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

Bagheri, S.

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Abstract

Optimization tasks in practice have multifaceted challenges as they are often *black box*, *subject to multiple equality and inequality constraints* and *expensive to evaluate*. The efficiency of a constrained optimizer has a crucial importance when it comes to selecting a suitable method for solving real-world optimization problems from industry with strict limitations of resources. In this dissertation we try to deal with the mentioned manifold challenges of the real-world optimization problems all at once.

The primary concern of this work is to develop new black box optimization algorithms which are generic enough to successfully handle a broad set of constrained optimization problems (COPs) *efficiently* and *without requiring apriori parameter tuning for different classes of the problems*. To achieve this goal we benefit from two main conceptual components in the development of new constrained solvers: 1. utilizing surrogate modeling techniques to use the limited available information about the black box functions as efficient as possible, 2. automatically adjusting sensitive problem-dependent parameters based on the information gained about the problems during the optimization procedure. The quality of the surrogates is also improved through novel self-adjusting procedures. This work eventuated in the development of two surrogate-assisted constrained solvers: SACOBRA and SOCU. It turns out that SACOBRA outperforms most other COP-solvers in solving the well-known G-problem suite and MOPTA08 (a COP from automotive industry), if the number of function evaluations is strongly limited.

Assuming that the black box objective and constraint functions have a structure, though unknown, makes the usage of mathematical models as surrogates meaningful. Both of the mentioned optimization frameworks benefit from employing surrogate models as a tool to predict the hidden structure of the black box objective and constraint functions. SACOBRA uses radial basis function interpolation (RBF) to model the objective and constraint functions. Investigating the effectiveness of the RBF surrogates (Ch. 3) yield several self-adjusting mechanisms to enhance the modeling quality. The online model selection mechanism (Ch. 8) is another self-adjusting element of SACOBRA, automatically selecting the best type of RBFs for each function during the optimization procedure.

SOCU (Ch. 5-6) is based on Efficient Global Optimization (EGO)¹ modified for constrained problems. The main distinction between SOCU and other EGO-based constrained solvers is SOCU's improved ability to direct the search toward the feasibility boundaries of the active constraints, where the optimal solution is located. Al-

¹Efficient Global Optimization (EGO) is aka Bayesian optimization.

though SOCU outperforms other EGO-based constrained solvers, it cannot compete with SACOBRA on COPs with higher dimensions. To gain more insights about both algorithms, we studied the similarities and differences of RBF and Kriging (Ch. 7).

The efficient equality handling approach in SACOBRA benefiting from surrogate models and a shrinking feasibility margin combined with a novel refine mechanism contributes to finding near-optimal solutions with high accuracy for most of the G-problems (Ch. 4). Finding a fully feasible solution by means of numerical methods for COPs with equality constraints is impossible. Therefore, it is difficult to compare the performances of different algorithms, as we should consider two values for each solution: its level of the constraint violation and objective value. To solve this dilemma we recommend to report a set of Pareto-optimal solutions for COPs with equality constraints optimizing both constraint violation and objective value.

To tackle the obstacles faced by SACOBRA in efficiently optimizing functions with high-conditioning, a self-adjusting online whitening algorithm attempts to improve the modeling phase of SACOBRA gradually as it learns more about the functions during the optimization procedure (Ch. 9).