Estimation of (small) reliable sets using a sequential Bayesian strategy
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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 the space of deterministic inputs and uncertain inputs.

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 $f : \mathbb{R}^n \times \mathbb{R}^m \rightarrow \mathbb{R}$. In this setting, $X$ is the space of deterministic inputs and $S$ is the space of uncertain inputs.

- Given a critical region $C \subseteq \mathbb{R}^n$ and a threshold $\alpha \in [0, 1]$, our objective is to estimate the "reliable" set

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

where $S$ is a random variable with known distribution $P_S$ on $S$.

3. A SUR criterion for the RSI problem

- Assuming $\xi \sim GP(\mu, k)$ 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 $\Gamma(\tau)$ as:

$$\tau(x, s) = \int_C \mathbb{1}(\xi(x, s) \in C) dP_S(s)$$

and $\Gamma(\tau) = \{x \in X, \tau(x, s) \leq \alpha\}$.

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

$$\mathcal{H}_{\alpha} = \int_X \min_{\pi} \tau(x, s) \leq \alpha$$

with $\pi(x) = P_S(\xi(x, s) \leq \alpha)$, where $P_S$ is the distribution of $\xi$ given the current information

$$\mathcal{I}_{\alpha} = \{X_1, S_1, \xi(X_1, S_1), \ldots, X_n, S_n, \xi(X_n, S_n)\}.$$

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

$$\{X_{n+1}, S_{n+1}\} = \arg\min_{x, s} \mathbb{E}_{\mathcal{I}_{n+1}} \mathcal{H}_{\alpha+1} | X_{n+1} = x, S_{n+1} = s$$

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

4. An approximated sampling criterion

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

$$\hat{\xi}(x, s) = \mathbb{1}(\xi(x, s) \in \Theta) \quad \text{if} \quad (x, s) \in \Theta$$

and $E_{\Theta} [\xi(x, s) | \Theta]$ otherwise.

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

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

$$\hat{J}_n(x, s) = \int_{n}^{M} \sum_{m=1}^{M} \sum_{i=1}^{M} k(\hat{\xi}(x, s), x, \hat{\xi}_i) \leq \alpha \approx J_n(x, s)$$

5. An SMC-based optimization algorithm

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

$$\Gamma_1(f) \supset \Gamma_2(f) \supset \cdots \supset \Gamma_n(f) = \Gamma(f)$$

such that $\Gamma_n(f)$ is "easy" to estimate knowing $\Gamma_{n-1}(f)$.

At each step $n$:

- Build a set $\tilde{S}_n \subset \hat{S}$ whose points are i.i.d. according to $P_S$.
- Generate a set of particles $\tilde{X}_n \subset X$ using sequential Monte Carlo with target distribution $q_{\pi}(x) = P_S(x \in \Gamma_n(f))$.
- Approximate $q_{\pi}(x) \approx \frac{1}{N} \sum_{i=1}^N \mathbb{1}(\xi(x, s) \in \Theta)$ for all $x \in \tilde{X}_n$.
- Sample $\tilde{X}_n$ particles according to $\sum_{i=1}^N q_{\pi}(x) \mathbb{1}(\xi(x, s) \in \Theta)$ (residual resampling).
- Move the particles according to a random walk Metropolis-Hastings algorithm.
- Draw a subset $\Theta \subset \tilde{S}_n \times \tilde{X}_n$ according to the distribution proportional to $\min\{p_{\pi}(x, s), 1 - p_{\pi}(x, s)\}$, with $p_{\pi}(x, s) = P_S(\xi(x, s) \in C)$.
- Minimize $\hat{J}_n$ on $\Theta$.
- If $\min_{(x, s) \in \Theta} \hat{J}_n(x, s) \leq \alpha$, set

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

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

