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SEQUENTIAL BAYESIAN INVERSION OF BLACK-BOX FUNCTIONS IN PRESENCE OF UNCERTAINTIES

Context & motivations

In engineering, many system design problems come down to finding design parameters for the system to operate under desired conditions. When time-consuming numerical simulations are used to assess the conditions of operation of such systems, it is essential to treat this problem—broadly known as "**inversion**"—using search methods that are very sparing in the number of simulations.

With this constraint in mind, we propose here a **sequential strategy** for a particular robust inversion problem that we call "**reliability-based inversion**" (**RBI**), in which the system has both **deterministic and uncertain inputs**. In this formulation, the objective is to retrieve the set of deterministic inputs such that the probability of the outputs exceeding a given level is greater than a threshold.

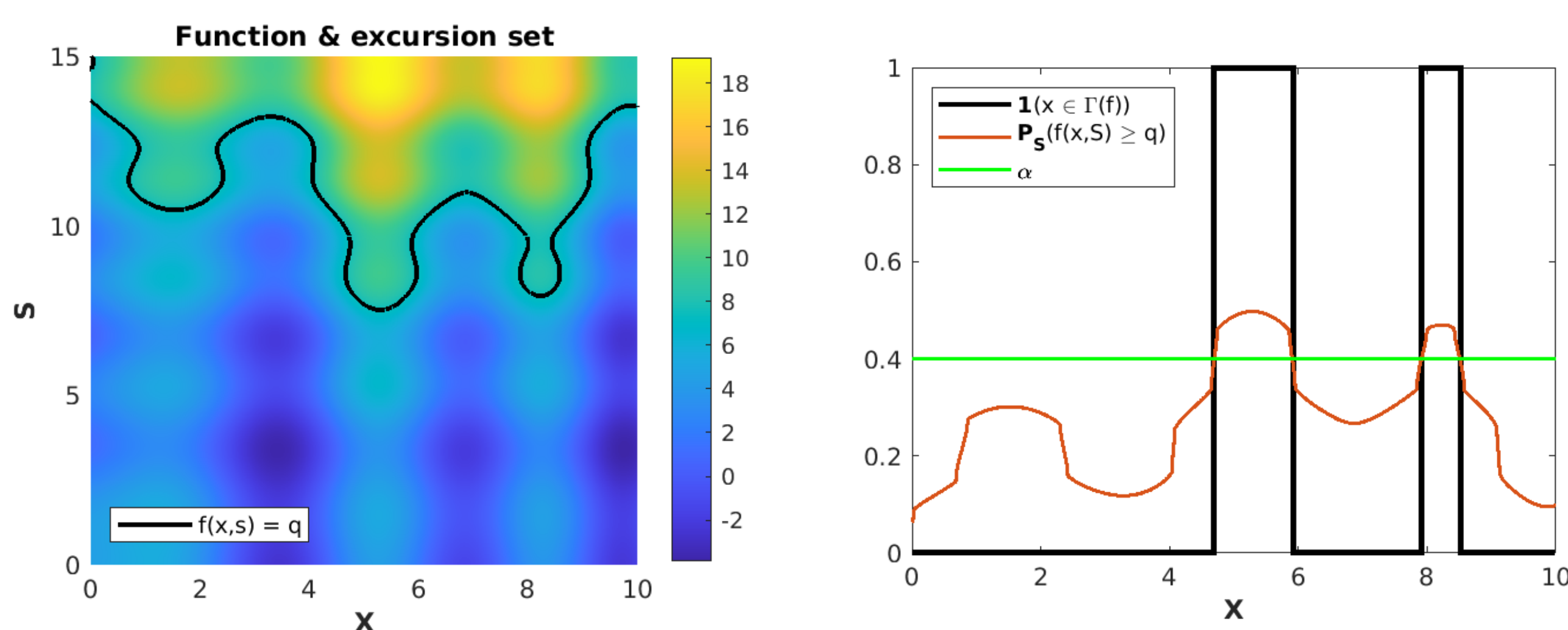
The reliability-based inversion (RBI) problem

We view our system as a **black-box function** $f : \mathbb{X} \times \mathbb{S} \mapsto \mathbb{R}$. In this setting, \mathbb{X} is the space of deterministic inputs and \mathbb{S} the space of **uncertain** inputs.

- Given a level $q \in \mathbb{R}$ and a threshold $\alpha \in]0, 1[$, **our objective is to approximate the set**

$$\Gamma(f) = \{x \in \mathbb{X} : \mathbb{P}(f(x, S) \geq q) \geq \alpha\}$$

where S is a random variable with **known distribution** \mathbb{P}_S on \mathbb{S} .



- Equivalently, we can formulate this problem as a **classification problem**, in which we wish to **approximate the classifier**

$$c(x) = \begin{cases} 1 & \text{if } x \in \Gamma(f) \\ 0 & \text{otherwise} \end{cases}$$

The Stepwise Uncertainty Reduction (SUR) principle

SUR strategies are a subset of the Bayesian strategies in which the points of evaluation are sequentially chosen by minimizing the expected future uncertainty on the object of interest, using a probabilistic surrogate of the unknown function.

- Consider $\xi \sim GP(\mu, k)$ a **Gaussian Process prior** on f , with μ and k respectively the mean and covariance functions of the process.
- We define the **current information** \mathcal{I}_n :

$$\mathcal{I}_n = \{(X_1, S_1, \xi(X_1, S_1)), \dots, (X_n, S_n, \xi(X_n, S_n))\}$$

- A SUR strategy choose the point **minimizing the expected future uncertainty**:

$$(X_{n+1}, S_{n+1}) \in \arg \min_{(x,s) \in \mathbb{X} \times \mathbb{S}} \mathbb{E}_n(U_{n+1} | X_{n+1} = x, S_{n+1} = s)$$

where:

- U_{n+1} is an uncertainty metric on the object of interest, depending on \mathcal{I}_{n+1}
- \mathbb{E}_n expectation with respect to \mathbb{P}_n , the distribution of ξ given \mathcal{I}_n

SUR approaches have been successfully used for the resolution of several problems regarding expensive-to-evaluate black box, including optimization [VW09; MTZ78], function fitting, and more standard inversion problems. [Bec+12]

Construction of a SUR criterion for the RBI problem

- Let us define the **integrated process** τ and $\Gamma(\xi)$ the associated **random excursion set** above the threshold α :

$$\tau(\xi, x) = \int_{\mathbb{S}} \mathbb{1}(\xi(x, s) \geq q) \mathbb{P}_S(ds) \quad \text{and} \quad \Gamma(\xi) = \{x \in \mathbb{X}, \tau(\xi, x) \geq \alpha\}$$

- We consider the uncertainty metric U_n defined by

$$U_n = \int_{\mathbb{X}} \tilde{p}_n(x)(1 - \tilde{p}_n(x)) dx$$

with $\tilde{p}_n(x) = \mathbb{P}_n(\tau(\xi, x) \geq \alpha)$

The link between the metric and the **uncertainty of the random set** $\Gamma(\xi)$ can be seen more clearly by remarking that:

$$U_n = \int_{\mathbb{X}} \mathbb{V}_n(\mathbb{1}(x \in \Gamma(\xi))) dx$$

with \mathbb{V}_n the conditional variance given \mathcal{I}_n

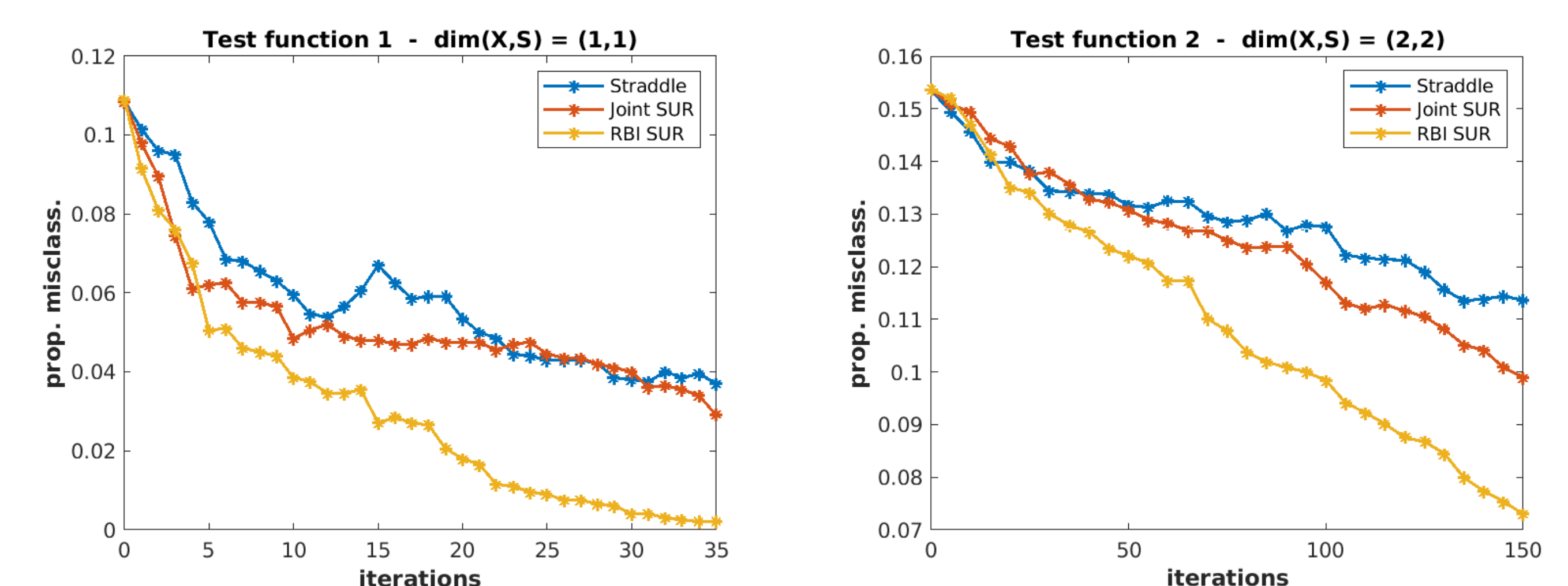
- The conditional distributions of $\tau(\xi, x)$ are **intractable**: the SUR criterion does not admit an analytic expression.
- Monte Carlo simulations**: ξ being Gaussian, we can generate ξ_1, \dots, ξ_M sample paths of ξ under \mathbb{P}_n

$$\frac{1}{M} \sum_{m=1}^M \mathbb{1}(\tau(\xi_m, x) \geq \alpha) \xrightarrow[M \rightarrow +\infty]{a.s.} \mathbb{P}_n(\tau(\xi, x) \geq \alpha) = \tilde{p}_n(x)$$

For each candidate point (x, s) , the sample paths are **reconditioned** according to values sampled from the distribution of $\xi(x, s)$ given \mathcal{I}_n

Numerical results

We compare, iteration by iteration, the proportion of misclassified points obtained with our method to the ones of methods focusing on the excursion set in the joint space $\mathbb{X} \times \mathbb{S}$ of design and uncertainties: the **straddle criterion** [Bry+05] and a **SUR approach** to standard inversion problems. [Bec+12]



Empirical evidences show that our method **generally outperforms** state of the art joint space inversion methods. Moreover, in all the test cases, the new SUR strategy never lags behind the others approaches considered.

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