Exploitation of Multiple Surrogate Models in Multi-Point Infill Sampling Strategies

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ABSTRACT

This work presents interesting multi-point search algorithms exploiting several surrogate models, implemented in MINAMO, the multi-disciplinary optimization platform of Cenaero. Many types of surrogate models are used in the literature with their own forces and weaknesses. More generally, each one models differently a given problem and provides its own representation of the reality. The idea of this paper is to exploit simultaneously different types of surrogate models in order to catch automatically their forces and to outshine some of their weaknesses. This strategy is based on a multi-point enrichment at each iteration, each candidate point being provided by one kind of surrogate model and/or criterion. This strategy can be tuned by selecting different infill criteria, based on different surrogate models, in order to improve more specifically different aspects such as feasibility, exploration and/or exploitation. The performance of this surrogate-based optimization framework is illustrated on well-known constrained benchmark problems available in the literature (such as GX-functions and MOPTA08 test cases). Good performance both in terms of identification of feasible regions and objective gains is demonstrated.

CCS CONCEPTS

• **Theory of computation** → **Online learning algorithms**; **Active learning**; • **Computing methodologies** → *Machine learning approaches*; *Modeling methodologies*; • **Mathematics of computing** → *Evolutionary algorithms*.

KEYWORDS

surrogate-based optimization, infill sampling criteria, multi-point, constrained design problems.

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1 INTRODUCTION

A globally effective approach to optimization problems based on computationally expensive high-fidelity computations lies in the exploitation of surrogate models. They act as cheap-to-evaluate alternatives to the original model reducing the computational cost, while still providing improved designs. A wide variety of techniques are available to build these models, such as Radial Basis Function Networks (RBFN) or Kriging, which all have their advantages and drawbacks, see [5]. The underlying principle of Surrogate-Based Optimization (SBO) consists in accelerating the optimization process by essentially exploiting surrogates for the objective and constraint evaluations, with a minimal number of function calls to the high-fidelity model for keeping the computational time within affordable limits [4].

One of the more popular approaches to select update points in a SBO framework is the maximization of the Expected Improvement (EI), see e.g. [8]. Studies have adapted EI to find multiple update points [6, 12], which is the topic of this study. Using multiple updates is far from a new idea, having been notably explored by Schonlau [12]. With the availability of parallel computing becoming commonplace, formulation of multiple update infill criteria has received further attention in past years [14].

Many works have been done on the use of multiple surrogates with success to enhance the robustness of the optimization process, see e.g. [1, 3, 11, 13].

2 MULTIPLE SURROGATES-BASED OPTIMIZATION STRATEGY

The purpose of this paper is to use multi-point strategies with multiple surrogate models based on multiple instance of evolutionary algorithms by using different infill criteria. Infill sampling criteria aims to extract knowledge from the surrogate models to find potential interesting areas for model refinement in order to strike a balance between model exploitation and exploration (and possibly feasibility). Two infill criteria have been considered in this work :

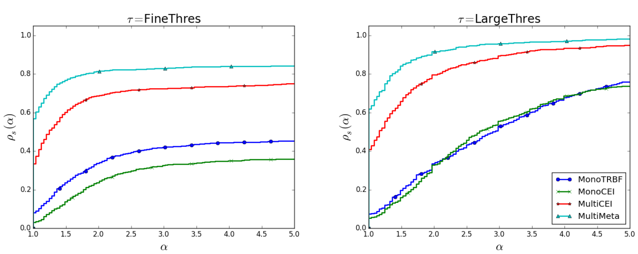
- Deb's constraint tournament selection criterion [2] ;
- Constrained expected improvement (CEI) [10].

The main idea of our multi-point surrogate-based optimization framework is to perform two evolutionary algorithms in parallel either based on different types of surrogate models or based on different infill criteria. In these strategies, two points will be evaluated at each iteration.

The following mono- and multi-point strategies will be compared :

- `MonoTRBF` : Mono-point strategy using an auto-tuned RBF (TRBF) meta-model and Deb's constraint tournament selection to deal with contraints ;
- `MonoCEI` : Mono-point strategy using a Kriging model and CEI as infill strategy ;
- `MultiCEI` : Multi-point strategy with two evolutionary algorithms, the first one exploiting Deb's constraint tournament selection with a TRBF model, the second one based on CEI infill criterion with a Kriging meta-model. This strategy combines `MonoTRBF` and `MonoCEI` strategies ;
- `MultiMeta` : Multi-point strategy with two evolutionary algorithms, both searches are based on Deb's constraint tournament selection but with either a TRBF model or a Kriging model.

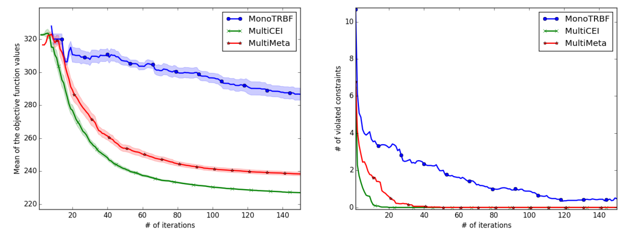
Figure 1 allows to compare globally the different strategies on the whole set of benchmark problems via the performance profiles (introduced in [9]). We can observe that both multi-point strategies are very interesting compared to mono-point strategies, in terms of efficiency as well as robustness.



(a) Fine Threshold (b) Large Threshold

Figure 1: Performance profiles of the different strategies on the GX test cases. Percentage of solved problems with respect to α.

The proposed strategies have also been compared on the MOPTA08 automotive problem, a benchmark test defined by Jones [7] which enables to assess the efficiency of optimization algorithms in a highly constrained, high-dimensional design space. It defines a design space with 124 parameters, for an optimization problem with a single objective and 68 inequality constraints. For the original benchmark problem, Jones [7] provides one feasible initial point. Since for real-world industrial applications, feasible points are typically not always available, the real challenge is to investigate the performance of our strategies if only unfeasible initial points are considered. For this purpose, a DoE of 125 points has been generated without including the feasible initial point, and the optimization has been launched in these unfavorable conditions. Figure 2 shows the convergence in terms of objective function and constraint violations (mean of 50 independent runs with 95% confidence interval) for the MOPTA08 problem. The multi-point strategies can help to reach faster the feasible region and with a good evolution of the objective function convergence compared to a classical mono-point strategy.



(a) Objective function (b) Number of violated constraints

Figure 2: Evolution of the optimization in terms of design iterations for MOPTA08 test case.

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