A stepwise uncertainty reduction strategy for the estimation of small quantile sets

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Abstract

Given a numerical simulator of a physical phenomenon or system, one often seeks to determine the set of inputs that lead to values with specified properties. Such problems are broadly known as *set inversion* problems.

This communication focuses on a particular robust formulation of such problems that we call *Quantile Set Inversion* (QSI) [1], in which the function of interest has both deterministic and uncertain inputs. In this formulation, given a vector-valued function $f : \mathbb{X} \times \mathbb{S} \mapsto \mathbb{R}^q$, a critical region $C \subset \mathbb{R}^q$, and a threshold $\alpha \in (0, 1)$, the object of interest is the set

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

where $\mathbb{X}$ and $\mathbb{S}$ are respectively the spaces of design and uncertain input variables, and S is a random vector with known probability distribution $\mathbb{P}_S$.

This object, which we call a *quantile set*, corresponds to the set of deterministic inputs such that the probability (w.r.t. the distribution of the uncertain inputs) that the output variables belong to a critical region is below a threshold. A simple scalar-valued example of such a problem is shown in Figure 1.

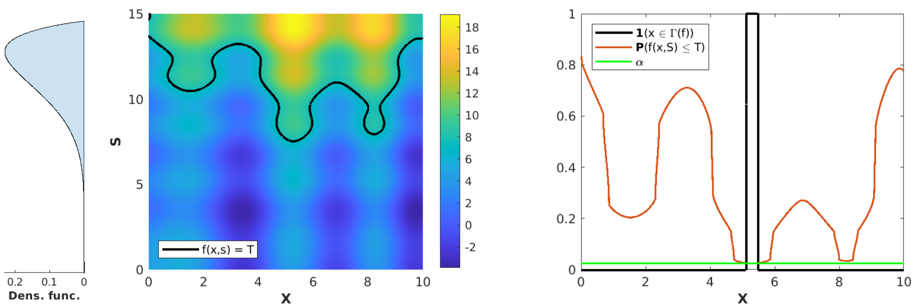

Figure 1: Scalar-valued example function (middle), probability density function associated to the distribution $\mathbb{P}_S$ of the uncertain input variable (left), and set of interest obtained with critical region $C = (-\infty, T]$ and threshold $\alpha = 0.025$ (right).

In the case of an *expensive-to-evaluate* function, the objective is to reach a good approximation of the set of interest using only a small, predetermined number of evaluations. The choice of the evaluation points must then be conducted carefully.

To address this set inversion problem, while taking into consideration the expensive-to-evaluate nature of the underlying function, we have proposed a sequential Bayesian strategy [1] based on the *Stepwise Uncertainty Reduction* (SUR) principle (see, e.g., [5] and references therein). Starting from a Gaussian process prior on the unknown function f, the strategy selects the next evaluation points by minimizing the expected future uncertainty about the *quantile set*, measured by a particular metric inspired by [3].

We propose, in this communication, an improvement of the method discussed in [1] to tackle more difficult problems where the quantile set is small with respect to the full input domain $\mathbb{X}$. In particular, we focus on the resolution of two defects arising in such context:

- An adaptive sequential Monte Carlo algorithm is introduced, in the spirit of [4], to tackle the difficulty of the sampling criterion optimization in the case of small quantile sets.
- The criterion is estimated using approximated Gaussian process sample paths [2], allowing an improvement in term of computation cost.

The performance of this strategy is illustrated by applying it to several test functions.

Short biography (PhD student)

With a backgroung in probability theory, statistics, machine learning and quantitative finance, Romain Ait Abdelmalek-Lomenech began his PhD in October 2021 with CentraleSupélec, under the supervision of Emmanuel Vazquez and Julien Bect. His work aims at developing new Bayesian methods for the optimization/inversion of expensive-to-evaluate functions in presence of uncertain input variables.

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