MASCOT-NUM 2022
Clermont Ferrand, France
7-9 June 2022

Sequential Bayesian inversion of black-box functions in presence of uncertainties

R. Ait Abdelmalek-Lomenech
Université Paris-Saclay, CNRS, CentraleSupélec, Laboratoire des signaux et systèmes (L2S)

Supervisor(s): E. Vazquez (L2S), J. Bect (L2S)

PhD expected duration: 2021 - 2024

Address: Laboratoire des Signaux et Systèmes, CentraleSupelec,
3 rue Joliot Curie, 91190 Gif-sur-Yvette

E-mail: Romain.Ait@centralesupelec.fr

Abstract:

Given an expensive-to-compute black-box function, we aim at finding the subset of points that leads to values of the function having prescribed properties.

In this communication, we focus on a particular robust formulation of this inversion problem that we call "Reliability-Based Inversion" (RBI), in which the function of interest has both deterministic and uncertain inputs. In this formulation, the objective is to retrieve the set of deterministic inputs such that the probability that the outputs exceed a given level is greater than a threshold.

More precisely, given a level $q \in \mathbb{R}$ and a threshold $\alpha \in]0,1[$, the object of interest in the RBI problem is the set

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

where f is a black-box function, $\mathbb{X}$ is a design space, S is a random vector with known probability distribution $\mathbb{P}_S$.

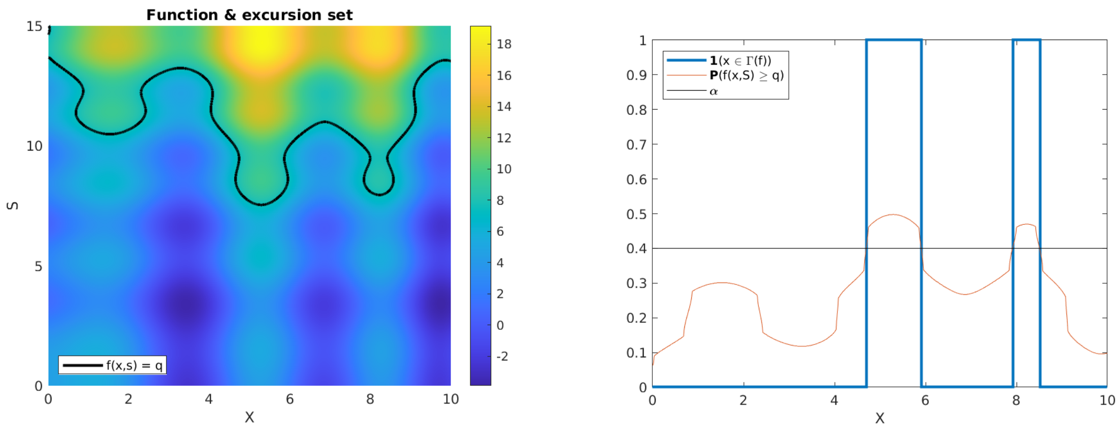

Figure 1: Excursion set of a function f over q (left) and associated set of interest (right).

When every call to the function is expensive—for example in the case of finite elements based simulations—the objective is to reach a good approximation of the set of interest given a small number of evaluations. The choice of the points of evaluation must then be conducted carefully.

To address this problem, we propose a sequential Bayesian strategy based on the Stepwise Uncertainty Reduction (SUR) framework. SUR strategies are Bayesian methods for selecting the evaluation points by minimizing the expected future uncertainty about the quantity of interest, measured by a particular metric. Such strategies have been used with success in a diverse range of problems: function fitting, optimization [4, 5], and more standard inversion problems [2, 1].

In this work, we postulate a Gaussian process prior ξ on the considered numerical simulator. The SUR strategy then aims at selecting the future points of evaluation by minimizing a criterion based on a "variance-like" uncertainty measure on the random set $\Gamma(\xi)$. We illustrate the performance of our method by applying it to several test functions. Those numerical experiments show that the developed strategy generally outperforms methods focusing on the excursion set in the joint space of design and uncertainties [2, 3] and never lags behind.

Joint work with J. Bect and E. Vazquez.

References

[1] D. Azzimonti, D. Ginsbourger, C. Chevalier, J. Bect, and Y. Richet. Adaptive design of experiments for conservative estimation of excursion sets. *Technometrics*, 63(1):13–26, 2019.

[2] J. Bect, D. Ginsbourger, L. Li, V. Picheny, and E. Vazquez. Sequential design of computer experiments for the estimation of a probability of failure. *Statistics and Computing*, 22(3):773–793, 2012.

[3] B. Bryan, J. Schneider, R. C. Nichol, C. J. Miller, C. R. Genovese, and L. Wasserman. Active learning for identifying function threshold boundaries. NIPS'05, pages 163–170, Cambridge, MA, USA, 2005. MIT Press.

[4] J. Mockus, V. Tiesis, and A. Zilinskas. The application of Bayesian methods for seeking the extremum. *Towards Global Optimization*, 2(117-129):2, 1978.

[5] J. Villemonteix, E. Vazquez, and E. Walter. An informational approach to the global optimization of expensive-to-evaluate functions. *J. of Global Optimization*, 44(4):509–534, 2009.

Short biography – With a backgroung in probability theory, statistics and machine learning, Romain began his PhD in October 2021 with CentraleSupélec. His work aims at developing new sequential Bayesian methods for the optimization/inversion of complex black-box functions.

This PhD thesis is funded by the French National Research Agency (ANR) in the context of the project SAMOURAI (ANR-20-CE46-0013).