Self-adjusting surrogate-assisted optimization techniques for expensive constrained black box problems

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Chapter 10

Conclusion and Outlook

10.1 Contributions

The primary goal of this thesis was to develop new constrained optimization algorithms which work reliably on a broad set of problems without the necessity of extensive parameter tuning to the problem at hand. To solve real-world COPs in a realistically affordable time, it is crucially important to use efficient techniques, i.e needing less than $50d$ function evaluations where d is the dimension of the problem. In this thesis, two new surrogate-assisted constrained optimization techniques, namely SACOBRA and SOCU, were proposed. SACOBRA, which has a self-adjusting parameter control capability, takes benefit of the radial basis function interpolation technique to model the expensive objective and constraint functions. To the best of our knowledge, SACOBRA is the most efficient derivative-free constrained solver on a large set of constrained optimization problems, the so-called G-problems and MOPTA08 from the automotive industry.

SOCU utilizes Gaussian process aka Kriging as surrogate for modeling the objective function and the probability of feasibility. SOCU, which is a constrained optimizer employing the efficient global optimization methodology (EGO), outperforms the other EGO-based constrained optimizers, although its overall performance is not as good as SACOBRA on the higher dimensional benchmarks tested in this work.

The main ingredients of SACOBRA contributing to its good performance on a widely varying set of constrained optimization problems can be listed as follows:

- Self-adjusting parameter control capability described in **Ch. 3**.
- Equality handling approach introduced and investigated in **Ch. 4**.
- Online model selection mechanism discussed in **Ch. 8**.

Ch. 3 describes the self-adjusting parameter control functionality of the SACOBRA framework in detail. In this chapter we collected evidence supporting that each of the adaptive control elements of the SACOBRA play a role in boosting up the overall performance of SACOBRA over a large set of COPs with various characteristics. All the suggested control elements work automatically without any prior knowledge about the problem but based on the information gathered about the black box functions after the initialization step or within the optimization procedure in an online manner. The self-adjusting control elements in SACOBRA can be categorized into two groups: (I) automatic linear or nonlinear transformation of the objective and constraint functions (II) adjustment or selection of parameters which control the exploration/exploitation rate depending on the type of the problem. **Bottom line:** SACOBRA, the derivative-free surrogate assisted constrained optimizer, unlike many other optimization techniques, does not require a parameter tuning procedure at hand. The sensitive parameters in SACOBRA are automatically controlled based on the features that can be extracted from the limited information gained after initialization and during the optimization procedure. SACOBRA is able to successfully solve about 80% of the G-problems with a fixed configuration and without any further parameter tuning.

To efficiently handle equality constraints, SACOBRA uses a gradually shrinking feasibility margin, then a refine mechanism tries to move the found solution within the feasibility margin toward the actual feasible subspace by minimizing the sum of the squares of the equality constraint surrogates. SACOBRA with the equality handling extension is capable of finding near-optimal solutions with small constraint violation ($< 10^{-4}$) for 8 of the 11 G-problems with equality constraints[1], efficiently. To the best of our knowledge there are no other COP solvers that can produce such accuracy in less than 500 function evaluations for the challenging G-problems. Assessing the performance of SACOBRA compared to the other constrained solvers in a fair manner was not straight forward. This was because other works often report solutions with better objective values than the true optimal value without reporting the amount of constraint violation. Reporting a set of Pareto-optimal solutions, minimizing both objective function and maximum violation, enables a fair comparison between different algorithms and it gives the users the possibility to choose the most suitable solution based on their application. **Bottom line**: 1. SACOBRA with equality handling, benefiting from surrogate modeling and the gradually shrinking feasible margin combined with a refine mechanism, can approach the optimal solu-

[1] The three unsolved problems G20, G21 and G22 are very challenging for most of the constrained solvers due to their high dimensionality and number of the active constraints. The true optimal solutions for G20 and G22 are not known.

tions of most of the G-problems with equality constraints significantly more efficient than other constrained solvers. 2. It is recommended to report a set of Pareto-optimal solutions for black box COPs with equality constraints, instead of a single solution.

Since there are many different types of radial basis functions that can be used for the RBF interpolation one could ask: "Which RBF should I use to model a function as accurate as possible with a limited number of evaluated scatter points?". The answer to this question is not trivial and it depends on many factors, e.g. type of the function to model, number of available points and the way these points are distributed in the input space, some of which are not available in the black box expensive setup. As it is discussed and referred in **Ch. 8**, there are studies indicating that different RBFs perform differently on different functions. SACOBRA initially used cubic RBFs to model objective and constraint functions. However, the fact that in most cases real-world COPs have objective and constraint functions of different types and nature, motivated us to develop an online model selection mechanism which chooses the best fit for any of the objective and constraint functions during the optimization process. The online model selection successfully improves the overall performance of SACOBRA on the whole set of 24 G-problems. Our investigation about the effectiveness of this approach compared to the SACOBRA with a fixed RBF reveals two main advantages: 1. COPs which have objective and constraint functions of different types clearly benefit from using different types of RBFs for their objective and constraints functions. 2. the dynamic nature of the proposed model selection allows to update the best model type for each function when the number and distribution of the points change. **Bottom line:** It is beneficial to use different RBF types for modeling different functions at different stages of the optimization procedure and it is possible to do it in an efficient manner. This approach boosts SACOBRA's performance by 10% on the whole set of 24 G-problems. Clearly, the online model selection mechanism can be applied to any other sequential surrogate-assisted optimizer.

In **Ch. 7** we bring a brief comparison between the Kriging and RBF interpolation. Although the RBF interpolation does not provide any uncertainty measure by its nature, we formulated an uncertainty measure for them by means of analogy to Kriging. So that SOCU, modeling the probability of feasibility, can also utilize any arbitrary RBF kernel including, cubic RBF, augmented cubic, etc. Comparing two SOCU variances one with the augmented cubic RBF and the other one with Kriging as the modeling technique, depicts that using RBF kernels is beneficial for SOCU in terms of efficiency and reliability.

10.2 Future Directions

Although SACOBRA can locate near-optimal solutions for most of the tested benchmarks with a small number of function evaluations, it fails – like other surrogate-assisted optimizers do – to solve COPs with highly multimodal objective functions. Development of surrogate-assisted optimizers which can provide reasonable models for highly multimodal functions remains a challenge and an interesting direction for further research.

Automatic selection of the most effective algorithm for solving an optimization task known as algorithm selection problem [146] is a hot topic in the optimization community. However, not many works are devoted to algorithm selection for *expensive constrained optimization problems* and most of the existing approaches rely on landscape analysis determined by features which demand many function evaluations in the search space. Development of efficient algorithm selection procedures with features especially designed for surrogate-assisted constrained solvers like SACOBRA is a possible future path.

Not all the challenging real-world optimization tasks can be formulated as single-objective optimization problems. The development of constrained or unconstrained multiobjective solvers is an attractive field in the optimization community as it is a relevant problem for many applications in practice. Extending SACOBRA to handle multiobjective problems efficiently with the assistance of RBF surrogates can be a relevant future direction. Recently, de Winter et al. [180] achieved promising results in solving a multiobjective constrained optimization problem (a ship design problem) by means of their proposed surrogate-assisted optimization technique which utilizes SACOBRA in combination with the S-Metric-Selection-based Efficient Global Optimization (SMS-EGO) algorithm.

Furthermore, noisy optimization problems cannot be handled with SACOBRA in its current form because SACOBRA mainly works with RBF interpolation. Adapting SACOBRA to the noisy setup is another important possible future work as many real-world problems are defined in noisy environments. Using RBF approximation instead of interpolation and also considering the uncertainty measure that was determined for RBF models in analogy to Gaussian process in Ch. 7 can be a starting point to this direction.