A Bayesian subset simulation approach to constrained global optimization of expensive-to-evaluate black-box functions

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Paul FELIOT · Julien BECT · Emmanuel VAZQUEZ

Abstract This talk addresses the problem of derivative-free global optimization of a real-valued function under multiple inequality constraints. Both the objective function and the constraint functions are assumed to be smooth, nonlinear, expensive-to-evaluate black-box functions. As a consequence, the number of evaluations that can be used to carry out the optimization is very limited. We focus in this work on the case of strongly constrained problems, where finding a feasible design, using such a limited budget of simulations, is a challenge in itself. The method that we propose to overcome this difficulty has its roots in the recent literature on Gaussian process-based methods for reliability analysis—in particular, the Bayesian Subset Simulation (BSS) algorithm of Li, Bect and Vazquez—and multi-objective optimization. More specifically, we consider a decreasing sequence of nested subsets of the design space, which is defined and explored sequentially using a combination of Sequential Monte Carlo (SMC) techniques and sequential Bayesian design of experiments. The proposed method obtains promising result on challenging test cases from the literature.

Keywords Optimization · Kriging · Gaussian Process · Subset Simulation · Sequential Monte Carlo

Mathematics Subject Classification (2000) 90C56 · 90C59 · 62K99 · 62L05 · 62P30

1 Context

This talk addresses the problem of derivative-free global optimization of a real-valued function under multiple inequality constraints:

$$\begin{cases} \text{Minimize} & f(x), \\ \text{Subject to} & x \in \mathbb{X} \quad \text{and} \quad c(x) \leq 0, \end{cases}$$

where f is the function to be minimized, $\mathbb{X} \subset \mathbb{R}^d$ is the design space and $c = (c_1, \ldots, c_q)$ is the vector of constraint functions, $c_j : \mathbb{X} \to \mathbb{R}$, $1 \leq j \leq q$.

Both the objective function f and the constraint functions c_j are assumed to be smooth, nonlinear, expensive-to-evaluate black-box functions. More specifically, it is assumed that the values of $f(x)$

Paul Feliot (corresponding author), Julien Bect, Emmanuel Vazquez
Institut de Recherche Technologique SystemX & Supélec
E-mail: firstname.lastname@irt-systemx.fr ou firstname.lastname@supelec.fr
IRT SystemX: 8, avenue de la Vauve, 91120 Palaiseau, France.
Supélec: 3 rue Joliot-Curie, 91192 Gif-sur-Yvette cedex, France.

and $c(x)$, for a given $x \in \mathbb{X}$, are provided simultaneously by a single call to some time-consuming computer program—a setup that typically applies to industrial design problems, where numerical simulations are used to mimic the actual physical behavior of the system to be designed. Such simulations may for instance require fluid dynamic, heat transfer or mechanical deformation computations and can take from a few hours to several days to compute.

The number of runs that can be afforded to carry out the optimization is therefore very limited. We focus in this work on the case of strongly constrained problems, where finding a feasible design, using such a limited budget of simulations, is a challenge in itself.

2 Proposed method

Global optimization methods have been investigated intensively for the last decades. When expensive-to-evaluate functions are involved, cheap-to-evaluate approximations of the objective and constraints functions—often referred to as surrogate models or meta-models—are classically relied upon. We adopt here a Bayesian approach, which provides not-only natural surrogate models for the expensive-to-evaluate functions that we have to deal with, but also an elegant framework to help design efficient optimization algorithms. More precisely, the objective function f and the constraint functions c_j are modeled as (independent) Gaussian processes, following a now classical approach that has been made popular by Jones et al. (1998) for unconstrained optimization problems. Subsequent developments for constrained optimization problems have been proposed by, among others, Schonlau et al. (1998); Sasena et al. (2002); Gramacy and Lee (2011); Parr et al. (2012); Picheny (2014a).

We focus in this talk on the case of strongly constrained problems, where the volume of the feasible space is small compared to the size of the design space. As a consequence, locating even a single feasible point becomes difficult and most existing Bayesian optimization methods, which require at least one feasible point to begin with, fail to be applicable. The method that we propose to overcome this difficulty has its roots in the literature on Bayesian sequential design of experiments for reliability analysis (see, e.g., Bect et al., 2012; Li et al., 2012)—estimating a failure region or a feasible set are very similar problems—and multi-objective optimization (see, e.g., Emmerich et al., 2006; Wagner et al., 2010; Picheny, 2014b). More specifically, we consider a decreasing sequence of nested subsets of the design space, which is defined and explored sequentially using a combination of Sequential Monte Carlo (SMC) techniques and sequential Bayesian design of experiments, in the spirit of Li et al. (2012); Benassi et al. (2012); Li (2012); Benassi (2013).

3 Results and future work

We are able to report good results on challenging test cases from the literature. Future work will include the extension of our method to multi-objective problems and the optimization of various aspects of our algorithm (Sequential Monte Carlo algorithm, sampling criterion...). Simulation failures should also be taken into account as they are inherent to complex industrial simulation codes. The performance of the method will be evaluated on a real-life industrial problem provided by Safran, with the contribution of Cenaero (optimization of the performances of a turbo-machine fan blade under aerodynamic, mechanic and acoustic constraints).

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