Targeting Well-Balanced Solutions in Bayesian Multi-Objective Optimization under a Restricted Budget

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Abstract:

Multi-objective optimization aims at minimizing m functions simultaneously: $\min_{\mathbf{x}\in X}(f_1(\mathbf{x}), .., f_m(\mathbf{x}))$. There does not exist one but several optimal solutions in the *non-domination* sense to this problem, and the goal is to determine and understand the Pareto set composed of all the best trade-off solutions between these objectives. When dealing with expensive-to-evaluate black box functions, approaches based on Gaussian Processes (GP) in the vein of EGO [2] have proven their effectiveness. These methods consist in building a surrogate (GP) which is sequentially updated by evaluating the computer code at *the most promising* design $\mathbf{x}^{(n+1)}$.

However, for extremely narrow budgets, and/or when the number of objectives is large, uncovering the entire Pareto set becomes out of reach even for these approaches. In the presence of many objectives, it may anyway be irrelevant to look for the whole front, as the latter will encompass too many solutions. For these reasons, we restrict the search to well-chosen parts of the Pareto set. This accelerates the problem resolution as only a subset of the objective space is considered. As an end-user would typically prefer solutions with equilibrated trade-offs between objectives over solutions favoring a part of them, we will focus on the central part of the Pareto front.

First, we define the center of a given continuous (or prolongated) Pareto front. Means for estimating the center of the unknown Pareto front which rely on conditional GP simulations are presented. That estimated point has to fairly represent the topology of the front, in spite of the parsimonious knowledge of the objective space. Then, three infill criteria which guide the optimization by selecting new inputs to be evaluated by the computer code are studied. They include the *Expected Hypervolume Improvement* [1] and a multi-objective version of the *Expected Improvement* [3]. They are tailored through some of their hyperparameters to enable them to target specific parts of the objective space. EHI [1] for example needs a reference point whose choice is crucial and will impact the search results. Ponweiser et al. [4] use the maximum objective values of all non-dominated points augmented by one for this reference point, the argument being that no Pareto optimal solution should be omitted. Here, the reference point is considered in a different way: it is used as a hyperparameter that enables EHI to restrict the search to chosen parts of the objective space. By choosing the reference point to be the estimated center of the Pareto front, potential solutions are sought in regions with equilibrated trade-offs. Note that this approach is more general than a linear aggregation of normalized objectives that only applies to convex Pareto fronts.

Once the algorithm has attained the center, only marginal gains would result from continuing this methodology. Therefore, a convergence criterion that triggers a new phase is defined. The stopping criterion is based on the local GP uncertainty at the estimated Pareto front center. The

new optimization phase broadens the targeted objective space considering both the remaining computational budget and the reduction of uncertainty, while keeping it centered, to offer a wider range of well-balanced solutions to the decision maker.

To assess the performance of the algorithm, a benchmark built from real-world airfoil aerodynamic data is used. It has variable dimension (3, 8 and 22), representing CAD parameters, and 2 to 4 aerodynamic objectives (lift and drag at various airfoil angles). It is observed that compared with standard techniques, the proposed methodology leads to a faster and a more precise convergence towards the center of the Pareto front. Typical convergences of the proposed and classical methods are given in Figure 1 for two objectives.

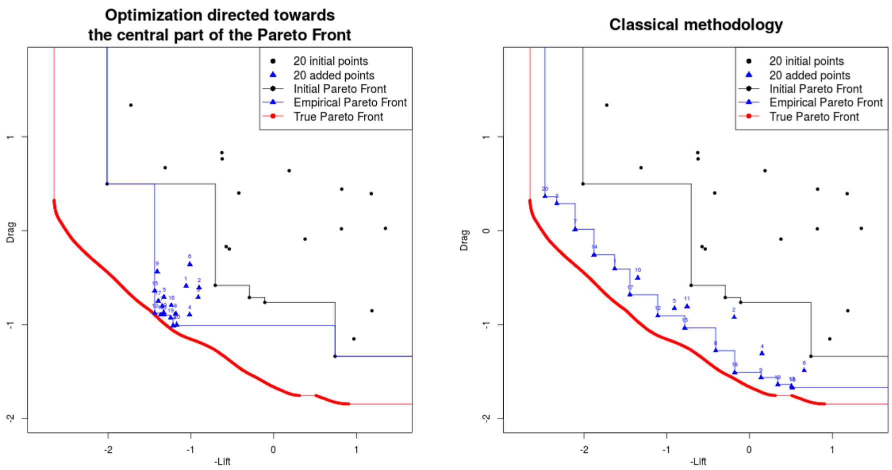

Figure 1: Two objectives optimization directed towards the estimated central part of the Pareto front (left). The initial Pareto front approximation (black) has only been improved in the region corresponding to well-balanced solutions. Compared with standard bayesian multi-objective optimization techniques (right), the proposed methodology focuses on the central part of the Pareto front where convergence is enhanced, instead of trying to find the whole front

References

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Short biography – David Gaudrie obtained his engineering degree from INSA Toulouse in Applied Mathematics in 2016. He started a PhD thesis about high dimensional multi-objective optimization in the context of expensive computer codes in November 2016. This thesis in funded by the automotive group PSA (CIFRE convention) in collaboration with the École des Mines de Saint-Étienne and the MIA department of INRA Toulouse.