Multi-Criteria Optimization for Hard Problems under Limited Budgets

Martin Zaefferer, Thomas Bartz-Beielstein, Martina Friese, Boris Naujoks, Oliver Flasch
Cologne University of Applied Sciences,
Faculty for Computer and Engineering Science,
51643 Gummersbach, Germany
{firstname.lastname}@fh-koeln.de

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1. INTRODUCTION

In this paper, we show how techniques from multi-criteria optimization (MCO) can be efficiently integrated into the framework of the sequential parameter optimization (SPO [1]) Toolbox (SPOT). We test for competitiveness against state-of-the-art approaches and determine how our approach can be employed to improve the robustness of a tuning process.

In many industrial optimization problems, the duration of a process feedback plays a major role in the optimization process. Large evaluation times restrict optimization processes to only a very limited number of evaluations. Moreover, almost every industrial optimization task features more than one quality criterion. Techniques from multi-criteria optimization were developed during the last decade to solve such tasks. The necessity to combine MCO techniques and optimization methods that require a very small number of function evaluations only, should be self-evident.

Research in combining MCO and surrogate model optimization is not a new topic. Various research in this topic has been performed (cf. [8]). In particular, Voutchkov and Keane [9] introduced a multi-criteria approach for sequentially improving on surrogate models and tested it on simple multi-criteria functions with very few function evaluations. Their approach is similar to multi criteria SPOT (MSPOT) suggested here and uses a subset of the test functions considered in our study, however, restricted to low dimensional decision spaces. SPOT has previously been applied to multi objective optimization itself, not as an MCO algorithm, but as a tuner for such algorithms.

2. MULTI-CRITERIA OPTIMIZATION WITH SPOT

Single objective SPOT generates an initial design of several points and evaluates it on the objective function. Based on these evaluation results, SPOT builds a surrogate model (e.g., a linear, Kriging, or tree-based model). Two approaches can be used to exploit that model. (i) The naive approach samples a large number of points, which are then evaluated on the surrogate model. The best will be suggested for exact evaluation. (ii) More sophisticated approaches seek for the optimum of the surrogate model. This process of building and exploiting the surrogate model is repeated sequentially until a termination criterion is fulfilled.

The multi criteria SPOT approach makes use of the same basic scheme, but builds one surrogate for each objective. In the naive approach here, points sampled on the surrogate models are sorted by their non-dominated sorting rank and (if necessary as a tie breaker) hypervolume contribution. In the sophisticated approach, NSGA2 [4] or SMS-EMOA [2] are used to find Pareto optimal points on the surrogates.

3. EXPERIMENTAL SETUP

Three different surrogate models were tested with MSPOT and SPOT, a Kriging model [6], a Random Forest (RF) model [3], and a Multivariate Adaptive Regression Splines (MARS) model [7].[1] Using these, we try to answer two research questions:

RQ 1. *Is there a competitive advantage of MSPOT over state-of-the-art MCO algorithms? (Case Study I)*

To answer this question, the MSPOT approach is compared to NSGA2 and SMS-EMOA on test functions ZDT1 to ZDT3, DTLZ1, and DTLZ2 [10, 5]. ZDT feature 30 decision variables, DTLZ1 7 and DTLZ2 12, respectively. The test problems are restricted to very few function evaluations to increase problem hardness, i.e., a few ten or few hundred function evaluations are allowed only. To show development beyond these limits we decided to run up to a maximum budget of 1000 function evaluations.

RQ 2. *Is* MSPOT*'s multi-criteria optimization approach advantageous for parameter optimization? (Case Study II)*

Robustness in solving minimization problems can be defined by using the following goals: (i) to minimize the mean $\overline{Y}$ of the objective function values, and (ii) to minimize the standard deviation $\mathrm{sd}(Y)$ of these. This paper considers the search for robust solutions as a multi-criteria optimization problem, handling both mentioned goals as objectives.

[1]The used R-packages SPOT, randomForest, mco and earth can be retrieved from the CRAN homepage, i.e. `http://cran.r-project.org`

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To test this approach, MSPOT is compared to single criteria SPOT. Both are employed to tune algorithms, namely an Evolution Strategy (ES) and a Simulated Annealing algorithm (SANN), which again are used to optimize simple single criteria test functions (Branin, SixHump, Rastrigin, Rosenbrock, MexicanHat, and Sphere). Single criteria SPOT only optimizes the quality of ES or SANN (minimal expected test function value) based on design points $\vec{x}$ (algorithm parameters). MSPOT optimizes a second objective, the standard deviation of y, to evaluate the robustness of the parameter setting $\vec{x}$. With three different surrogate models, two algorithms and six test functions, altogether $3 \times 2 \times 6 = 36$ configurations are considered.

4. EXPERIMENTAL RESULTS

4.1 Case Study I: Comparison

SPOT variants with MARS and RF performed significantly better than NSGA2 or SMS-EMOA on all test functions with few function evaluations. However, only invoking the MARS model continued to perform well beyond 500 function evaluations. SPOT with Kriging does not perform well at all. This is probably due to a too high input dimension for Kriging.

On the DTLZ functions, SMS-EMOA takes the lead on larger budgets after about 300 function evaluations. The exact crossing point varies for different settings. On the other hand, the MSPOT MARS variant performs best on ZDT even for larger budgets.

4.2 Case Study II: Robustness

To gain insight into problem complexity and structure, we performed a sweep over the search space first. One thousand design points were evaluated ten times. For each design point, mean value and standard deviation were calculated. As a result, in every experimental setup, $\mathrm{sd}(Y)$ and $\overline{Y}$ were correlated. We observed that a parameter setting $\vec{x}$, which results in a good mean function value, also shares a low standard deviation. The correlation between $\overline{Y}$ and $\mathrm{sd}(Y)$ increases for good parameter settings.

Afterwards, we analyzed which model performs best for each SPOT variant: MARS, Kriging, or RF. For both variants, Kriging performed best. Therefore, it was chosen for the final comparison of the SPOT variants. Standard SPOT determines a design point, whereas MSPOT generates a set of (Pareto optimal) design points. Since good design points, i.e., design points with a low $\overline{Y}$ value, are expected to have a low associated standard deviation (cf. results received for Case Study I), the design point with the best $\overline{Y}$ value was chosen from the Pareto front for the final comparison with SPOT. The MSPOT approach performed equally good or even slightly better than single criteria SPOT on every test function.

5. CONCLUSION AND OUTLOOK

A multi-criteria approach to SPO was outlined in this paper. It was shown that MSPOT can be applied successfully to solve MCO problems with a strictly limited budget.

CONCLUSION 1. *On lowest budgets, stated earlier to be most promising for* MSPOT*, it is shown that* MSPOT *methods outperform NSGA2 or SMS-EMOA on a majority of test functions.* □

Moreover, MSPOT was applied to single objective algorithm tuning, by considering the standard deviation of results as a second objective. Both SPOT and MSPOT were able to find good parameter settings. Results indicated that there is a high correlation between standard deviation and solution quality if the solution is in the vicinity of the optimum of these problems. It could be observed, that MSPOT can find better solutions than single objective SPOT on this problem type.

CONCLUSION 2. *Integrating the standard deviation of a solution as a second optimization criterion into the search process of SPO can be beneficial.* □

CONCLUSION 3. *If the algorithm improves during the optimization, the final $\overline{Y}$ values have a small standard deviation. If the optimization of the algorithm fails, the standard deviation remains relatively high.* □

Although conclusion 2 requires further investigation, we are optimistic that enhanced MSPOT variants might result in a performance boost.

The proposed MSPOT approach should be further improved: Several existing SPOT features can be integrated into MSPOT, e.g., an adaptation rule for the number of repeats on noisy problems or an optimization on the surrogate models. Moreover, the choice of the population sizes for the internal optimization of the surrogates should be independent of the used sequential budget. Additionally, MARS can be used with more sophisticated parameterizations. Using a more varied selection of test problems might also improve the relevance of the results found. Finally, a main focus of further research will be to test MSPOT on real industrial problems. Such applications are the driving force behind this research.

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