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Sequential Bayesian Inversion of Black-box Functions in Presence of Uncertainties

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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 \( f : X \times S \rightarrow \mathbb{R} \). In this setting, \( X \) is the space of deterministic inputs and \( S \) 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

\[
\Gamma(f) = \{ x \in X : P(f(x, S) \geq q) \geq \alpha \}
\]

where \( S \) is a random variable with known distribution \( P_S \) on \( S \).

- Equivalently, we can formulate this problem as a classification problem, in which we wish to approximate the classifier

\[
e(\mathbf{x}) = \begin{cases} 1 & \text{if } x \in \Gamma(f) \\ 0 & \text{otherwise} \end{cases}
\]

The 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 \( I_n \):

\[
I_n = \{(X_1, S_1, \xi(X_1, S_1)), \ldots, (X_n, S_n, \xi(X_n, S_n))\}
\]

- A SUR strategy choose the point minimizing the expected future uncertainty:

\[
(x_{n+1}, S_{n+1}) = \arg \min_{(x,s) \in X \times S} E_n(U_{n+1} | X_{n+1} = x, S_{n+1} = s)
\]

where:

- \( U_{n+1} \) is an uncertainty metric on the object of interest, depending on \( I_n \)
- \( E_n \) expectation with respect to \( P_n \), the distribution of \( \xi \) given \( I_n \)

SUR approaches have been successfully used for the resolution of several problems regarding expensive-to-evaluate black box, including optimization [VVW09; 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 \( \alpha \):

\[
\tau(\mathbf{x}, \mathbf{s}) = \int \mathbb{1}(\xi(\mathbf{x}, \mathbf{s}) \geq q) \, dP_{\mathbf{s}}(\mathbf{s})
\]

and

\[
\Gamma(\xi) = \{ \mathbf{x} \in X, \tau(\mathbf{x}, \mathbf{s}) \geq \alpha \}
\]

- We consider the uncertainty metric \( U_n \) defined by

\[
U_n = \int_X \tilde{p}_n(x)(1 - \tilde{p}_n(x)) \, dx
\]

with \( \tilde{p}_n(x) = P_n(\tau(\mathbf{x}, \mathbf{s}) \geq \alpha) \)

The link between the metric and the uncertainty of the random set \( \Gamma(\xi) \) can be seen more clearly by remarking that:

\[
U_n = \int_X V_n(\mathbb{1}(\xi(x) \in \Gamma(\xi))) \, dx
\]

with \( V_n \) the conditional variance given \( I_n \).

- The conditional distributions of \( \tau(\mathbf{x}, \mathbf{s}) \) are tractable: the SUR criterion does not admit an analytic expression.

- Monte Carlo simulations: \( \xi \) being Gaussian, we can generate \( \xi_1, \ldots, \xi_M \) sample paths of \( \xi \) under \( P_n \)

\[
\frac{1}{M} \sum_{\xi} \mathbb{1}(\tau(\mathbf{x}, \xi) \geq \alpha) \leq \mathbb{E}(\tau(\mathbf{x}, \xi) \geq \alpha) = \tilde{p}_n(x)
\]

For each candidate point \( (x, s) \), the sample paths are reconditioned according to values sampled from the distribution of \( \xi(x, s) \) given \( I_n \).

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 \( X \times S \) 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

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