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# A Bayesian approach to constrained multi-objective optimization

Paul FELIOT, Julien BECT, Emmanuel VAZQUEZ

IRT SystemX, Palaiseau, France & SUPELEC, Gif-sur-Yvette, France  
firstname.lastname@irt-systemx.fr or firstname.lastname@supelec.fr

**Abstract.** This paper addresses the problem of derivative-free multi-objective optimization of real-valued functions under multiple inequality constraints. Both the objective and constraint functions are assumed to be smooth, nonlinear, expensive-to-evaluate functions. As a consequence, the number of evaluations that can be used to carry out the optimization is very limited. The method we propose to overcome this difficulty has its roots in the Bayesian and multi-objective optimization literatures. More specifically, we make use of an extended domination rule taking both constraints and objectives into account under a unified multi-objective framework and propose a generalization of the expected improvement sampling criterion adapted to the problem. A proof of concept on a constrained multi-objective optimization test problem is given as an illustration of the effectiveness of the method.

## 1 Introduction

This paper addresses the problem of derivative-free multi-objective optimization of real-valued functions under multiple inequality constraints:

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

where  $f = (f_j)_{1 \leq j \leq p}$  is a vector of objective functions to be minimized,  $\mathbb{X} \subset \mathbb{R}^d$  is the search domain and  $c = (c_i)_{1 \leq i \leq q}$  is a vector of constraint functions. Both the objective functions  $f_j$  and the constraint functions  $c_i$  are assumed to be smooth, nonlinear functions that are expensive to evaluate. As a consequence, the number of evaluations that can be used to carry out the optimization is very limited. This setup typically arises when the values  $f(x)$  and  $c(x)$  for a given  $x \in \mathbb{X}$  correspond to the outputs of a computationally expensive computer program.

In this work, we consider a Bayesian approach to this optimization problem. The objective and constraint functions are modelled using a vector-valued Gaussian process and  $\mathbb{X}$  is explored using a sequential Bayesian design of experiments approach. More specifically, we focus on the Expected Improvement (EI) sampling criterion. This criterion was originally introduced in the context of single-objective, unconstrained optimization [10,13]. It was later extended to

handle constraints [7,16,18,20,21] and to address unconstrained multi-objective problems [4,17,23,9]. However, to the best of our knowledge, the general case of a constrained multi-objective problem has only been addressed very recently by [22]. In their paper, Shimoyama et al. consider three different Bayesian criteria for unconstrained multi-objective optimization and study the effect of multiplying the criteria by a probability of feasibility in order to handle the constraints.

The approach we propose to handle the constraints is based on an extended domination rule, in the spirit of [6,15,19], which takes both objectives and constraints into account under a unified framework. The extended domination rule makes it possible to derive a new expected improvement criterion to deal with constrained multi-objective optimization problems. Section 2 introduces the proposed method, while Section 3 presents a proof of concept on a classical test case from the literature. Results and future works are briefly discussed at the end of Section 3.

## 2 An expected improvement criterion for constrained multi-objective optimization

In this section, we present our extended domination rule and introduce a new expected improvement criterion suitable for constrained and unconstrained multi-objective problems. The new criterion is equivalent to the original EI on unconstrained single-objective problems and to Schonlau's extension to the constrained case [21] once a feasible point has been found. It is also similar to the formulation of [23] for unconstrained multi-objective problems and to that of [22] in the constrained case once a feasible point has been found. As such, it can be seen as a generalization of the above-mentioned criteria.

Denote by  $\mathbb{F} \subset \mathbb{R}^p$  and  $\mathbb{C} \subset \mathbb{R}^q$  the objective and constraint spaces respectively, and let  $\mathbb{Y} = \mathbb{F} \times \mathbb{C}$ . We shall say that  $y_1 \in \mathbb{Y}$  dominates  $y_2 \in \mathbb{Y}$ , which will be denoted by  $y_1 \triangleleft y_2$ , if  $\psi(y_1)$  dominates  $\psi(y_2)$  in the usual Pareto sense, where

$$\psi : \mathbb{F} \times \mathbb{C} \rightarrow \overline{\mathbb{R}}^p \times \mathbb{R}^q$$

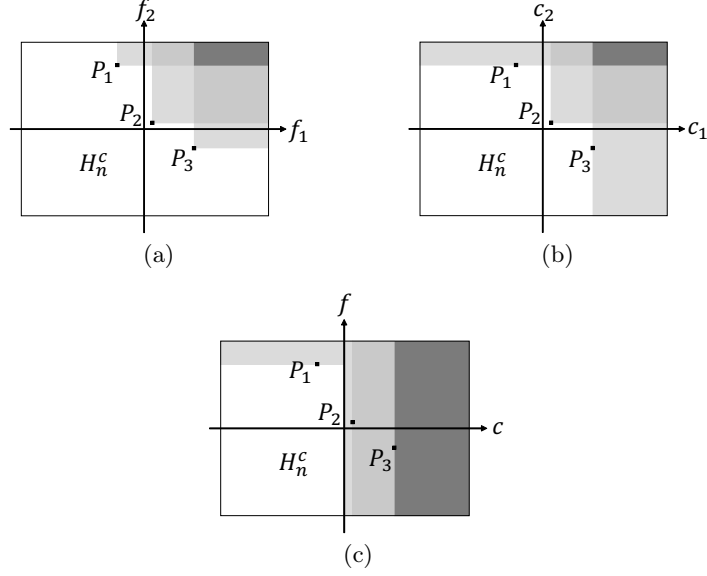
$$(y_f, y_c) \mapsto \begin{cases} (y_f, 0) & \text{if } y_c \leq 0, \\ (+\infty, \max(y_c, 0)) & \text{otherwise,} \end{cases}$$

In the above system of equations,  $\overline{\mathbb{R}}$  denotes the extended real line. For unconstrained problems, we simply take the usual domination rule on  $\mathbb{F}$ . Figure 1 illustrates this extended domination rule in different cases.

Assume now that  $\mathbb{Y}$  is bounded. Much like [4,23,17], we define the improvement yielded by a new observation as the increase of the dominated hypervolume:

$$I_N(x_{N+1}) = |H_{N+1}| - |H_N|,$$

where  $H_N$  is the subset of  $\mathbb{Y}$  dominated by the solutions observed so far  $(f(x_1), c(x_1)), \dots, (f(x_N), c(x_N))$  and  $|\cdot|$  denotes the usual (Lebesgue) volume measure in  $\mathbb{R}^{p+q}$ . The corresponding expected improvement criterion can be written as



**Fig. 1.** Illustration of the extended domination rule in different situations. The region dominated by each point is represented by a shaded area. Darker shades of gray indicate overlapping regions. (a) Feasible solutions are compared to their objective values using the usual domination rule in the objective space. (b) Non-feasible solutions are compared component-wise with respect to their constraint violations using the usual domination rule applied in the constraint space. (c) Feasible solutions always dominate non-feasible solutions; other cases are handled as in the first two figures.

$$\begin{aligned}
\text{EI}_N(x_{N+1}) &= \mathbb{E}_N((I_N(x_{N+1}))) \\
&= \mathbb{E}_N\left(\int_{\mathbb{Y} \setminus H_N} \mathbb{1}_{\xi(x_{N+1}) \triangleleft y} dy\right) \\
&= \int_{\mathbb{Y} \setminus H_N} \mathbb{P}_N(\xi(x_{N+1}) \triangleleft y) dy
\end{aligned}$$

where  $\mathbb{P}_N$  denotes the probability conditional to the observations and  $\xi$  is a vector-valued Gaussian model for  $(f, c)$ .

Even though the integrand of the EI formula can be readily computed analytically, its integration is not trivial due to the combinatorial nature of the problem [8,2,5]. To overcome this difficulty, we propose to use a Sequential Monte Carlo (SMC) approximation [3,11,12,1]:

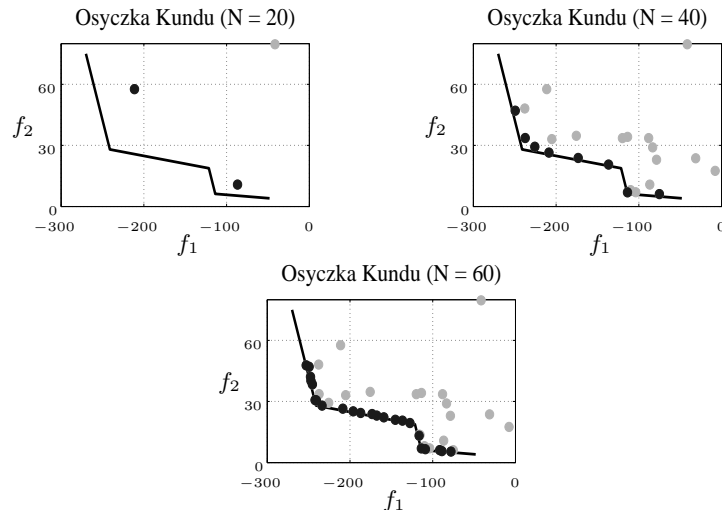
$$\text{EI}_N(x_{N+1}) \approx \sum_{i=1}^n w_i \mathbb{P}_N(\xi(x_{N+1}) \triangleleft y_i),$$

where  $\mathcal{Y}_N = (w_i, y_i)_{1 \leq i \leq n}$  is a weighted sample that targets the uniform density on  $\mathbb{Y} \setminus H_N$ .

### 3 Proof of concept

In this paper, we illustrate the behavior of our new optimization strategy using the Osyczka and Kundu test problem [14] for constrained multi-objective optimization ( $d = 6$ ,  $p = 2$ ,  $q = 6$ ). The algorithm is initialized using a Latin Hypercube sample of 18 samples and proceeds using the above mentioned criterion. Figure 2 shows the convergence of the algorithm at different steps of the optimization.

We are also able to report good results on other challenging test cases from the literature and future communications will include a comparison of our method to reference optimization methods. More details about the SMC procedure will also be proposed.



**Fig. 2.** Test results on Osyczka and Kundu test problem with, from left to right,  $N = 20$ , 40 and 60 evaluations. Only feasible points are shown on the figures. The dark dots represent non-dominated observations while the light gray dots represent dominated ones. The dark curve represents the target Pareto front.

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