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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.

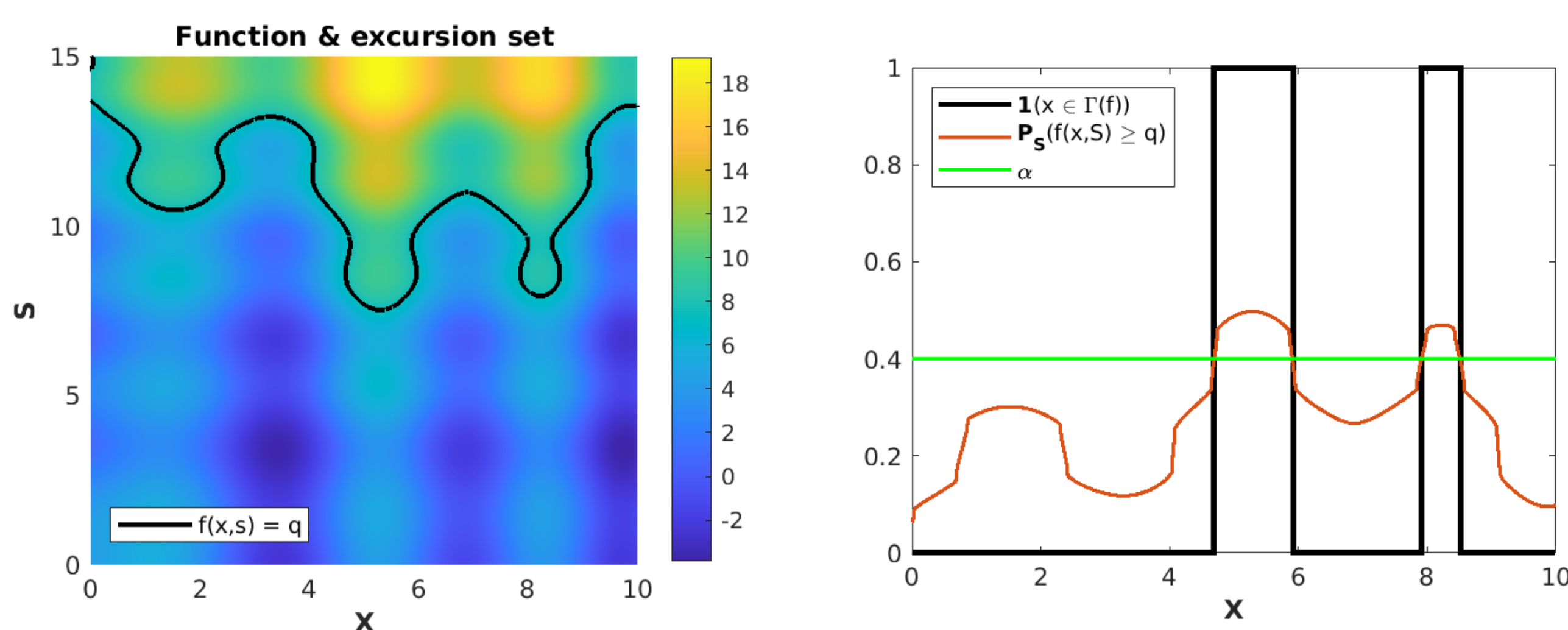
## The reliability-based inversion (RBI) problem

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  $\mu$  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  $\xi$  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**  $\tau$  and  $\Gamma(\xi)$  the associated **random excursion set** above the threshold  $\alpha$ :

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

- 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  $\mathcal{I}_n$

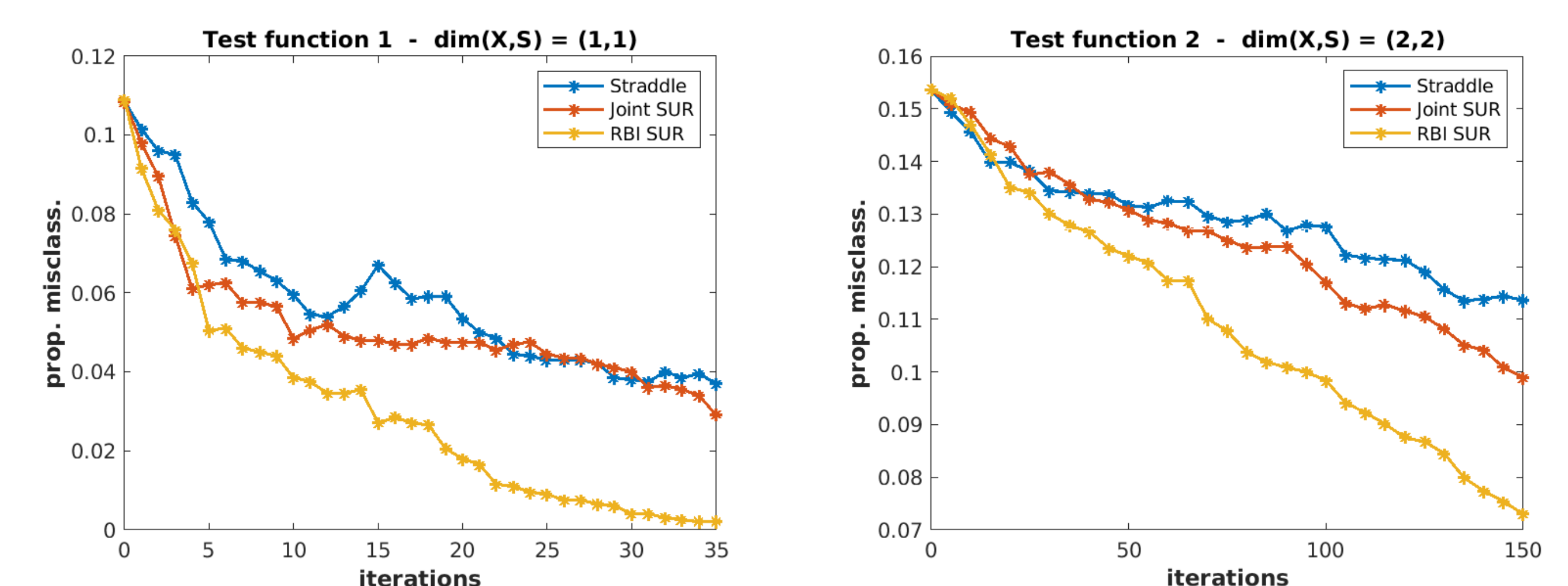
- The conditional distributions of  $\tau(\xi, x)$  are **intractable**: the SUR criterion does not admit an analytic expression.
- Monte Carlo simulations**:  $\xi$  being Gaussian, we can generate  $\xi_1, \dots, \xi_M$  sample paths of  $\xi$  under  $\mathbb{P}_n$

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

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.

## References

- [Bec+12] J. Bect et al. "Sequential design of computer experiments for the estimation of a probability of failure". In: *Statistics and Computing* 22.3 (2012), pp. 773–793.
- [Bry+05] B. Bryan et al. "Active Learning for Identifying Function Threshold Boundaries". In: *Proceedings of the 18th International Conference on Neural Information Processing Systems*. NIPS'05. 2005.
- [MTZ78] J. Mockus, V. Tiesis, and A. Zilinskas. "The Application of Bayesian Methods for Seeking the Extremum". In: *Towards Global Optimization* 2.117–129 (1978), p. 2.
- [VW09] J. Villemonteix, E. Vazquez, and E. Walter. "An Informational Approach to the Global Optimization of Expensive-to-Evaluate Functions". In: *J. of Global Optimization* 44.4 (Aug. 2009), pp. 509–534.