial DoEs of size 10 of type LHS Maximin.

Line plots on Figure 6 show the approximation error along the iterations of the enrichment. Firstly, it can be observed that the improvement of the approximation error during the enrichment is slower than in dimension 2, which is consistent with the increasing difficulty of the problem in higher dimension. Moreover, we observe that SUR Bichon performs better than SUR Vorob'ev whatever the chosen estimator, with respect to the robustness to outliers but also on average, especially from the 300th iteration. In addition, it is clear from Figure 6 (a) and (c) that naive estimator $\hat{\Gamma}_1$ gives a more robust approximation error than $\hat{\Gamma}_2$, with SUR Bichon enrichment. We thus decide to present the numerical results in the following of the section for $\hat{\Gamma}_1$ only.

We focus on one of the outliers of Figure 6 (b) for which the enrichment strategy is based on SUR Vorob'ev. For an extreme case, we represent in pairwise projection the points of a Sobol' sequence of size $5 \cdot 10^3$ on \mathbb{X} belonging to $\hat{\Gamma}_1 \Delta \Gamma^*$, with $\hat{\Gamma}_1$ the estimator obtained after 600 iterations (see Figure 7). There are only 55 misclassified points observed for SUR Bichon, against 247 in the case of SUR Vorob'ev. Moreover, among the 247 points for the case SUR Vorob'ev, 191 correspond to $\hat{\Gamma} \setminus \Gamma^*$ (unfeasible points that are predicted feasible), whereas the remaining misclassified points correspond to feasible points that were predicted unfeasible (as for 2D example). This allows to further illustrate the robustness of SUR Bichon compared to SUR Vorob'ev. A comparable study was carried out on the other extreme runs as well as on the non-extreme ones. The results showed that the configuration for the other extreme run is comparable to that in Figure 7 while the configurations for the non-extreme runs are all more or less similar and relatively balanced in terms of number of misclassified points between SUR Bichon and SUR Vorob'ev criteria.

The characteristic statistical values of the empirical distribution for the approximation error are given in Figure 2 for both SUR Bichon and SUR Vorob'ev. It can be confirmed that except at the beginning where enrichment is not yet sufficient, SUR Bichon performs better for all indicators than SUR Vorob'ev, and not only in terms of robustness (see e.g. the quantile of order 5% or the median).

In summary, the tests on Hartmann-rescaled function in dimension 6 with $T = -1.6$, further highlight the robustness of SUR Bichon compared to SUR Vorob'ev, in dimension higher than 2. In addition to the robustness, it was also observed that in this 6 dimensional case, beyond about 300 iterations, SUR Bichon performs better than SUR Vorob'ev, even without considering the outliers.

The robustness of SUR Bichon can be explained by its exploratory capability forced by the kriging standard deviation in factor of the SUR Bichon formulation (see Section 2.2). Besides, the Vorob'ev expectation is strongly dependent on the stationarity assumption of the underlying Gaussian process (Appendix D), which has an influence on the enrichment, since the enrichment with SUR Vorob'ev is based on the Vorob'ev deviation (Appendix A), and then on the Vorob'ev expectation. This could explain the lack of robustness of SUR Vorob'ev. Indeed, in practice the

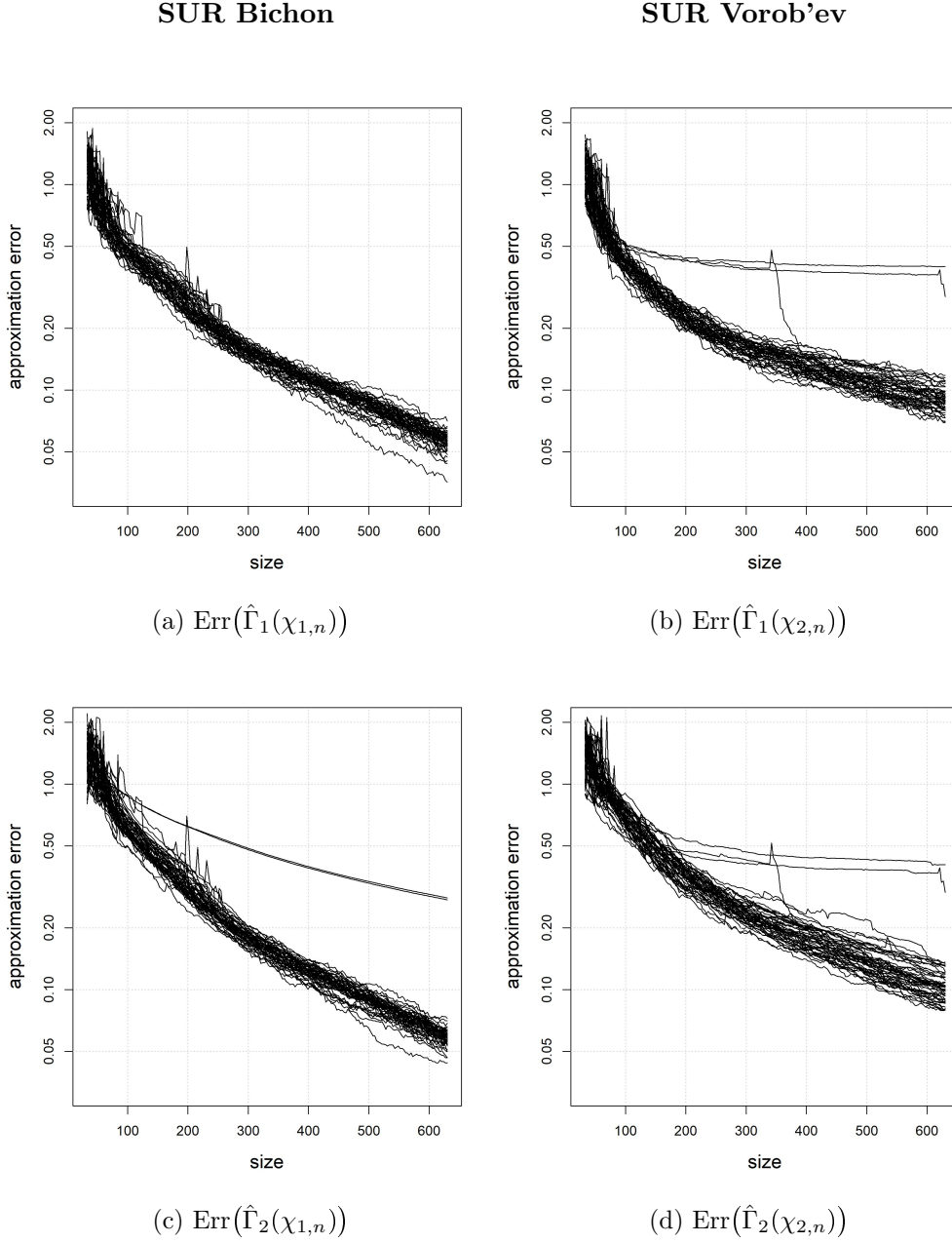


Figure 6: Line plots (with logarithmic scale) of the approximation error $\mathbb{P}_{\mathbb{X}}(\hat{\Gamma}_i(\chi_{j,n})\Delta\Gamma^*)/\mathbb{P}_{\mathbb{X}}(\Gamma^*)$ (with a Sobol' sequence of size 10^4) for the different criteria during 600 iterations, for Hartmann-rescaled function inversion ($d = 6$) with $T = -1.6$, for 50 different initial DoEs of size 30 of type LHS Maximin, for $\kappa = 1$ and with n.points= 10^4 . Left column: SUR Bichon with naive estimator (a) and Vorob'ev estimator (c). Right column: SUR Vorob'ev with naive estimator (b) and Vorob'ev estimator (d).

stationarity hypothesis is never rigorously checked (unless the model is defined as a given realization of a stationary Gaussian process). Eventually, the calculation of the Vorob'ev criterion is sensitive to the determination of the Vorob'ev threshold α^* (see Appendix A). However, we have verified that the determination of α^* was not the problem for the robustness of SUR Vorob'ev by checking the numerical simplicity of the minimum search for the function $\alpha \mapsto |\mathbb{E}[\mathbb{P}_{\mathbb{X}}(\Gamma)|\mathcal{E}_n] - \mathbb{P}_{\mathbb{X}}(Q_\alpha)|$.

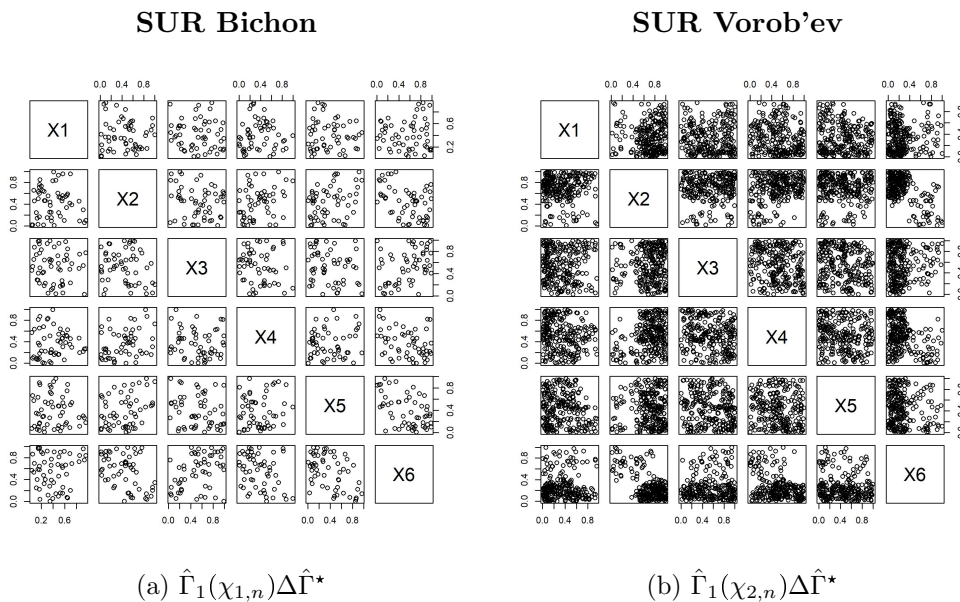


Figure 7: Pairwise projection plot of $\hat{\Gamma}_1\Delta\Gamma^*$ for a 5.10^3 -Sobol' sequence, for the two criteria after 600 iterations, for Hartmann-rescaled function inversion ($d = 6$) with $T = -1.6$, for a particular initial DoE of size 30 where SUR Bichon outperforms on SUR Vorob'ev, for $\kappa = 1$ and for n.points= 10^4 . Left column: SUR Bichon. Right column: SUR Vorob'ev.

Crit. ($\times 100$)	ite = 99		ite = 300		ite = 600	
	SUR B.	SUR V.	SUR B.	SUR V.	SUR B.	SUR V.
Mean	40.42	35.05	13.92	16.55	5.61	9.94
Median	40.32	34.72	13.92	15.28	5.66	8.83
Quantile 5%	34.14	28.84	12.09	12.74	4.62	7.17
Quantile 95%	46.67	44.40	15.38	29.42	6.45	11.63
Standard Deviation	3.98	4.48	0.99	6.14	0.61	5.26
Interquartile Range	5.26	4.56	1.13	1.81	0.68	1.75

Table 2: Summary of empirical distributions of the approximation error $\mathbb{P}_{\mathbb{X}}(\hat{\Gamma}\Delta\Gamma^*)/\mathbb{P}_{\mathbb{X}}(\Gamma^*)$ (with a Sobol' sequence of size 10^4) for the different criteria after 99, 300 and 600 iterations, for Hartmann-rescaled function inversion ($d = 6$) with $T = -1.6$, for 50 different initial DoEs of size 30 of type LHS Maximin, for $\kappa = 1$ and with n.points= 10^4 .

5 Conclusion

In the framework of solving inversion problems using Gaussian Process Regression, we have proposed a new SUR criterion based on the Bichon criterion for DoE enrichment. Numerical simulations have demonstrated its good exploratory behavior, as far as its robustness from different points of view. Indeed, our new criterion is robust with the stationarity assumption of the underlying Gaussian process. Moreover, it is robust to the geometry of the set to be retrieved, in particular in terms of number of connected components.

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A Basics on Vorob’ev Theory and corresponding SUR strategy

A.1 Vorob’ev expectation

In this part, the notion of expectation for random closed sets in the sense of Vorob’ev is defined from Molchanov [2005]. The framework is a compact set $\mathbb{X} \subset \mathbb{R}^d$ and a random closed set Γ of \mathbb{X} . It is recalled that $\Gamma : \Omega \rightarrow \mathcal{C}$ is a random closed set if it is a measurable function on the probability space $(\Omega, \mathcal{F}, \mathbb{P})$ with values in the set of all compacts of \mathbb{X} in the sense that:

$$\forall C \in \mathcal{C}, \{w \in \Omega, \Gamma(w) \cap C \neq \emptyset\} \in \mathcal{F}. \quad (25)$$

Let’s define the parametric family $\{Q_\alpha\}_{\alpha \in [0,1]}$ of Vorob’ev quantiles is defined by:

$$Q_\alpha := \{x \in \mathbb{X} : p(x) := \mathbb{P}(x \in \Gamma) \geq \alpha\}, \forall \alpha \in [0, 1]. \quad (26)$$

The elements of $\{Q_\alpha\}_{\alpha \in [0,1]}$ are called the Vorob’ev quantiles of the random closed set Γ and the function p is called the coverage function of Γ .

To define the expectation of the random closed set Γ , Molchanov [2005] comes back to the expectation of a real random variable: the measure of the Γ set $\mathbb{P}_{\mathbb{X}}(\Gamma)$. From the parametric family

of Vorob'ev quantiles (see (26)), the expectation of Γ in the sense of Vorob'ev is then defined as the Vorob'ev quantile of measure equal (or the closest one higher) to the expectation of the measure of Γ . More precisely, the Vorob'ev expectation of a random closed set Γ is the set Q_{α^*} , where α^* is defined as the Vorob'ev threshold by

$$\forall \alpha > \alpha^*, \mathbb{P}_{\mathbb{X}}(Q_\alpha) < \mathbb{E}[\mathbb{P}_{\mathbb{X}}(\Gamma)] \leq \mathbb{P}_{\mathbb{X}}(Q_{\alpha^*}), \quad (27)$$

where $\mathbb{P}_{\mathbb{X}}$ denotes the Lebesgue measure on \mathbb{X} . α^* is called the Vorob'ev threshold.

Remark 1.

- Based on Equation (26)), the function $\alpha \mapsto \mathbb{P}_{\mathbb{X}}(Q_\alpha)$ is decreasing on $[0, 1]$.
- The uniqueness of α^* in the definition is easily checked. The existence of such α^* in the definition of Vorob'ev expectation is based on the decreasing and continuity to the left of the function $\alpha \mapsto \mathbb{P}_{\mathbb{X}}(Q_\alpha)$ which is itself guaranteed by the superior semi-continuity of the coverage function p (see Molchanov [2005] page 23).
- The continuity of the function $\alpha \mapsto \mathbb{P}_{\mathbb{X}}(Q_\alpha)$ ensures equality $\mathbb{P}_{\mathbb{X}}(Q_{\alpha^*}) = \mathbb{E}[\mathbb{P}_{\mathbb{X}}(\Gamma)]$ in the definition of Vorob'ev expectation.

In the particular case where Γ is given by $\Gamma := \{\mathbf{x} \in \mathbb{X}, \xi(\mathbf{x}) \leq T\}$ with ξ a stochastic process indexed by \mathbb{X} with continuous trajectories conditioned on the event \mathcal{E}_n corresponding to n evaluations of ξ and T a fixed threshold, Γ is a random closed set ([Molchanov, 2005, page 3]). A sufficient condition to obtain a stochastic process with continuous trajectories is to consider a separable Gaussian process with continuous mean and covariance kernel of type Matérn 3/2 or 5/2 ([Paciorek, 2003, pages 35 and 44]). Moreover, in this case, the function $\alpha \mapsto \mathbb{P}_{\mathbb{X}}(Q_\alpha)$ is continuous and so the equality $\mathbb{P}_{\mathbb{X}}(Q_{\alpha^*}) = \mathbb{E}[\mathbb{P}_{\mathbb{X}}(\Gamma) | \mathcal{E}_n]$ is verified. It is also important to notice that naive estimator $\hat{\Gamma}_1$ is almost surely equal to the median of Vorob'ev (quantile of order 1/2). Indeed, by noting ϕ the distribution function of the standard normal distribution,

$$\begin{aligned} \hat{\Gamma}_1 &= \{\mathbf{x} \in \mathbb{X}, m_n(\mathbf{x}) \leq T\} \\ &\stackrel{\text{a.s.}}{=} \left\{ \mathbf{x} \in \mathbb{X}, \frac{T - m_n(\mathbf{x})}{\sigma_n(\mathbf{x})} \geq 0 \text{ and } \sigma_n(\mathbf{x}) \neq 0 \right\} \\ &= \left\{ \mathbf{x} \in \mathbb{X}, \phi\left(\frac{T - m_n(\mathbf{x})}{\sigma_n(\mathbf{x})}\right) \geq \phi(0) \text{ and } \sigma_n(\mathbf{x}) \neq 0 \right\} \text{ as } \phi \text{ increases} \\ &\stackrel{\text{a.s.}}{=} \left\{ \mathbf{x} \in \mathbb{X}, p_n(\mathbf{x}) \geq \frac{1}{2} \right\} \\ &= Q_{\frac{1}{2}}, \end{aligned} \quad (28)$$

where p_n is the coverage function $p_n(\mathbf{x}) := \mathbb{P}(\xi(\mathbf{x}) \leq T | \mathcal{E}_n)$.

Repeating the previous calculation and replacing 1/2 by the Vorob'ev threshold α^* , we obtain :

$$Q_{\alpha^*} \stackrel{\text{a.s.}}{=} \{\mathbf{x} \in \mathbb{X}, m_n(\mathbf{x}) \leq T - \phi^{-1}(\alpha^*) \sigma_n(\mathbf{x})\} \quad (29)$$

A.2 Vorob'ev deviation

The introduction of the concept of Vorob'ev deviation is used to define residual uncertainty $\mathcal{H}_n(\mathbf{x})$ in a SUR strategy. Let's start by introducing the notion of distance between two random closed sets.

The average distance $d_{\mathbb{P}_{\mathbb{X}}}$ with respect to a measure $\mathbb{P}_{\mathbb{X}}$ on all pairs of random closed sets included in \mathbb{X} is defined by: for all random closed sets Γ_1, Γ_2 defined on \mathbb{X} ,

$$d_{\mathbb{P}_{\mathbb{X}}}(\Gamma_1, \Gamma_2) := \mathbb{E}[\mathbb{P}_{\mathbb{X}}(\Gamma_1 \Delta \Gamma_2)] \quad (30)$$

where Δ is the random symmetric difference: $\forall \omega \in \Omega, \Gamma_1 \Delta \Gamma_2(\omega) := (\Gamma_1 \setminus \Gamma_2)(\omega) \cup (\Gamma_2 \setminus \Gamma_1)(\omega)$. In addition, the function $d_{\mathbb{P}_{\mathbb{X}}}$ checks the properties of a distance.

The following proposition Molchanov [2005] justifies the choice of the Vorob'ev quantile family to define the Vorob'ev expectation and also allows to define the Vorob'ev deviation. Moreover, when $\mathbb{E}[\mathbb{P}_{\mathbb{X}}(\Gamma)] = \mathbb{P}_{\mathbb{X}}(Q_{\alpha^*})$ (especially in the case of $\Gamma := \{\mathbf{x} \in \mathbf{X}, \xi(\mathbf{x}) \leq T\}$ with ξ a stochastic process indexed by \mathbb{X} with continuous trajectories), the condition $\alpha^* \geq \frac{1}{2}$ is no longer necessary (see [El Amri, 2019, page 28] for the proof)

Proposition 2. *Noting Q_{α^*} the Vorob'ev expectation of the random closed set Γ and assuming that $\alpha^* \geq \frac{1}{2}$, it results that: for any measurable set M included in \mathbb{X} such that $\mathbb{P}_{\mathbb{X}}(M) = \mathbb{E}[\mathbb{P}_{\mathbb{X}}(\Gamma)]$,*

$$d_{\mathbb{P}_{\mathbb{X}}}(\Gamma, Q_{\alpha^*}) \leq d_{\mathbb{P}_{\mathbb{X}}}(\Gamma, M) \quad (31)$$

The Vorob'ev deviation of the random set Γ is defined as the quantity $d_{\mathbb{P}_{\mathbb{X}}}(\Gamma, Q_{\alpha^*})$. The Vorob'ev deviation quantifies the variability of the random closed set Γ relative to its Vorob'ev expectation.

A.3 SUR Vorob'ev criterion

Once the basic elements of Vorob'ev theory are introduced, the associated SUR strategy is simply defined from the definition of SUR strategies via Equation (16) by taking:

$$\mathcal{H}_n := \mathbb{E}[\mathbb{P}_{\mathbb{X}}(\Gamma \Delta Q_{n, \alpha_n^*}) | \mathcal{E}_n] \quad \text{and} \quad \mathcal{H}_{n+1}(\mathbf{x}) := \mathbb{E}[\mathbb{P}_{\mathbb{X}}(\Gamma \Delta Q_{n+1, \alpha_{n+1}^*}) | \xi(\mathbf{x}), \mathcal{E}_n] \quad (32)$$

where Q_{n, α_n^*} denotes the Vorob'ev expectation conditioned on \mathcal{E}_n and Q_{n+1, α_{n+1}^*} the Vorob'ev expectation conditioned on \mathcal{E}_n and the addition of the point $(\mathbf{x}, \xi(\mathbf{x}))$ to the DoE. The idea behind (32) is to take as residual uncertainty, the variation with respect to the Vorob'ev expectation of the random closed set Γ , with $\Gamma := \{\mathbf{x} \in \mathbf{X}, \xi(\mathbf{x}) \leq T\}$. With the assumption that $\alpha_{n+1}^* = \alpha_n^*$ and by re-injecting the quantity $\mathcal{H}_{n+1}(\mathbf{x})$ of (32) in the \mathcal{J}_n criterion (16), it is possible to find a simplified formulation involving only an integral of a simple quantity Chevalier [2013]. This quantity is dependent on the cumulative distribution functions of the standard normal distribution and the bivariate centered normal distribution with given covariance matrix. Such a formulation then allows less time consuming computations and therefore is implemented in the package *KrigInv* (Chevalier et al. [2014]).

B Kriging update formulas

In the context of SUR strategies, the quantity $\mathcal{J}_n(\mathbf{x})$ in Equation (16) for a fixed \mathbf{x} is usually simplified thanks to formulas of kriging and conditionally on the point $(\mathbf{x}, \xi(\mathbf{x}))$ added to the DoE, and more particularly using the kriging standard deviation. Indeed, contrary to the trend, the kriging standard deviation does not depend on surrogate model observations. For instance the recurrent formula, used in Chevalier [2013] is efficient for calculating kriging model in the context of universal kriging and when the kriging parameters β and θ do not need to be re-estimated. These kriging update formulas are given for all \mathbf{y}, \mathbf{y}' in \mathbb{X}^2 by

$$m_{n+1}(\mathbf{y}) = m_n(\mathbf{y}) + k_n(\mathbf{y}, \mathbf{x}^{(n+1)}) k_n(\mathbf{x}^{(n+1)}, \mathbf{x}^{(n+1)})^{-1} \left(g(\mathbf{x}^{(n+1)}) - m_n(\mathbf{x}^{(n+1)}) \right), \quad (33)$$

$$\sigma_{n+1}^2(\mathbf{y}) = \sigma_n^2(\mathbf{y}) - k_n^2(\mathbf{y}, \mathbf{x}^{(n+1)}) \sigma_n^2(\mathbf{x}^{(n+1)})^{-1}, \quad (34)$$

$$k_{n+1}(\mathbf{y}, \mathbf{y}') = k_n(\mathbf{y}, \mathbf{y}') - k_n(\mathbf{y}, \mathbf{x}^{(n+1)}) k_n(\mathbf{x}^{(n+1)}, \mathbf{x}^{(n+1)})^{-1} k_n(\mathbf{y}', \mathbf{x}^{(n+1)}), \quad (35)$$

with $\mathbf{x}^{(n+1)}$ the $n + 1$ th observation point.

As for SUR strategies, it is possible to generalize these formulas in the case of simultaneous additions of q points (Chevalier [2013]). The advantage of these formulas is that the expressions of

m_n , σ_n , and k_n are reused to reduce computational time. It is particularly useful in SUR strategies where many evaluations of the kriging formulas may be required for the numerous evaluations of the sampling criterion (in the context of its minimization (16)). Finally, it can be shown that these kriging formulas still coincide with the Gaussian process conditional formulas in the context of universal kriging (see Appendix A of Chevalier [2013] for a proof).

C Proof of the explicit formula for SUR Bichon

The interest of this appendix is to propose a demonstration of Proposition 1, allowing to give an explicit expression of SUR Bichon. Let's start by stating and proving an intermediate lemma.

Lemma 2. *Let N be a standard Gaussian random variable and $(a, b) \in \mathbb{R}^2$ such that $a < b$, then:*

$$\mathbb{E}[N\mathbf{1}_{[a,b]}(N)] = -\varphi(b) + \varphi(a) \quad (36)$$

where φ is the probability density function of the standard normal distribution.

Proof.

$$\mathbb{E}[N\mathbf{1}_{[a,b]}(N)] = \frac{1}{\sqrt{2\pi}} \int_a^b te^{-\frac{t^2}{2}} dt = \frac{1}{\sqrt{2\pi}} \left[-e^{-\frac{t^2}{2}} \right]_a^b = -\varphi(b) + \varphi(a) \quad (37)$$

□

Proposition 1. *For all \mathbf{x}, \mathbf{z} belonging to \mathbb{X}^2 , we have:*

$$\begin{aligned} & \mathbb{E} \left[\left(\kappa\sigma_{n+1}(\mathbf{z}) - |T - \xi(\mathbf{z})| \right)^+ \middle| \mathcal{E}_n \right] \\ &= (m_n(\mathbf{z}) - T) \left[2\phi\left(\frac{T - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})}\right) - \phi\left(\frac{T^- - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})}\right) - \phi\left(\frac{T^+ - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})}\right) \right] \\ & \quad - \sigma_n(\mathbf{z}) \left[2\varphi\left(\frac{T - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})}\right) - \varphi\left(\frac{T^- - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})}\right) - \varphi\left(\frac{T^+ - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})}\right) \right] \\ & \quad + \varepsilon_{\mathbf{x}}(\mathbf{z}) \left[\phi\left(\frac{T^+ - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})}\right) - \phi\left(\frac{T^- - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})}\right) \right] \end{aligned} \quad (38)$$

where $\varepsilon_{\mathbf{x}}(\mathbf{y}) := \kappa\sigma_{n+1}(\mathbf{z})$, $T^\pm := T \pm \varepsilon_{\mathbf{x}}(\mathbf{z})$, φ and ϕ denote the probability density and cumulative distribution functions of the standard normal distribution, respectively.

Proof.

For the proof only and for the sake of lightening the notations, we note \mathbb{E}_n the conditional expectation $\mathbb{E}[\cdot | \mathcal{E}_n]$. In addition, the expression to be calculated is separated into three terms that are calculated separately. Specifically:

$$\begin{aligned} \mathbb{E}_n \left[\left(\kappa\sigma_{n+1}(\mathbf{z}) - |T - \xi(\mathbf{z})| \right)^+ \right] &= \mathbb{E}_n \left[\left(\varepsilon_{\mathbf{x}}(\mathbf{z}) - |T - \xi(\mathbf{z})| \right) \mathbf{1}_{[T^-, T^+]}(\xi(\mathbf{z})) \right] \\ &= \mathbb{E}_n \left[\varepsilon_{\mathbf{x}}(\mathbf{z}) \mathbf{1}_{[T^-, T^+]}(\xi(\mathbf{z})) \right] - \mathbb{E}_n \left[(T - m_n(\mathbf{z}) + m_n(\mathbf{z}) - \xi(\mathbf{z})) \mathbf{1}_{[T^-, T]}(\xi(\mathbf{z})) \right] \\ & \quad + \mathbb{E}_n \left[(T - m_n(\mathbf{z}) + m_n(\mathbf{z}) - \xi(\mathbf{z})) \mathbf{1}_{[T, T^+]}(\xi(\mathbf{z})) \right] \end{aligned}$$

$$\begin{aligned}
 &= \underbrace{\mathbb{E}_n \left[\varepsilon_{\mathbf{x}}(\mathbf{z}) \mathbf{1}_{[T^-, T^+]}(\xi(\mathbf{z})) \right]}_{\textcircled{1}} + \underbrace{(T - m_n(\mathbf{z})) \left[\mathbb{E}_n \left[\mathbf{1}_{[T, T^+]}(\xi(\mathbf{z})) \right] - \mathbb{E}_n \left[\mathbf{1}_{[T^-, T]}(\xi(\mathbf{z})) \right] \right]}_{\textcircled{2}} \\
 &\quad - \underbrace{\left[\mathbb{E}_n \left[(m_n(\mathbf{z}) - \xi(\mathbf{z})) \mathbf{1}_{[T^-, T]}(\xi(\mathbf{z})) \right] - \mathbb{E}_n \left[(m_n(\mathbf{z}) - \xi(\mathbf{z})) \mathbf{1}_{[T, T^+]}(\xi(\mathbf{z})) \right] \right]}_{\textcircled{3}} \quad (39)
 \end{aligned}$$

The calculation of the three terms separately is as follows:

$$\begin{aligned}
 \textcircled{1} &:= \mathbb{E}_n \left[\varepsilon_{\mathbf{x}}(\mathbf{z}) \mathbf{1}_{[T^-, T^+]}(\xi(\mathbf{z})) \right] \\
 &= \varepsilon_{\mathbf{x}}(\mathbf{z}) \mathbb{E}_n \left[\mathbf{1}_{\left[\frac{T^- - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})}, \frac{T^+ - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})} \right]} \left(\frac{\xi(\mathbf{z}) - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})} \right) \right] \\
 &= \varepsilon_{\mathbf{x}}(\mathbf{z}) \left[\phi \left(\frac{T^+ - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})} \right) - \phi \left(\frac{T^- - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})} \right) \right] \quad (40)
 \end{aligned}$$

$$\begin{aligned}
 \textcircled{2} &:= (T - m_n(\mathbf{z})) \left[\mathbb{E}_n \left[\mathbf{1}_{[T, T^+]}(\xi(\mathbf{z})) \right] - \mathbb{E}_n \left[\mathbf{1}_{[T^-, T]}(\xi(\mathbf{z})) \right] \right] \\
 &= (m_n(\mathbf{z}) - T) \left[\mathbb{E}_n \left[\mathbf{1}_{[T^-, T]}(\xi(\mathbf{z})) \right] - \mathbb{E}_n \left[\mathbf{1}_{[T, T^+]}(\xi(\mathbf{z})) \right] \right] \\
 &= (m_n(\mathbf{z}) - T) \left[2\phi \left(\frac{T - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})} \right) - \phi \left(\frac{T^- - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})} \right) - \phi \left(\frac{T^+ - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})} \right) \right] \quad (41)
 \end{aligned}$$

For the calculation of $\textcircled{3}$, the use of the lemma 2 is necessary, using the notations of it.

$$\begin{aligned}
 \textcircled{3} &:= - \left[\mathbb{E}_n \left[(m_n(\mathbf{z}) - \xi(\mathbf{z})) \mathbf{1}_{[T^-, T]}(\xi(\mathbf{z})) \right] - \mathbb{E}_n \left[(m_n(\mathbf{y}) - \xi(\mathbf{z})) \mathbf{1}_{[T, T^+]}(\xi(\mathbf{z})) \right] \right] \\
 &= \sigma_n(\mathbf{z}) \left[\mathbb{E}_n \left[\left(\frac{\xi(\mathbf{z}) - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})} \right) \mathbf{1}_{\left[\frac{T^- - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})}, \frac{T - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})} \right]} \left(\frac{\xi(\mathbf{z}) - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})} \right) \right] \right. \\
 &\quad \left. - \mathbb{E}_n \left[\left(\frac{\xi(\mathbf{z}) - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})} \right) \mathbf{1}_{\left[\frac{T - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})}, \frac{T^+ - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})} \right]} \left(\frac{\xi(\mathbf{z}) - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})} \right) \right] \right] \\
 &= \sigma_n(\mathbf{z}) \left[\mathbb{E} \left[N \mathbf{1}_{\left[\frac{T^- - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})}, \frac{T - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})} \right]}(N) \right] - \mathbb{E} \left[N \mathbf{1}_{\left[\frac{T - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})}, \frac{T^+ - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})} \right]}(N) \right] \right] \\
 &= -\sigma_n(\mathbf{z}) \left[2\varphi \left(\frac{T - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})} \right) - \varphi \left(\frac{T^- - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})} \right) - \varphi \left(\frac{T^+ - m_n(\mathbf{z})}{\sigma_n(\mathbf{z})} \right) \right] \quad (42)
 \end{aligned}$$

The expected result is then obtained by re-injecting the expressions of $\textcircled{1}$, $\textcircled{2}$, and $\textcircled{3}$ obtained in Equations (40) to (42) in Equation (39). \square

Remark 2.

• In this proof of the proposition 1, the fact that $m_n(\mathbf{z})$, $\sigma_n(\mathbf{z})$, $\varepsilon_{\mathbf{x}}(\mathbf{z})$ and T^\pm are constant with respect to $\xi(\mathbf{z})$ is implicitly used, in particular to output $m_n(\mathbf{z})$, $\sigma_n(\mathbf{z})$ and $\varepsilon_{\mathbf{x}}(\mathbf{z})$ of the conditional expectation \mathbb{E}_n , but also for the renormalization of $\xi(\mathbf{z})$ and the transition to the density probability and cumulative distribution functions of the standard normal distribution.

D Robustness of estimators with respect to the GP stationarity assumption.

A certain instability of the approximation error was observed at the beginning of the enrichment in Figures 4 and 6 in the case of estimator $\hat{\Gamma}_2$ corresponding to Vorob'ev expectation, in comparison to $\hat{\Gamma}_1$ naive estimator. This robustness of naive estimator $\hat{\Gamma}_1$ compared to $\hat{\Gamma}_2$ can be explained by the fact that naive estimator corresponds to the median of Vorob'ev (Appendix A, equation (28)). Indeed, even if the notions of expectation and median of Vorob'ev are not similar to the classical ones, the property of minimizing the first absolute central moment of the median is preserved when extending the notion of median to the framework of Vorob'ev random sets (Molchanov [2005] page 178). It is also possible to "read" the lack of robustness on Equation (29) of Appendix A which is recalled below:

$$Q_{\alpha^*} \stackrel{\text{a.s.}}{=} \{ \mathbf{x} \in \mathbb{X}, m_n(\mathbf{x}) \leq T - \phi^{-1}(\alpha^*) \sigma_n(\mathbf{x}) \}.$$

Knowing the strong dependence of the σ_n term on the stationarity condition of the process, it is straightforward that the term $\phi^{-1}(\alpha^*) \sigma_n(\mathbf{x})$ plays an important role in the non-robustness of $\hat{\Gamma}_2 = Q_{\alpha^*}$ estimator, compared to naive estimator $\hat{\Gamma}_1$ where this term $\phi^{-1}(\alpha^*) \sigma_n(\mathbf{x})$ does not appear.

To illustrate this robustness issue, we define the Loggruy function in dimension 2 as follows:

$$\forall \mathbf{x} \in \mathbb{R}^2, \text{Loggruy}(\mathbf{x}) = 10 \log_{10} \left(3.6 + 10^4 \left(\sum_{i=1}^2 (\mathbf{x}_i - \mathbf{a}_i)^2 - r^2 \right) \times \dots \times \left(\sum_{i=1}^2 (\mathbf{x}_i - \mathbf{e}_i)^2 - r^2 \right) \right) \quad (43)$$

with $(\mathbf{a}_i)_i = \begin{pmatrix} 0.153 \\ 0.939 \end{pmatrix}$; $(\mathbf{b}_i)_i = \begin{pmatrix} 0.854 \\ 0.814 \end{pmatrix}$; $(\mathbf{c}_i)_i = \begin{pmatrix} 0.510 \\ 0.621 \end{pmatrix}$; $(\mathbf{d}_i)_i = \begin{pmatrix} 0.207 \\ 0.386 \end{pmatrix}$; $(\mathbf{e}_i)_i = \begin{pmatrix} 0.815 \\ 0.146 \end{pmatrix}$
and $r := 0.07$.

The threshold chosen is $T = 10 \log_{10}(3.6)$ and the corresponding Γ^* excursion set (Equation (1)) is composed of 5 disconnected components. This function is particularly interesting in our context, since it has strong gradients at the edges of the domain and weaker gradients in the middle, where the different zones of the Γ^* excursion set are located (Figure 8c). This means that the stationarity assumption of the kriging meta-model cannot be verified.

Figure 8 represents in the case of an enrichment of 100 and 200 points of SUR Vorob'ev, from an initial DoE of size 10, the contour lines of the coverage probability p_n and the kriging mean m_n . Estimators $\hat{\Gamma}_1$ and $\hat{\Gamma}_2$ are also represented and compared to Γ^* . An irregularity is observed for the contour lines of p_n either after 100 or 200 iterations. But, m_n is relatively accurate even after 100 iterations. $\hat{\Gamma}_2$ estimator is then less efficient than $\hat{\Gamma}_1$ estimator.

In summary, $\hat{\Gamma}_2$ estimator related to Vorob'ev theory is more dependent on the stationarity hypothesis than $\hat{\Gamma}_1$ naive estimator, and this is essentially explained by the construction of Vorob'ev expectation which is more sensitive to the kriging standard deviation (Equation (29)). Consequently, the approximation error $\text{Err}(\hat{\Gamma}_2(\chi_{j,n}))$ is more dependent on the stationarity hypothesis than the naive approximation error $\text{Err}(\hat{\Gamma}_1(\chi_{j,n}))$.

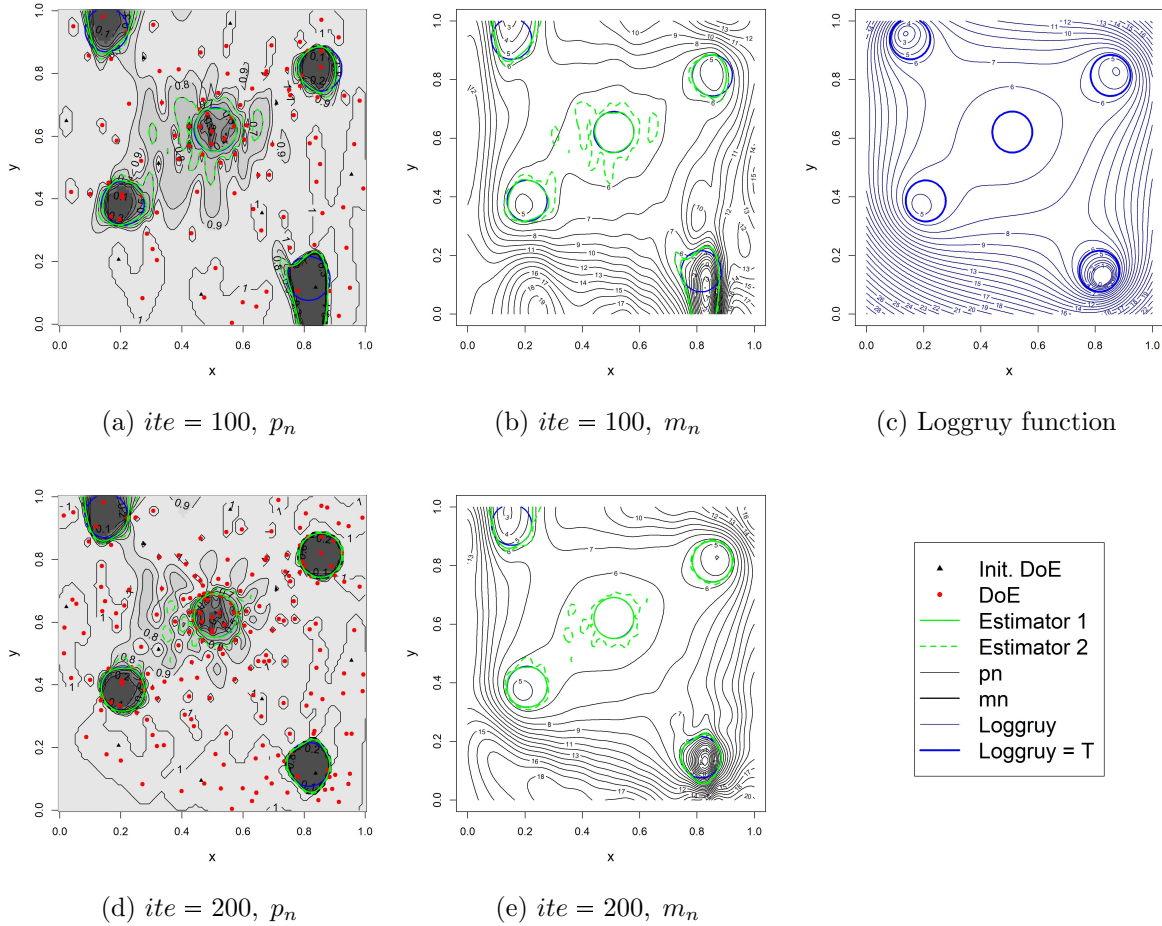


Figure 8: At left and center, representation of the two $\hat{\Gamma}_1$ and $\hat{\Gamma}_2$ estimators after 100 iterations (first line) and 200 iterations (second line) for SUR Vorob'ev, and with the contour lines of p_n (first column) and m_n (second column), in comparison with the true excursion set (top right), for Loggruy function inversion ($d = 2$) with $T = 10 \log_{10}(3.6)$, for a particular initial DoE of size 10.