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# ESTIMATION OF (SMALL) RELIABLE SETS USING A SEQUENTIAL BAYESIAN STRATEGY

## 1. Context & motivations

In engineering, many system design problems involve finding parameters for a system to operate under desired conditions. When time-consuming simulations are used to assess the operating conditions of such systems, it is essential to use search methods that minimize the number of simulations.

Here, we propose a **SUR sequential strategy** [Bec+12] for a problem we refer to as **“reliable set inversion” (RSI)** [Ait+22], in which the system has both **deterministic and uncertain inputs**. In this problem, the objective is to estimate the set of deterministic inputs such that the probability of the outputs exceeding a given level is lower than a threshold.

We specifically focus on the case where the set to retrieve is relatively **small** compared to the space of deterministic inputs.

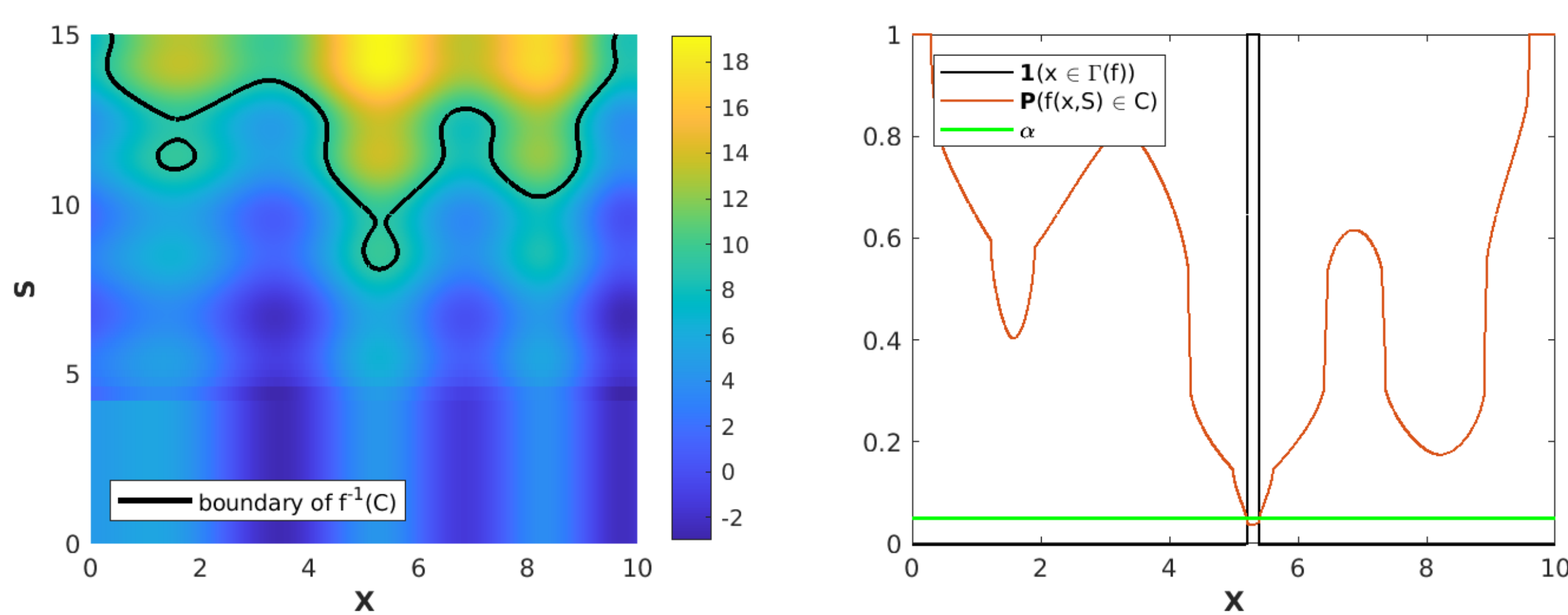
## 2. The reliable set inversion (RSI) problem

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

- Given a critical region  $C \subset \mathbb{R}^q$  and a threshold  $\alpha \in ]0, 1[$ , **our objective is to estimate the “reliable” set**

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

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



## 3. A SUR criterion for the RSI problem

- Assuming  $\xi \sim \text{GP}(\mu, k)$  is a **Gaussian Process prior** on  $f$ , with  $\mu$  and  $k$  respectively the mean and covariance functions of the process, define the **integrated process**  $\tau$  and the associated **random excursion set**  $\Gamma(\xi)$  as:

$$\tau(\xi, x) = \int_{\mathbb{S}} \mathbb{1}(\xi(x, s) \in C) d\mathbb{P}_S(s) \quad \text{and} \quad \Gamma(\xi) = \{x \in \mathbb{X}, \tau(\xi, x) \leq \alpha\}.$$

- Define an uncertainty measure  $\mathcal{H}_n$ :

$$\mathcal{H}_n = \int_{\mathbb{X}} \min(\pi_n(x), 1 - \pi_n(x)) dx,$$

with  $\pi_n(x) = \mathbb{P}_n(\tau(\xi, x) \leq \alpha)$ , where  $\mathbb{P}_n$  is the distribution of  $\xi$  given the current information

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

- The proposed SUR strategy chooses the point **minimizing the expected future uncertainty**:

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

where  $\mathbb{E}_n$  is the conditional expectation with respect to  $\mathcal{I}_n$ .

## 4. An approximated sampling criterion

- Given a discrete approximation grid  $\tilde{\mathbb{X}} \times \tilde{\mathbb{S}}$  and a subset  $\Theta \subset \tilde{\mathbb{X}} \times \tilde{\mathbb{S}}$ , define the discretized approximated process [Azz+16]

$$\tilde{\xi}(x, s) = \begin{cases} \xi(x, s) & \text{if } (x, s) \in \Theta \\ \mathbb{E}_n[\xi(x, s) | \xi(\Theta)] & \text{otherwise.} \end{cases}$$

- Monte Carlo simulations:** Given a candidate point  $(\check{x}, \check{s}) \in \Theta$  and a quantization  $(w_i, z_i)_{i=1, \dots, I}$  of the distribution of  $\xi(\check{x}, \check{s})$  given  $\mathcal{I}_n$ , we can generate sample paths  $\tilde{\xi}_1^i, \dots, \tilde{\xi}_M^i$  of  $\tilde{\xi}$  on  $\tilde{\mathbb{X}} \times \tilde{\mathbb{S}}$  conditional to  $\mathcal{I}_n$  and  $\{\xi(\check{x}, \check{s}) = z_i\}$ .

Then we can write an approximated criterion  $\tilde{J}_n$  on  $\Theta$

$$\tilde{J}_n(\check{x}, \check{s}) = \sum_{i=1}^I \frac{w_i}{M} \sum_{m=1}^M \sum_{x \in \tilde{\mathbb{X}}} \mathbb{1}(\tau(\tilde{\xi}_m^i, x) \leq \alpha) \approx J_n(\check{x}, \check{s})$$

## 5. An SMC-based optimization algorithm

Considering the small volume of  $\Gamma(f)$  relatively to  $\mathbb{X}$ , the idea is to build a sequence of sets of decreasing volume

$$\Gamma_1(f) \supset \Gamma_2(f) \supset \dots \supset \Gamma_T(f) = \Gamma(f)$$

such that  $\Gamma_{t+1}(f)$  is “easy” to estimate knowing  $\Gamma_t(f)$ .

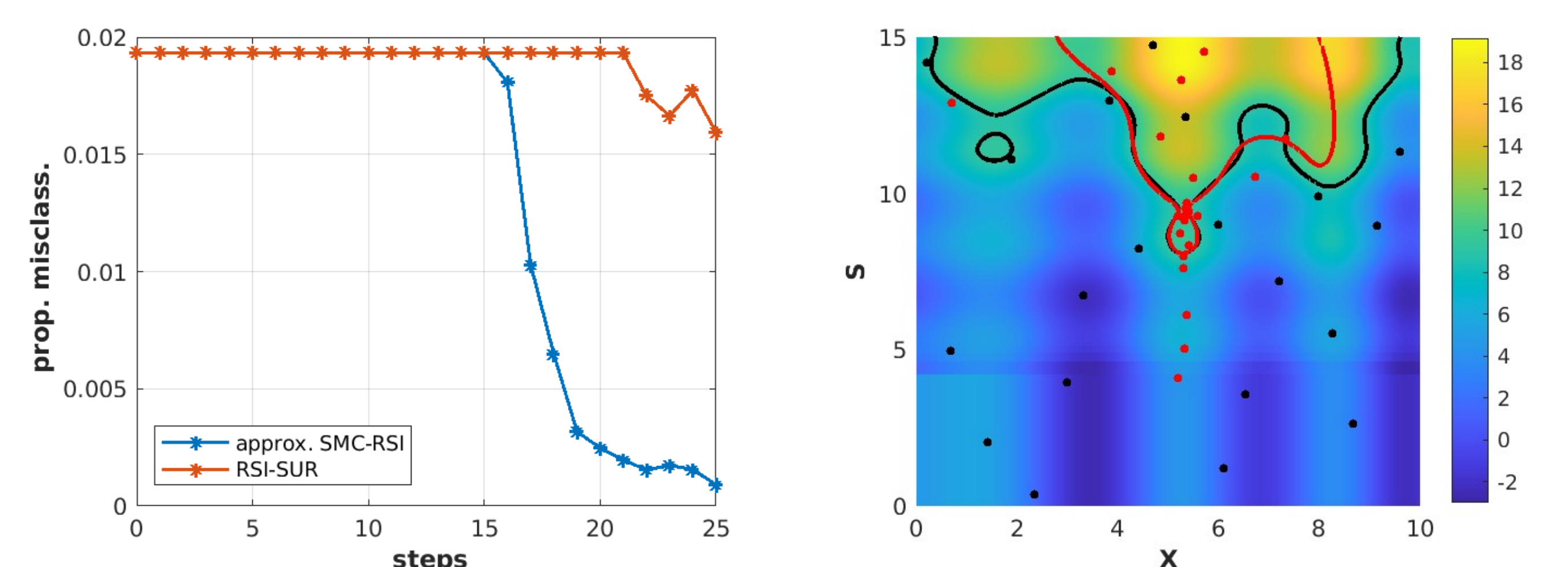
**At each step  $n$ :**

- Build a set  $\tilde{\mathbb{S}}_n \subset \mathbb{S}$  whose points are i.i.d. according to  $\mathbb{P}_S$ .
- Generate a set of particles  $\tilde{\mathbb{X}}_n \subset \mathbb{X}$  using sequential Monte Carlo with target distribution  $\pi_n^t(x) = \mathbb{P}_n(x \in \Gamma_t(\xi))$ 
  - Approximate  $q_n(x) \propto \frac{\pi_n^t(x)}{\pi_{n-1}^t(x)}$  for all  $x \in \tilde{\mathbb{X}}_n$ .
  - Sample  $n_X$  particles according to  $\sum_{x \in \tilde{\mathbb{X}}_n} q_n(x) \delta_{\{x\}}$  (residual resampling).
  - Move the particles according to a random walk Metropolis-Hastings algorithm.
- Draw a subset  $\Theta \subset \tilde{\mathbb{X}}_n \times \tilde{\mathbb{S}}_n$  according to the distribution proportional to  $\min(p_n(x, s), 1 - p_n(x, s))$ , with  $p_n(x, s) = \mathbb{P}_n(\xi(x, s) \in C)$ .
- Minimize  $\tilde{J}_n$  on  $\Theta$ .
- If  $\min_{(x, s) \in \Theta} \tilde{J}_n(x, s)$  is less than a threshold, set

$$\Gamma_{t+1}(f) = \left\{ x \in \mathbb{X} : \mathbb{P}(f(x, S) \in C) \leq q_\beta \left( \mathbb{P}_n(\xi(x, S) \in C), x \in \tilde{\mathbb{X}}_n \right) \right\}.$$

## 6. Numerical results

We compare, on an artificial example, the median of the proportion of misclassified points obtained with our improved method to the one obtained with the previous RSI-SUR sampling criterion.



## References

- [Ait+22] R. Ait Abdelmalek-Lomenech et al. *Bayesian sequential design of computer experiments to estimate reliable sets*. 2022. arXiv: 2211.01008 [stat.ML].  
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[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.