

Reliability-based inversion: Stepwise uncertainty reduction strategies?

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Reliability-based inversion problem

Consider $f : \mathbb{X} \times \mathbb{S} \mapsto \mathbb{R}$ an **expensive to compute black-box** numerical simulator with inputs

- $x \in \mathbb{X}$: design input.
- $s \in \mathbb{S}$: uncertain input.

We assume that \mathbb{S} is equipped with a **known** probability distribution $\mathbb{P}_{\mathbb{S}}$.

Example: f the electrical production of a wind farm, depending on

- x the design of the wind turbine
- s the climatic conditions

Reliability-based inversion (RBI) problem

Given $q \in \mathbb{R}$, $\alpha \in]0, 1[$, and $S \sim \mathbb{P}_S$, we define the set of interest as

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

with the associated function $c(x) = \mathbb{1}(x \in \Gamma(f))$

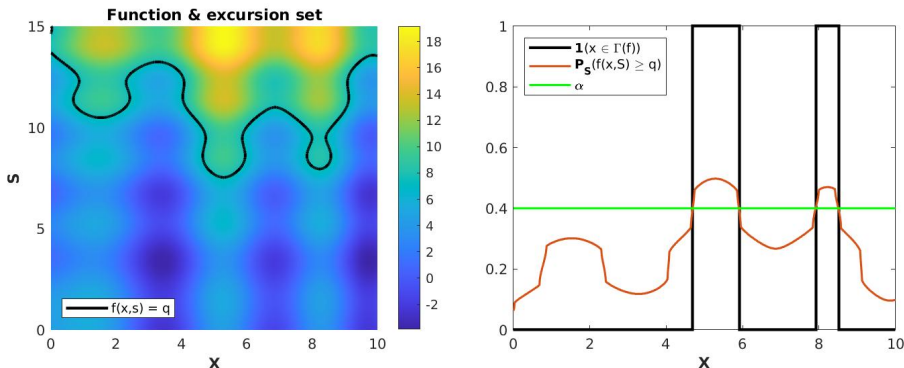


Figure: Excursion set of f over q (left) and set of interest (right).

Reliability-based inversion (RBI) problem

Objective:

Construct a good approximation $\hat{\Gamma}(f)$ of $\Gamma(f)$, given a (generally small) budget of N calls to f .

\implies “Reliability-based” inversion problem (RBI)

\implies Careful decision rule for the choice of the points of evaluations

$$\{(X_1, S_1), \dots, (X_N, S_N)\}$$

We propose a Stepwise Uncertainty Reduction (SUR) strategy to this end.

Let ξ be a Gaussian process (GP) prior on f

$$\xi \sim GP(\mu, k)$$

with μ a mean function and k a covariance kernel.

Main interests of GPs :

- Tractable conditional distributions
- Conditioning formula for sample paths

\implies Common assumption in Bayesian optimization and black-box inference.

SUR strategies principle:

Given current information \mathcal{I}_n

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

choose the point minimizing the expected future uncertainty.

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

where:

- U_{n+1} uncertainty metric depending on \mathcal{I}_{n+1}
- \mathbb{E}_n expectation w.r.t. \mathbb{P}_n , the distribution of ξ knowing \mathcal{I}_n

Examples of SUR strategies:

Let $\mu_n(x, s) = \mathbb{E}_n(\xi(x, s))$ and $\sigma_n^2(x, s) = \mathbb{E}_n((\xi(x, s) - \mu_n(x, s))^2)$, respectively the kriging mean and variance of $\xi(x, s)$ knowing \mathcal{I}_n

- Function fitting: ALC [CGJ94]

$$\begin{aligned} U_n &= \mathbb{E}_n \left(\|\xi - \mu_n\|_{L^2(\mathbb{X} \times \mathbb{S})}^2 \right) \\ &= \int_{\mathbb{X} \times \mathbb{S}} \sigma_n^2(x, s) d(x, s) \end{aligned}$$

- Optimization: IAGO [VW09]

$$U_n = \mathbb{H}_n \left(\arg \min_{(x, s) \in \mathbb{X} \times \mathbb{S}} \xi(x, s) \right)$$

where \mathbb{H}_n is the entropy w.r.t. \mathbb{P}_n

- Standard inversion in the joint space $\mathbb{X} \times \mathbb{S}$ [Bec+12]: approximate the excursion set

$$\gamma(f) = \{(x, s) \in \mathbb{X} \times \mathbb{S}, f(x, s) \geq q\}$$

$$U_n = \int_{\mathbb{X} \times \mathbb{S}} p_n(x, s) (1 - p_n(x, s)) d(x, s)$$

with $p_n(x, s) = \Phi\left(\frac{\mu_n(x, s) - q}{\sigma_n(x, s)}\right)$ where Φ is the c.d.f of the standard Gaussian distribution.

We introduce the integrated process and the associated set of interest:

$$\tau(\xi, x) = \int_{\mathbb{S}} \mathbb{1}(\xi(x, s) \geq q) \mathbb{P}_S(ds)$$

and

$$\Gamma(\xi) = \{x \in \mathbb{X}, \tau(\xi, x) \geq \alpha\}$$

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

Remark

The metric U_n can be rewritten:

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

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

Issue: The distribution of $\tau(\xi, x)$ is intractable

The process ξ being Gaussian, we can generate ξ_1, \dots, ξ_M sample paths of ξ under \mathbb{P}_n

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

The paths are then reconditioned for every candidate point (x, s) , according to values sampled from the posterior distribution of $\xi(x, s)$.

A SUR method for RBI

Sequential choice of evaluation points according to

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

When the budget of N evaluations is reached, we define

$$\hat{\Gamma}(f) = \{x \in \mathbb{X}, \hat{\tau}(f, x) \geq \alpha\}$$

with $\hat{\tau}(f, x)$ approximation constructed from the final model.

Simplest choice of $\hat{\tau}(f, x)$:

$$\hat{\tau}(f, x) = \tau(\mu_N, x)$$

with $\mu_N = \mathbb{E}_N(\xi)$, the posterior mean function of ξ knowing \mathcal{I}_N

\implies Can be obtained easily, ξ being Gaussian.

Numerical experiments

Two test functions:

$$f_1(x, s) = g_1(x, s) + \sin(x^{1.4}) + \sin(y^{1.4})$$

- $\mathbb{X} \times \mathbb{S} = [0, 10] \times [0, 15]$
- g_1 the Branin-Hoo function
- $\mathbb{P}_S = \mathcal{U}([0, 15])$

Function & excursion set

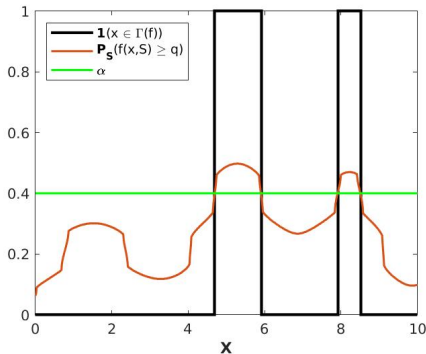
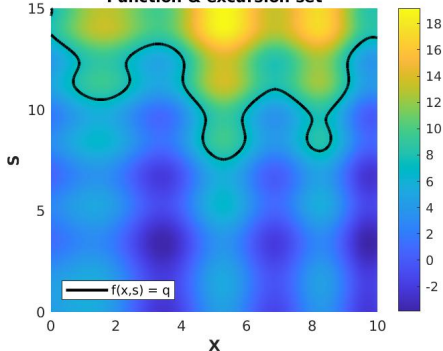


Figure: Excursion set of f_1 (left), set of interest for $q = 7.5$ & $\alpha = 0.4$. (right)

Numerical experiments

$$f_2(x, s) = \frac{1}{2}(g_2(x_1, s_1) + g_2(x_2, s_2))$$

- $\mathbb{X} \times \mathbb{S} = [-2, 2]^2 \times [-1, 1]^2$
- g_2 the six-hump camel-back function
- $\mathbb{P}_S = \mathcal{U}([-1, 1]^2)$

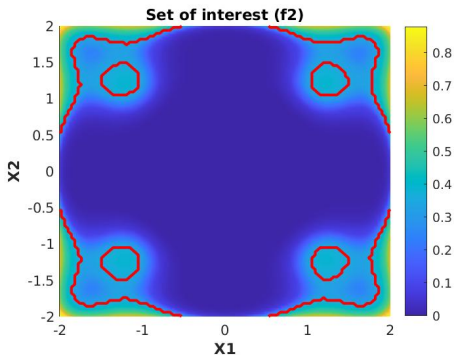


Figure: Set of interest of f_2 for $q = 2.15$ and $\alpha = 0.35$.

Numerical experiments

Speed of convergence compared to the one of methods reducing uncertainty on the excursion set in the joint space:

- Straddle heuristic [Bry+05]
- Standard SUR inversion

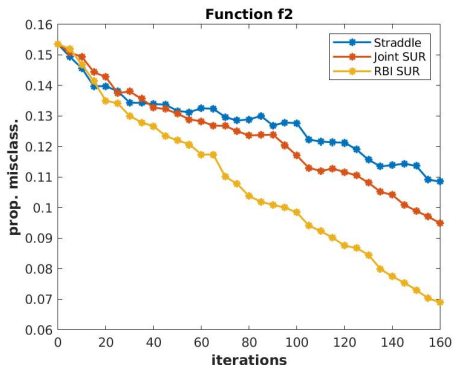
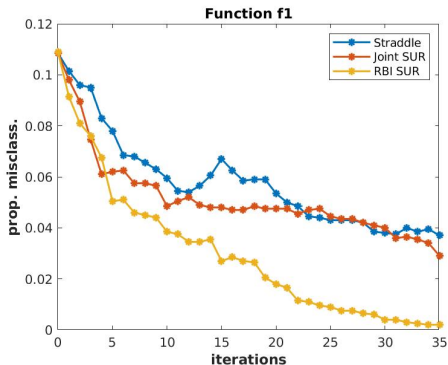


Figure: Median of the proportion of misclassification vs. number of iterations - (50 runs).

Numerical experiments

Illustration: Sequential overview of an application of the strategy.

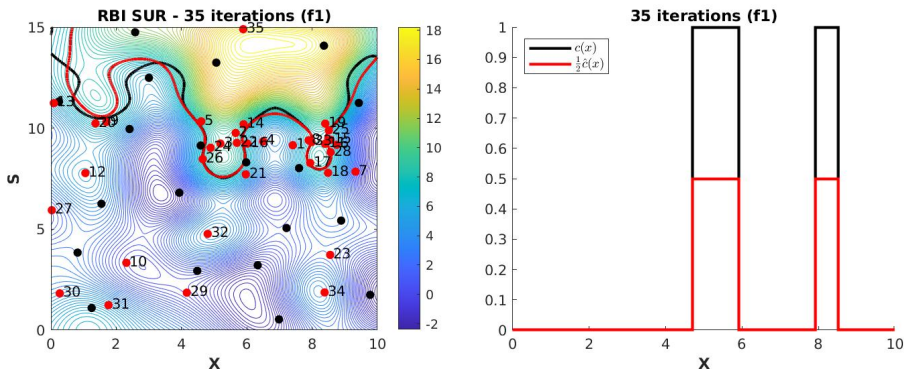


Figure: Example of design and estimation obtained.

Numerical experiments

In some cases, the strategy performs similarly to the SUR inversion in the joint space. We consider f_3 the Hartman4 function:

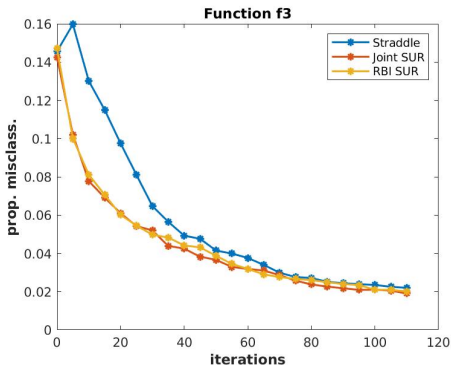


Figure: Median of the proportion of misclassification vs. number of iterations - (50 runs).

⇒ RBI-SUR method never lags behind for all the functions tested.

Conclusion:

- RBI dedicated SUR method tends to converge faster than standard methods focusing on the excursion set in the joint space $\mathbb{X} \times \mathbb{S}$.
- Drawback: based on expensive conditioning of GPs sample paths.

Open questions:

- In a simplified framework: consistency of the strategy?
- Efficient sampling of the set of candidate points.
- Approximation of the integrals.



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Appendix

Illustration: Design obtained by our strategy vs. design obtained by SUR method on the excursion set in the joint space.

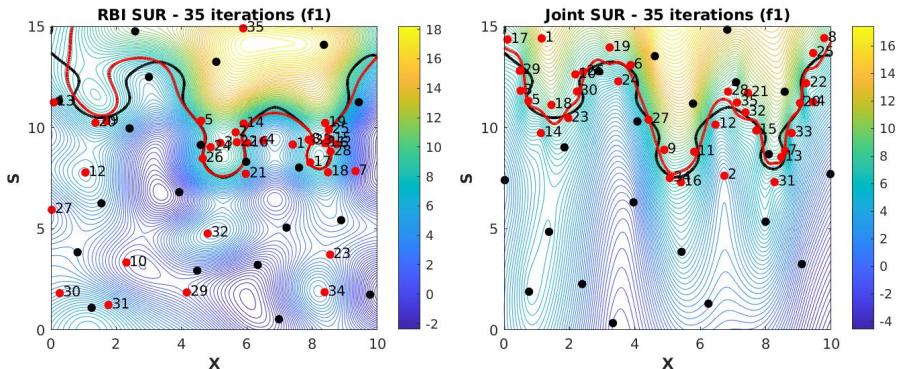


Figure: Our strategy (left), standard SUR on the joint space (right).

Parameters for the numerical simulations:

Test function f_1 :

- Covariance kernel: anisotropic Matérn.
- Number of initial (random) points: 20.
- Number of candidate points: 400.
- Number of trajectories: 250.

Test function f_2 :

- Covariance kernel: anisotropic Matérn.
- Number of initial (random) points: 40.
- Number of candidate points: 1600.
- Number of trajectories: 500.