Bayesian sequential design of computer experiments to estimate reliable sets

Romain Ait Abdelmalek-Lomenech, Julien Bect, Vincent Chabridon, Emmanuel Vazquez

▶ **To cite this version:**

Romain Ait Abdelmalek-Lomenech, Julien Bect, Vincent Chabridon, Emmanuel Vazquez. Bayesian sequential design of computer experiments to estimate reliable sets. 2022. hal-03835704v1

HAL Id: hal-03835704

https://centralesupelec.hal.science/hal-03835704v1

Preprint submitted on 1 Nov 2022 (v1), last revised 7 Nov 2023 (v3)

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Distributed under a Creative Commons Attribution - NonCommercial - NoDerivatives 4.0 International License

Bayesian sequential design of computer experiments to estimate reliable sets

Romain Ait Abdelmalek-Lomenech*[1], Julien Bect[1], Vincent Chabridon[2], and Emmanuel Vazquez[1]

[1]Université Paris-Saclay, CNRS, CentraleSupélec, Laboratoire des Signaux et Systèmes, 91190 Gif-sur-Yvette, France
[2]EDF R&D, 6 Quai Watier, 78401 Chatou, France

November 1, 2022

Abstract

We consider an unknown multivariate function representing a system—such as a complex numerical simulator—taking both deterministic and uncertain inputs. Our objective is to estimate the set of deterministic inputs leading to outputs whose probability (with respect to the distribution of the uncertain inputs) to belong to a given set is controlled by a given threshold. To solve this problem, we propose a Bayesian strategy based on the Stepwise Uncertainty Reduction (SUR) principle to sequentially choose the points at which the function should be evaluated to approximate the set of interest. We illustrate its performance and interest in several numerical experiments.

Keywords: Gaussian processes, Active learning, Design of computer experiments, Stepwise Uncertainty Reduction, Set inversion, Uncertainty quantification.

*The authors gratefully acknowledge the National French Research Agency (ANR) for funding this work in the context of the project SAMOURAI (ANR-20-CE46-0013).

1 Introduction

When dealing with a numerical model of a physical phenomenon or a system, one is often interested in estimating the set of input parameters leading to outputs being in a given range. Such *set inversion* problems (Jaulin and Walter, 1993) arise in a large variety of frameworks. In particular, *robust* versions of this problem in which some inputs are considered uncertain have appeared recently in the literature, with applications to nuclear safety (Chevalier, 2013; Marrel et al., 2022), flood defense optimization (Richet and Bacchi, 2019) and pollution control systems (El Amri et al., 2021), for instance.

Following Richet and Bacchi (2019), we focus on a robust formulation of the set inversion problem that we call *reliable set inversion* (RSI). We consider a system modeled by an unknown continuous function $f : \mathbb{X} \times \mathbb{S} \mapsto \mathbb{R}^q$, where $\mathbb{X}$ and $\mathbb{S}$ are bounded subsets of $\mathbb{R}^{d_x}$ and $\mathbb{R}^{d_s}$ respectively, representing deterministic and uncertain input variables. We model uncertain input variables by a random variable S with known distribution $\mathbb{P}_S$ on $\mathbb{S}$. Then, given a critical region $C \subset \mathbb{R}^q$ and a threshold $\alpha \in (0, 1)$, our objective is to estimate the set

$$\Gamma(f) = \{x \in \mathbb{X} : \mathbb{P}(f(x, S) \in C) \leq \alpha\}, \tag{1}$$

which we call *reliable set*, and which corresponds to the points in $\mathbb{X}$ where the probability that $f(x, S)$ falls in the critical region C is controlled by α. Using the language of machine learning, we can also formulate this problem as that of learning a classifier $\mathbb{X} \mapsto \{0, 1\}$ as close as possible to the indicator function $\mathbb{1}_{\Gamma(f)}$.

At each iteration n, the function f can be evaluated at a unique point (x_n, s_n). The result of an evaluation is a possibly noisy observation

$$Z_n^{\text{obs}} = f(x_n, s_n) + \epsilon_n, \tag{2}$$

the deterministic case ($\epsilon_n = 0$) corresponding to the case of deterministic simulators.

When the numerical model f is computationally expensive, it is important to estimate $\Gamma(f)$ using a small number of evaluations of f only. With this constraint in mind, we propose in this article a sequential Bayesian strategy based on the Stepwise Uncertainty Reduction (SUR) principle (Vazquez and Piera-Martinez, 2006; Villemonteix et al., 2009; Vazquez and Bect, 2009; Bect et al., 2012, 2019). Given a quantity of interest derived from f, the starting point of a SUR-based strategy is to view f as a sample path of a random process, generally a Gaussian process (GP). Then, evaluation points are chosen sequentially to minimize at each step a measure of uncertainty about the quantity of interest given past and future evaluation results.

The structure of the article is as follows: in the next two sections, we present our framework and a brief overview of the literature on Bayesian set inversion strategies, with

a particular emphasis on SUR-based approaches. The core contribution of this article is Section 4, which is about the construction of SUR sampling criteria for the RSI problem. Section 5 demonstrates the performance of our approach on numerical examples.

Acknowledgement. *The authors have become aware, at the occasion of the SIAM Conference on Uncertainty Quantification (UQ22) in Atlanta, of related research work conducted by Charlie Sire (IRSN, France) and co-authors (Sire, 2022). The research presented in this article has been carried out independently of theirs.*

2 Framework

In the following, we consider a function $f : \mathbb{D} \mapsto \mathbb{R}$, where $\mathbb{D} = \mathbb{X}$ or $\mathbb{D} = \mathbb{X} \times \mathbb{S}$, depending on whether there are stochastic input variables, and where $\mathbb{X}$ and $\mathbb{S}$ are defined as above. For the RSI problem, we adopt a Bayesian approach to sequentially choose the evaluation points $D_1, D_2, \ldots \in \mathbb{D}$ of f and estimate $\Gamma(f)$ from evaluation results. We assume that we observe, at each selected point D_n, a response $Z_n^{\text{obs}} = f(D_n) + \epsilon_n$, where the ϵ_n's are independent zero-mean Gaussian random variables—possibly with variance zero, which corresponds to the case of a deterministic simulator. We consider a GP prior denoted by $\xi \sim \text{GP}(\mu, k)$ about the unknown function f, where μ and k are mean and covariance functions (see, e.g., Santner et al., 2003; Rasmussen and Williams, 2006).

Denote by $\mathbb{P}_n$ the conditional probability given $\mathcal{I}_n = \{(D_1, Z_1^{\text{obs}}), \ldots, (D_n, Z_n^{\text{obs}})\}$. Bayesian strategies use at each iteration n a *sampling criterion* (also called acquisition function) J_n or G_n based on the distribution of ξ under $\mathbb{P}_n$, to choose the evaluation points sequentially as:

$$D_{n+1} \in \operatorname*{argmin}_{d \in \mathbb{D}} J_n(d) \quad \text{or} \quad D_{n+1} \in \operatorname*{argmax}_{d \in \mathbb{D}} G_n(d)\,.$$

We review in the following sections two families of such criteria.

Notations. $\mathbb{E}_n = \mathbb{E}\left(\cdot \mid \mathcal{I}_n\right)$ will denote the conditional expectation associated with $\mathbb{P}_n$, $\mu_n(x)$ and $\sigma_n(x)$ the conditional (posterior) mean and standard deviation of $\xi(x)$, and $p_n(x) = \mathbb{P}_n(\xi(x) \in C)$ the conditional (posterior) probability that $\xi(x)$ belongs to C.

3 Overview of Bayesian strategies for set inversion

3.1 Maximal uncertainty sampling

We review in this section a first family of sampling criteria, which corresponds to the general idea of "maximal uncertainty sampling", i.e., sampling at the location $x \in \mathbb{X}$ where the uncertainty about $\mathbb{1}_C(\xi(x))$ and/or $\xi(x)$ is maximal. The literature on such criteria only deals, to the best of our knowledge, with the deterministic case $\mathbb{D} = \mathbb{X}$, when f is a real-valued function ($q = 1$), and when $C = [T; +\infty)$, for a given $T \in \mathbb{R}$. In this setting, the set inversion problem reduces to the estimation of the set $\gamma(f) = \{x \in \mathbb{X} : f(x) \leq T\}$.

A natural approach to this problem is to select the point at which the probability of misclassification is maximal (Bryan et al., 2005): this leads to the sampling criterion $G_n(x) = \min(p_n(x), 1 - p_n(x))$. Maximizing this criterion leads to selecting a point X_{n+1} such that $p_n(X_{n+1})$ is as close as possible—and if possible equal—to $1/2$. Several equivalent criteria lead to the same choice of sampling point, including the variance or the entropy (Bryan et al., 2005) of the classification indicator $\mathbb{1}_C(\xi(x))$, or the "learning function U" of Echard et al. (2011).

Some sampling criteria operate a trade-off between the posterior variance of ξ and its proximity to the threshold T. This is the case, for instance, for the family of criteria defined by $G_n(x) = \mathbb{E}_n\left[\max\left(0, (\kappa\sigma_n(x))^\delta - |\xi(x) - T|^\delta\right)\right]$, with $\kappa > 0$ and $\delta \in \{1, 2\}$. Those sampling criteria, inspired by the *expected improvement* criterion for optimization (Mockus et al., 1978; Jones et al., 1998), were introduced separately by Bichon et al. (2008) ($\delta = 1$) and Ranjan et al. (2008) ($\delta = 2$). Similarly, Bryan et al. (2005) proposed the *straddle heuristic*, in which the sampling criterion is $G_n(x) = \kappa\sigma_n(x) - |\mu_n(x) - T|$, with $\kappa = \Phi^{-1}(0.975) \approx 1.96$, where Φ^{-1} stands for the quantile function of the normal distribution.

3.2 Stepwise uncertainty reduction

SUR strategies (see, e.g., Bect et al., 2019, and reference therein) are a special case of the Bayesian approach in which the evaluation points are sequentially chosen by minimizing the *expected future uncertainty* about the quantity of interest. More precisely, a SUR strategy starts by defining a measure of uncertainty $\mathcal{H}_n$ at each step n, that depends on information $\mathcal{I}_n$. Then, a sampling criterion J_n is built by considering the expectation of $\mathcal{H}_{n+1}$ conditional on $\mathcal{I}_n$ and the action of choosing a new evaluation point at d (notice that $\mathcal{H}_{n+1}$ depends on the unknown outcome of the evaluation at d):

$$J_n : d \mapsto \mathbb{E}_n\left[\mathcal{H}_{n+1} \mid D_{n+1} = d\right] . \tag{3}$$

Note that instead of minimizing the criterion J_n, one can also maximize the information gain $G_n : d \mapsto \mathcal{H}_n - J_n(d)$. SUR-based strategies have been shown to be particularly effective on various estimation problems.

We now give more details and first focus on the case of deterministic inversion. Several approaches have been developed in the past years.

For instance, Vazquez and Piera-Martinez (2006); Vazquez and Bect (2009) propose to estimate the volume of an excursion set using the uncertainty measure

$$\mathcal{H}_n = \Big(\int_{\mathbb{X}} \sqrt{\min(p_n(x), 1 - p_n(x))}\, \mathrm{d}x \Big)^2, \tag{4}$$

where $\min(p_n(x), 1-p_n(x))$ is the probability of misclassification using the classifier $\mathbb{E}_n[\mathbb{1}_{\gamma(\xi)}(x)]$. Bect et al. (2012) suggest other uncertainty measures, such as, for instance,

$$\mathcal{H}_n = \int_{\mathbb{X}} \min(p_n(x), 1 - p_n(x))\, \mathrm{d}x, \tag{5}$$

and

$$\mathcal{H}_n = \int_{\mathbb{X}} p_n(x)(1 - p_n(x))\, \mathrm{d}x, \tag{6}$$

which corresponds to the integrated posterior variance of the indicator function $\mathbb{1}_{\gamma(\xi)}(x)$. (Note that the problem of estimating the volume of an excursion set is directly linked to that of set inversion.) Picheny et al. (2010) propose a *targeted Integrated Mean Square Error* (tIMSE) based on the uncertainty metric

$$\mathcal{H}_n = \int_{\mathbb{X}} \sigma_n^2(x)\, \mathbb{P}_n \left(|\xi(x) - T| \leq \beta \right)\, \mathrm{d}x\,, \tag{7}$$

for some $\beta > 0$. For the sake of brevity, we refer the reader to Chevalier et al. (2013), Chevalier (2013), Marques et al. (2018), Azzimonti et al. (2021), and Duhamel et al. (2022) for other examples of uncertainty metrics and corresponding SUR criteria applicable to the deterministic set inversion problem.

We now turn to the case of reliable set inversion. Chevalier (2013) considers the task of estimating the set $\{x \in \mathbb{X} : \max_{s \in \mathbb{S}} f(x, s) \leq T\}$. In this setting, the proposed uncertainty measure is

$$\mathcal{H}_n = \int_{\mathbb{X}} p_n^{\vee}(x)(1 - p_n^{\vee}(x))\mathrm{d}x, \tag{8}$$

where $p_n^{\vee}(x) = \mathbb{P}_n(\max_{s \in \mathbb{S}} \xi(x, s) \leq T)$. In the work of El Amri et al. (2021), the objective instead is to estimate the set $\{x \in \mathbb{X} : \mathbb{E}(f(x, S)) \leq T\}$. To this end, the authors propose a hybrid SUR strategy to choose, sequentially, the deterministic component x and stochastic component s of each new evaluation point.

Remark 1 *SUR methods have been applied to other problems beyond the scope of set inversion, notably for optimization (see, e.g., Villemonteix et al., 2009).*

4 Construction of SUR strategies for RSI

4.1 Sampling criteria

Our objective is to estimate the reliable set $\Gamma(f)$ defined by (1) using evaluation results modeled by (2). Consider the random process

$$\tau(x) \;=\; \int_{\mathbb{S}} \mathbb{1}_C\left(\xi(x,s)\right) \mathrm{d}\mathbb{P}_S(s) \;=\; \mathbb{P}_S\big(\{s \in \mathbb{S} \,:\, \xi(x,s) \in C\}\big), \tag{9}$$

which corresponds to the volume with respect to $\mathbb{P}_S$ of the excursion of the process $\xi(x,\,\cdot\,)$ in C. Using τ, notice that $\Gamma(\xi)$ can be written as

$$\Gamma(\xi) = \{x \in \mathbb{X} \,:\, \tau(x) \leq \alpha\}\,. \tag{10}$$

In the following, we propose two sampling criteria for the RSI problem.

First approach. Given a sequence of estimators $\widehat{\Gamma}_n$ of $\Gamma(\xi)$, we propose to use as uncertainty measure the volume of the difference between $\Gamma(\xi)$ and its estimators:

$$\mathcal{H}_n^{(m)} = \lambda(\Gamma(\xi)\,\Delta\,\widehat{\Gamma}_n)\,, \quad n \geq 1. \tag{11}$$

where λ is the Lebesgue measure on $\mathbb{R}^{d_x}$.

The SUR strategy derived from (11) consists in minimizing at each step the criterion

$$J_n^{(m)}(x,s) = \mathbb{E}_n\left[\lambda(\Gamma(\xi)\Delta\widehat{\Gamma}_{n+1}) \mid (X_{n+1}, S_{n+1}) = (x,s)\right]\,. \tag{12}$$

Approaches using the symmetric difference have been used in different contexts (see, e.g., Chevalier, 2013; Azzimonti et al., 2021).

It is straightforward to see that $\mathcal{H}_n^{(m)}$ correspond to the integrated probability of misclassification associated to the classifier $\mathbb{1}_{\widehat{\Gamma}_n}$. When considering the Bayes-optimal estimator

$$\widehat{\Gamma}_n = \{x \in \mathbb{X} \,:\, \pi_n(x) > \frac{1}{2}\}, \tag{13}$$

where $\pi_n(x) = \mathbb{P}_n(\tau(x) \leq \alpha)$, the uncertainty metric $\mathcal{H}_n^{(m)}$ can be expressed as follows.

Proposition 1 *For $\widehat{\Gamma}_n = \{x \in \mathbb{X} \,:\, \pi_n(x) > \frac{1}{2}\}$, we have*

$$\mathcal{H}_n^{(m)} = \int_{\mathbb{X}} \min(\pi_n(x),\, 1 - \pi_n(x))\,\mathrm{d}x\,. \tag{14}$$

Second approach. A second possibility is to focus instead on the IMSE of the soft classifiers π_n and to define the uncertainty measure

$$\mathcal{H}_n^{(v)} = \mathbb{E}_n\Big[\int_X \big(\mathbb{1}_{\Gamma(\xi)}(x) - \pi_n(x)\big)^2 \,\mathrm{d}x\Big]\,. \tag{15}$$

Proposition 2 *We have*

$$\mathcal{H}_n^{(v)} = \int_{\mathbb{X}} \mathrm{Var}_n\left(\mathbb{1}_{\Gamma(\xi)}(x)\right)\mathrm{d}x = \int_{\mathbb{X}} \pi_n(x)(1-\pi_n(x))\,\mathrm{d}x\,. \tag{16}$$

The SUR strategy derived from (15) consists in minimizing at each step the criterion

$$J_n^{(v)}(x,s) = \mathbb{E}_n\left[\mathcal{H}_{n+1}^{(v)} \mid (X_{n+1},S_{n+1}) = (x,s)\right]\,. \tag{17}$$

Remark 2 *It is instructive to compare the sampling criteria $J_n^{(m)}$ and $J_n^{(v)}$ to those proposed by Bect et al. (2012), and to notice the formal resemblance, if replacing p_n by π_n and $\gamma(\xi)$ by $\Gamma(\xi)$.*

4.2 Approximation of the criteria

In this section, we discuss the numerical approximation of

$$J_n^{(m)}(x^\star,\, s^\star) = \int_{\mathbb{X}} \mathbb{E}_n\left[\min(\pi_{n+1}(x), 1-\pi_{n+1}(x)) \mid (X_{n+1},S_{n+1}) = (x^\star,\, s^\star)\right]\mathrm{d}x$$

at a given point $(x^\star, s^\star) \in \mathbb{X}\times\mathbb{S}$. (The same methodology can be applied to $J_n^{(v)}$.)

Two difficulties arise for the numerical evaluation of $J_n^{(m)}$ (and $J_n^{(v)}$). First, the integrand

$$\mathbb{E}_n\left[\min(\pi_{n+1}(x), 1-\pi_{n+1}(x)) \mid (X_{n+1},S_{n+1}) = (x^\star,s^\star)\right] \tag{18}$$

does not admit—to the best of the authors knowledge—an analytic expression as in Chevalier et al. (2014) because τ is not a Gaussian process.

In order to propose a practical algorithm, we propose to estimate (18) using quantization of the distribution $\mathbb{P}_S$ together with Monte Carlo simulations of the process ξ, in the spirit of Villemonteix et al. (2009) and Bect et al. (2012).

Let us consider $\tilde{\mathbb{S}}$ a finite subset of $\mathbb{S}$, and $(w(s))_{s\in\tilde{\mathbb{S}}}$ a family of real numbers such that $\mathbb{P}_{\tilde{S}} = \sum_{s\in\tilde{\mathbb{S}}} w(s)\delta_s$ is a "good" approximation of $\mathbb{P}_S$, where δ_s denotes the Dirac measure at s. This can be achieved, naively, by defining $\tilde{\mathbb{S}}$ as a collection of i.i.d samples from $\mathbb{P}_S$ and fixing $w \propto 1$. In the case of a distribution $\mathbb{P}_S$ with a density g with respect to the Lebesgue measure, another solution is to use a sufficiently large space-filling design $\tilde{\mathbb{S}}$ of $\mathbb{S}$ and set $w(s) \propto g(s)$. The reader can refer to Graf and Luschgy (2000) for more information about quantization.

Let $\{Z_1, \ldots, Z_N\}$ be a collection of independent samples drawn from the distribution of $\xi(x^\star, s^\star)$ given $\mathcal{I}_n$. It is well known that we can easily simulate M sample paths $\{\xi_{i,1}, \ldots, \xi_{i,M}\}$ of $\xi(x, \cdot)$ over $\tilde{\mathbb{S}}$, under $\mathbb{P}_n(\cdot \mid \xi(x^\star, s^\star) = Z_i)$, using the conditioning formula for Gaussian processes. Given a point $x \in \mathbb{X}$, set

$$\tilde{\pi}^i_{n+1}(x) = \frac{1}{M} \sum_{m=1}^{M} \left(\sum_{s \in \tilde{\mathbb{S}}} w(s)\, \mathbb{1}_C(\xi_{i,m}(x,s)) \right). \tag{19}$$

Then it is easy to show, using the law of large numbers, that

$$\tilde{\pi}^i_{n+1}(x) \xrightarrow[M\to\infty]{\text{a.s.}} \mathbb{P}\left(\xi(x, \tilde{S}) \in C \mid \mathcal{I}_n\,,\, \xi(x^\star, s^\star) = Z_i\right), \tag{20}$$

with $\tilde{S} \sim \mathbb{P}_{\tilde{S}}$. As a consequence, for a sufficiently large M, it is possible to use

$$j^x_n(x^\star, s^\star) = \frac{1}{N} \sum_{i=1}^{N} \min(\tilde{\pi}^i_{n+1}(x), 1 - \tilde{\pi}^i_{n+1}(x)) \tag{21}$$

as an approximation of (18).

The second issue is the approximation of the integral over $\mathbb{X}$ arising in $J^{(m)}_n(x^\star, s^\star)$. As simple solution (to be improved in future work) is to estimate the integral using a finite subset $\tilde{\mathbb{X}}$ of $\mathbb{X}$ (for instance, a Latin Hypercube design or the first terms of a Sobol sequence). The criterion $J^{(m)}_n(x^\star, s^\star)$ is then approximated, up to a multiplicative constant, by

$$\tilde{J}^{(m)}_n(x^\star, s^\star) \;=\; \sum_{x \in \tilde{\mathbb{X}}} j^x_n(x^\star, s^\star). \tag{22}$$

Algorithm 1 summarizes the numerical procedure.

Algorithm 1 Procedure to choose a new point of evaluation according to $J^{(m)}_n$

For each candidate point $(x^\star, s^\star)$:

1. Generate N samples $\{Z_1, ..., Z_N\}$ of $\xi(x^\star, s^\star)$ with respect to $\mathbb{P}_n$
2. For $i = 1, ..., N$
   2.1 Generate M samples paths of ξ on $\tilde{\mathbb{X}} \times \tilde{\mathbb{S}}$ according to $\mathbb{P}_n(\cdot \mid \xi(x^\star, s^\star) = Z_i)$
   2.2 Compute $\tilde{\pi}^i_{n+1}(x)$ using (19), for all $x \in \tilde{\mathbb{X}}$
3. Calculate the approximation $\tilde{J}^{(m)}_n(x^\star, s^\star)$ of the criterion according to (22)

Remark 3 *For better numerical efficiency, the simulations of the sample paths of ξ under $\mathbb{P}_n(\cdot \mid \xi(x^\star, s^\star) = Z_i)$ is preferably carried out using successive reconditioning of sample paths. A description of this procedure is given by Villemonteix et al. (2009), Section 5.1.*

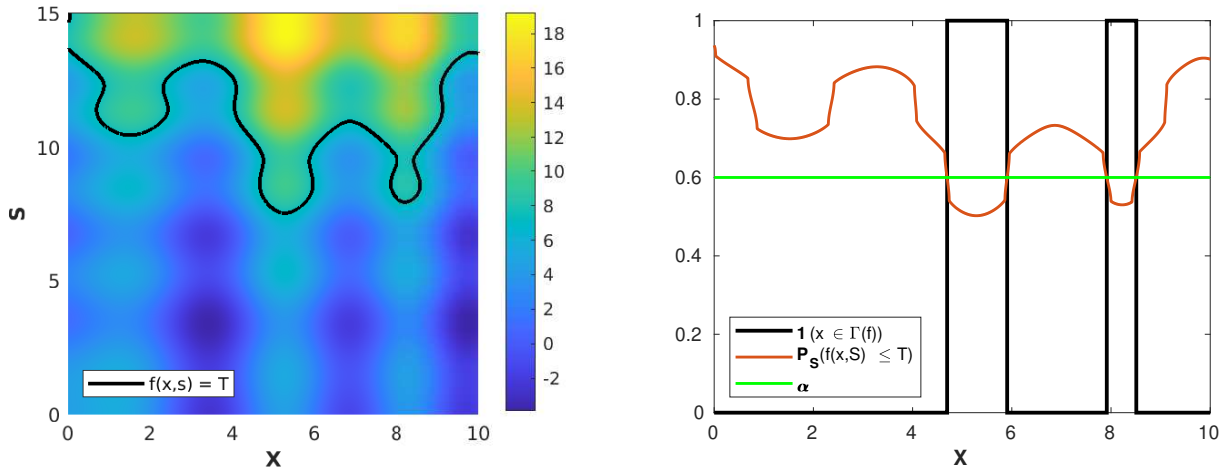

Figure 1: Representation of f_1 (left) and the associated reliable set (right).

5 Numerical applications

5.1 Test functions and benchmark methods

To evaluate the performances of the sampling criteria in Section 4, we focus on two artificial examples, with scalar output values ($q = 1$) and noise-free observations.

The first test function (see Figure 1) is a modified Branin-Hoo function f_1 defined on $\mathbb{X} = [0; 10]$ and $\mathbb{S} = [0; 15]$ by

$$f_1(x, s) = \frac{1}{12} b(x, s) + 3 \sin\left(x^{\frac{5}{4}}\right) + 3 \sin\left(s^{\frac{5}{4}}\right), \tag{23}$$

where b is the Branin function $b(x, s) = \left(s - \frac{5.1x^2}{4\pi^2} + \frac{5x}{\pi} - 6\right)^2 + 10\left(1 - \frac{1}{8\pi}\right)\cos(x) + 10$. We take $C = (-\infty; T]$ with $T = 7.5$, $\alpha = 0.6$ and $\mathbb{P}_S$ the uniform distribution on $\mathbb{S}$.

The second test function is defined on $\mathbb{X} = [-2; 2]^2$ and $S = [-1; 1]^2$ by

$$f_2\left((x_1, x_2), (s_1, s_2)\right) = c(x_1, s_1) + c(x_2, s_2), \tag{24}$$

with c the two-hump Camel function $c(x, s) = \left(4 - 2.1x^2 + \frac{x^4}{3}\right) x^2 + xs + (4s^2 - 4)s^2$. We take $C = (-\infty; T]$ with $T = 2.15$, $\alpha = 0.65$ and $\mathbb{P}_S$ the uniform distribution on $\mathbb{S}$. The corresponding reliable set $\Gamma(f_2)$ is shown in Figure 2.

We compare the results obtained with our sampling criteria $J_n^{(m)}$ and $J_n^{(v)}$ to several other Bayesian methods. Due to the absence in the literature of strategies dealing with the precise problem exposed in this work, we focus on methods aiming at approximating the set $\gamma(f) = \{(x, s) \in \mathbb{X} \times \mathbb{S} : f(x, s) \in C\}$. It is clear indeed that perfect knowledge of $\gamma(f)$ implies perfect knowledge of $\Gamma(f)$.

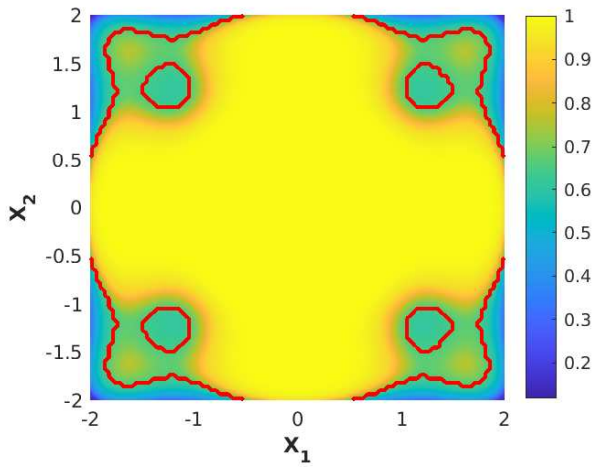

Figure 2: Representation of the probability of excursion and $\Gamma(f_2)$.

More precisely, we compare our results to those obtained with the misclassification and straddle criteria (see Section 3.1) and with the SUR-based criteria $J_n^{(m),\,\mathrm{joint}}$ and $J_n^{(v),\,\mathrm{joint}}$, corresponding respectively to the uncertainty metrics (5) and (6) for the random set $\gamma(\xi)$. As a baseline method, we also include the results obtained with random sampling of the evaluation points.

5.2 Implementation details

For every strategy and test function considered, we use a GP prior with an unknown constant mean and an anisotropic Matérn covariance function. At each iteration of the algorithm, the parameters of the Gaussian prior are estimated using the restricted maximum likelihood (ReML) method (see, e.g., Stein, 1999).

The new sampling criteria are numerically approximated as described in Section 4.2. At each iteration, $\tilde{\mathbb{X}}$ and $\tilde{\mathbb{S}}$ are (pseudo-)maximin random Latin hypercubes (LHC), obtained by selecting the best maximin design among a collection of 1000 random LHC. For f_1, we take $\mathrm{card}(\tilde{\mathbb{X}}) = \mathrm{card}(\tilde{\mathbb{S}}) = 30$ and for f_2, we take $\mathrm{card}(\tilde{\mathbb{X}}) = \mathrm{card}(\tilde{\mathbb{S}}) = 40$. Also, for each candidate point $(x^\star, s^\star)$, we use 50 sample values Z_i of $\xi(x^\star, s^\star)$ given $\mathcal{I}_n$, and 500 sample paths over $\tilde{\mathbb{X}} \times \tilde{\mathbb{S}}$ of ξ under $\mathbb{P}_n(\,\cdot \mid \xi(x^\star, s^\star) = Z_i)$.

For all methods (except random sampling), the sampling criterion is optimized using an exhaustive search over the finite subset $\tilde{\mathbb{D}} = \tilde{\mathbb{X}} \times \tilde{\mathbb{S}}$. The SUR criteria $J_n^{(m),\,\mathrm{joint}}$ and $J_n^{(v),\,\mathrm{joint}}$ are discretized over $\tilde{\mathbb{D}}$ as well.

All the experiments are carried using out Matlab and the *STK* toolbox (Bect et al., 2022).

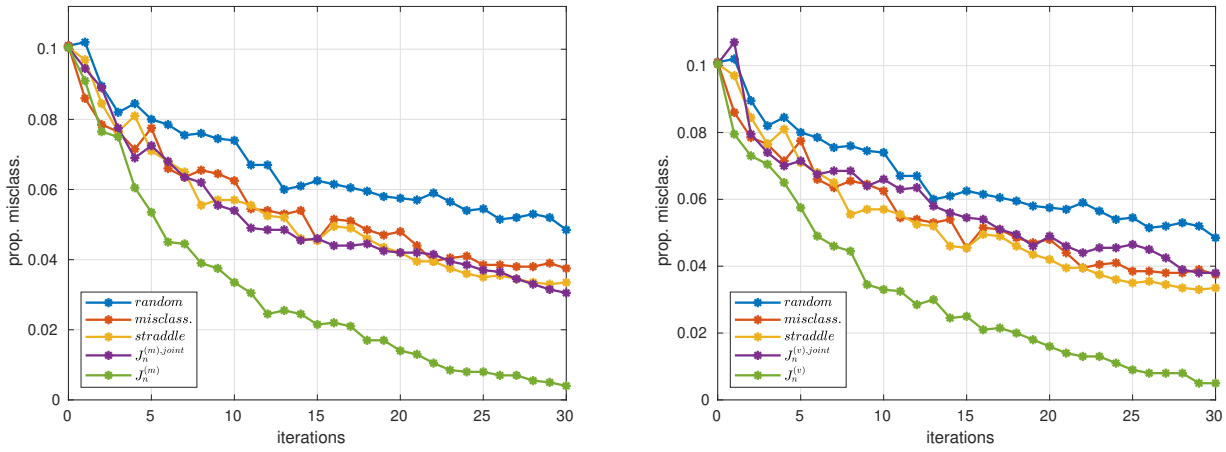

Figure 3: Median of the proportion of misclassified points vs. number of iterations, for 50 repetitions of the algorithms on the test function f_1.

5.3 Results

The different algorithms are repeated 50 times on the test function f_1 and 25 times on f_2, using different random LHC as initial designs. Following the rule of thumb consisting of taking an initial design of size ten times the dimension of the problem (Loeppky et al., 2009), we use respectively initial designs of size 20 and 40 for f_1 and f_2.

We compare the proportions of wrongly classified points obtained on a prediction grid composed of the product of two Sobol sequences, each composed of 1000 points respectively from $\mathbb{X}$ and $\mathbb{S}$. Considering that the Bayes-optimal estimator (13) is too expensive to compute (using heavy Gaussian sample paths simulations on the prediction grid), we use instead the estimator

$$\widehat{\Gamma}_n = \{x \in \mathbb{X} \,:\, \mathbb{E}_n(\tau(x)) \leq \alpha\}. \tag{25}$$

From the results in Figure 3 and Figure 4, observe that the new sampling criteria perform better on the RSI problem than the state-of-the-art methods focusing on the excursion set $\gamma(f)$ in the joint space of deterministic and uncertain inputs. These differences in performance can be explained, from a heuristic viewpoint, by the fact that in the joint space, the new criteria tend to concentrate the evaluations around specific zones of $\gamma(f)$ which are particularly relevant for the approximation of $\Gamma(f)$. This phenomenon, linked to the geometry of the excursion set $\gamma(f)$, can be visualized on Figure 5.

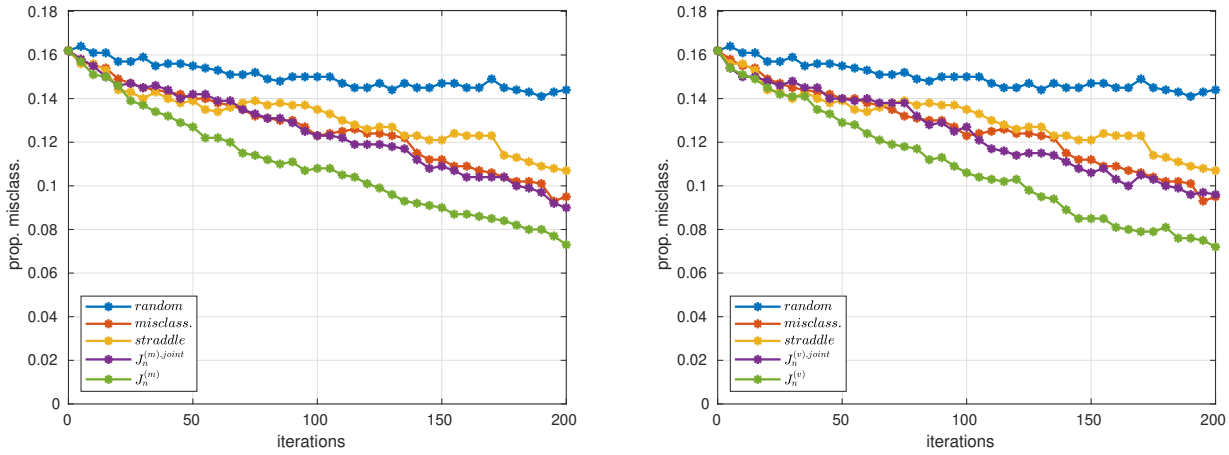

Figure 4: Median of the proportion of misclassified points vs. number of iterations, for 25 repetitions of the algorithms on the test function f_2.

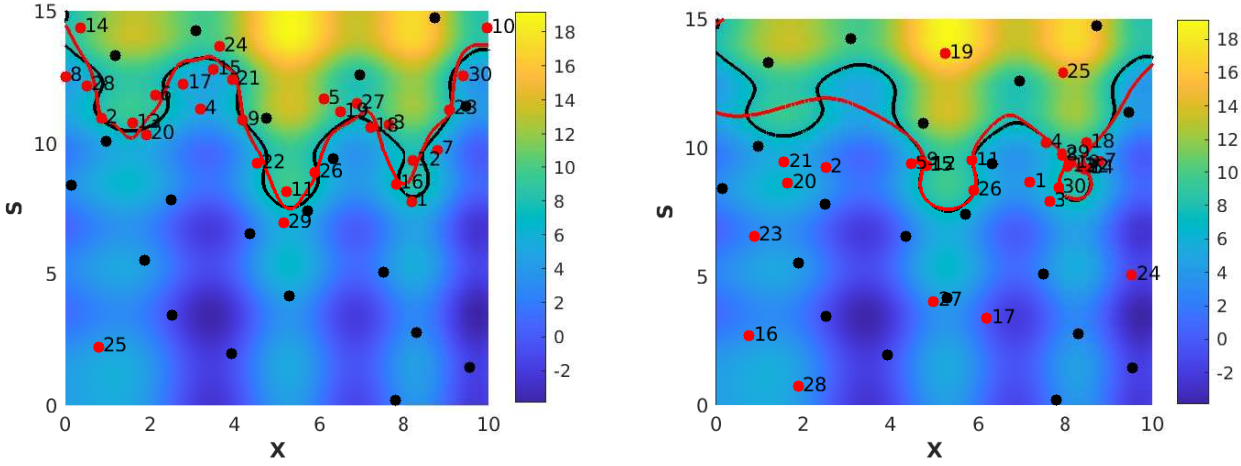

Figure 5: Examples of sequential design obtained after $n = 30$ iterations on the function f_1, with the criteria $J_n^{(m),\,\text{joint}}$ (left) and $J_n^{(m)}$ (right) and an initial design of 20 points (black dots). Black curve represents the boundary of $\gamma(f)$, red curve the boundary of $\gamma(\mu_n)$.

6 Conclusion

This article presents SUR-based strategies for the reliable set inversion problem. The practical interest of the proposed method is illustrated on two artificial test problems, on which methods that do not take advantage of the specificity of the RSI problem are outperformed. However, this gain in performance comes at the cost of a high numerical complexity, in relation with the heavy use of conditioned Gaussian processes simulations. Future work will concentrate on making the method applicable to harder test problems (higher input dimensions, smaller probabilities, etc.) and on demonstrating its practical relevance to real-life examples.

References

Azzimonti, D., D. Ginsbourger, C. Chevalier, J. Bect, and Y. Richet (2021). Adaptive design of experiments for conservative estimation of excursion sets. *Technometrics 63*(1), 13–26.

Bect, J., F. Bachoc, and D. Ginsbourger (2019). A supermartingale approach to Gaussian process based sequential design of experiments. *Bernoulli 25*(4A), 2883–2919.

Bect, J., D. Ginsbourger, L. Li, V. Picheny, and E. Vazquez (2012). Sequential design of computer experiments for the estimation of a probability of failure. *Statistics and Computing 22*, 773–793.

Bect, J., E. Vazquez, et al. (2022). STK: a Small (Matlab/Octave) Toolbox for Kriging. Release 2.7.0.

Bichon, B. J., M. S. Eldred, L. P. Swiler, S. Mahadevan, and J. M. McFarland (2008). Efficient global reliability analysis for nonlinear implicit performance functions. *AIAA Journal 46*(10), 2459–2468.

Bryan, B., R. C. Nichol, C. R. Genovese, J. Schneider, C. J. Miller, and L. Wasserman (2005). Active learning for identifying function threshold boundaries. In Y. Weiss, B. Schölkopf, and J. Platt (Eds.), *Advances in Neural Information Processing Systems*, Volume 18. MIT Press.

Chevalier, C. (2013). *Fast uncertainty reduction strategies relying on Gaussian process models*. Ph. D. thesis, University of Bern.

Chevalier, C., J. Bect, D. Ginsbourger, E. Vazquez, V. Picheny, and Y. Richet (2014). Fast parallel kriging-based stepwise uncertainty reduction with application to the identification of an excursion set. *Technometrics 56*(4), 455–465.

Chevalier, C., D. Ginsbourger, J. Bect, and I. Molchanov (2013). Estimating and quantifying uncertainties on level sets using the Vorob'ev expectation and deviation with Gaussian process models. In D. Uciński, A. C. Atkinson, and M. Patan (Eds.), *mODa 10 – Advances in Model-Oriented Design and Analysis*, pp. 35–43. Springer.

Duhamel, C., C. Helbert, M. Munoz Zuniga, C. Prieur, and D. Sinoquet (2022). A SUR version of the Bichon criterion for excursion set estimation. HAL preprint hal-03780559v1.

Echard, B., N. Gayton, and M. Lemaire (2011). Ak-mcs: An active learning reliability method combining kriging and monte carlo simulation. *Structural Safety 33*(2), 145–154.

El Amri, R., C. Helbert, M. Munoz Zuniga, C. Prieur, and D. Sinoquet (2021). Set inversion under functional uncertainties with Gaussian Process Regression defined in the joint space of control and uncertain. HAL preprint hal-02986558v2.

Graf, S. and H. Luschgy (2000). *Foundations of Quantization for Probability Distributions*. Lecture Notes in Mathematics. Springer.

Jaulin, L. and E. Walter (1993). Set inversion via interval analysis for nonlinear bounded-error estimation. *Automatica 29*(4), 1053–1064.

Jones, D. R., M. Schonlau, and W. J. Welch (1998). Efficient global optimization of expensive black-box functions. *Journal of Global Optimization 13*, 455–492.

Loeppky, J. L., J. Sacks, and W. J. Welch (2009). Choosing the sample size of a computer experiment: A practical guide. *Technometrics 51*(4), 366–376.

Marques, A., R. Lam, and K. Willcox (2018). Contour location via entropy reduction leveraging multiple information sources. In *Advances in Neural Information Processing Systems 31 (NeurIPS 2018)*, pp. 1–11.

Marrel, A., B. Iooss, and V. Chabridon (2022). The icscream methodology: Identification of penalizing configurations in computer experiments using screening and metamodel—applications in thermal hydraulics. *Nuclear Science and Engineering 196*(3), 301–321.

Mockus, J. B., V. Tiesis, and A. Žilinskas (1978). *The application of Bayesian methods for seeking the extremum*, Volume 2, pp. 117–129.

Picheny, V., D. Ginsbourger, O. Roustant, R. T. Haftka, and N.-H. Kim (2010). Adaptive designs of experiments for accurate approximation of a target region. *Journal of Mechanical Design 132*(7).

Ranjan, P., D. Bingham, and G. Michailidis (2008). Sequential experiment design for contour estimation from complex computer codes. *Technometrics 50*(4), 527–541.

Rasmussen, C. E. and C. K. I. Williams (2006). *Gaussian processes for machine learning*. Adaptive computation and machine learning. MIT Press.

Richet, Y. and V. Bacchi (2019). Inversion algorithm for civil flood defense optimization: Application to two-dimensional numerical model of the Garonne river in france. *Frontiers in Environmental Science 7*(160), 1–16.

Santner, T. J., B. J. Williams, and W. I. Notz (2003). *The Design and Analysis of Computer Experiments*. Springer Series in Statistics. Springer.

Sire, C. (2022). Robust inversion under uncertainty for flooding risk analysis. Talk given at SIAM Conference on Uncertainty Quantification (UQ22), MS10, April 12, Atlanta.

Stein, M. L. (1999). *Interpolation of spatial data: some theory for kriging*. Springer.

Vazquez, E. and J. Bect (2009). A sequential Bayesian algorithm to estimate a probability of failure. Volume 42, pp. 546–550.

Vazquez, E. and M. Piera-Martinez (2006). Estimation of the volume of an excursion set of a gaussian process using intrinsic kriging. *arXiv preprint math/0611273*.

Villemonteix, J., E. Vazquez, and E. Walter (2009). An informational approach to the global optimization of expensive-to-evaluate functions. *Journal of Global Optimization 44*, 509–534.