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

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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.

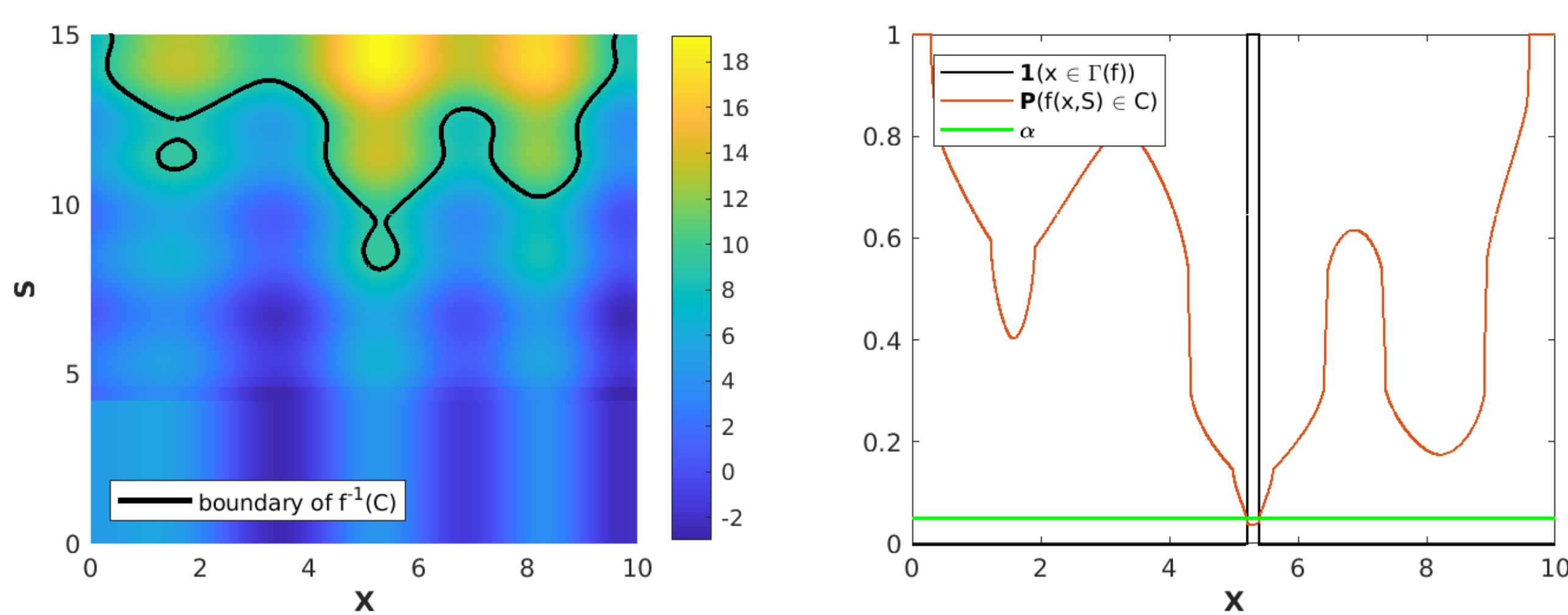
2. The reliable set inversion (RSI) problem

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 μ and k respectively the mean and covariance functions of the process, define the **integrated process** τ 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 ξ 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 ξ_1^i, \dots, ξ_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 Θ

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

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 $\Gamma_t(f)$.

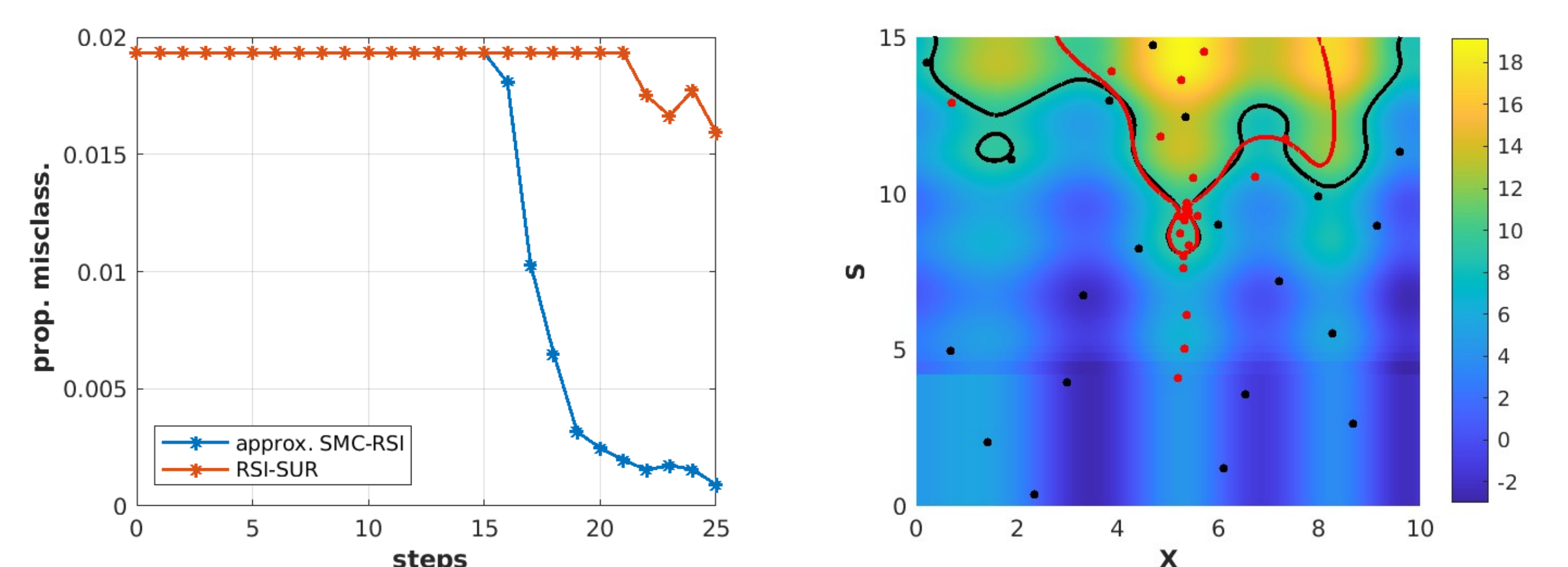
At each step n :

- 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 Θ .
- 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

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