

Model-Based Multi-objective Optimization: Taxonomy, Multi-Point Proposal, Toolbox and Benchmark

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Abstract. Within the last 10 years, many model-based multi-objective optimization algorithms have been proposed. In this paper, a taxonomy of these algorithms is derived. It is shown which contributions were made to which phase of the MBMO process. A special attention is given to the proposal of a set of points for parallel evaluation within a batch. Proposals for four different MBMO algorithms are presented and compared to their sequential variants within a comprehensive benchmark. In particular for the classic ParEGO algorithm, significant improvements are obtained. The implementations of all algorithm variants are organized according to the taxonomy and are shared in the open-source R package mlrMBO.

Keywords: Expected improvement · Hypervolume · Kriging · Performance indicator · Surrogate model

1 Introduction

In recent years, the use of surrogate models for partly replacing the actual objective function allowed multi-objective optimization techniques to be applied to real-world problems in an efficient way [16]. The resulting combinations of surrogate models and optimization algorithms are denoted as model-based multi-objective

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optimization (MBMO) algorithms in the following. In the early algorithms, surrogate models have been fitted, and have then been used for the optimization in replacement of the actual objective functions. No sequential update has been performed. If a validation is performed at all, only the finally selected solution has been evaluated on the actual problem.

Since 2005, sequential approaches – using the surrogate to decide on new points to evaluate and update the model in an iterative fashion – have been proposed. Most of these approaches are based on ideas of the popular Efficient Global Optimization (EGO) procedure [13]. Early work in the multi-objective scenario has either scalarized the objectives [15] to allow EGO to be directly used or has optimized EGO’s figure of merit for different models in parallel using MOEA [11, 19]. Later, also set-based improvement criteria, specifically designed for multi-objective optimization, have been defined [1, 9, 14, 18, 23]. Until now, the algorithms as a whole were considered as a contribution to the field of MBMO. In order to better distinguish the actual contributions, a first taxonomy of existing MBMO approaches is introduced in this paper.

Due to the enormous growth of parallel computing power and the advantages of performing real experiments in batches, allowing more than one point to be proposed per iteration (batch processing) is of great interest. Right now, only one multi-objective approach exists [23] (see [3] for a comparison of methods and a new approach in the single-objective case). As a consequence, possibilities to integrate batch proposals into existing MBMO algorithms are proposed in the paper. In particular for set-based improvement criteria in MBMO, this is done for the first time, to the best of our knowledge.

The taxonomy is introduced in section 2. In section 3, it is shown how the existing algorithms can be classified using the concepts of the taxonomy. The ideas for allowing a batch proposal within specific algorithm classes are proposed in section 4. All covered algorithms are integrated into the R toolbox *mlrMBO* for model-based optimization (MBO), whose software design closely reflects the presented taxonomy. The toolbox is briefly presented in section 5. The MBMO algorithms are compared on a comprehensive benchmark, which is described and evaluated in section 6. The paper is concluded by a summary of the results and an outlook on possible further improvements.

2 Taxonomy

The taxonomy of the MBMO approaches is based on the standard procedure of a sequential MBO algorithm, whose phases are shown on the left of Fig. 1. First, an initial design is evaluated on the actual, expensive objective function in order to train the surrogate model. In principle, all available design-of-experiment (DOE) techniques can be used. Due to its connection to the established Kriging models [13], however, Latin Hypercube Sampling (LHS) is applied in almost all existent MBMO approaches, and hence explicitly mentioned as an option.

For model fitting, two approaches are established. In the straightforward variant, an individual surrogate model is built for each objective function. In order to