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

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Summary

Real-world optimization problems can be found everywhere from day-to-day tasks to complex scientific, industrial or business problems. In many engineering fields development of accurate simulation software, replacing real experiments, provided the possibility of finding an optimal design for large complex systems which are highly parametrized. Searching for an optimal design is often subjected to multiple constraints such as geometrical limitations, stability, safety, budget, etc., making only a subset of designs feasible. Industrial design optimization aka simulation-based optimization refers to a class of problems where their objective and/or constraint functions are black box meaning that they do not have an explicit algebraic formulation. The fact that the objective and constraint function of such problems can only be evaluated through time-expensive simulation runs, is why efficiency of an optimizer has critical importance in this field. Therefore, we can state that many real-world optimization problems are *black box*, *expensive* to evaluate, *subject to multiple constraints* and *high-dimensional*. The main focus of this thesis is to develop suitable optimizers to tackle the mentioned challenges in an efficient manner.

The attempts to solve real-world optimization problems are often involved with breaking down the problems and handling each mentioned challenge in an isolated fashion. In **Chapter 2** we give a brief survey about the existing optimization methods suitable for addressing black box unconstrained and constrained optimization problems. Very limited studies are devoted to address all the demanding challenges of the real-world optimization problems simultaneously.

In this dissertation we introduce two methods for solving black box expensive constrained optimization problems (COPs). The introduced solvers are evaluated on two real-world COPs and a set of 24 well-studied toy problems known as the G-problems suite [107]. MOPTA08 [92] is a large scale mass optimization problem in the auto industry. This problem which was introduced by a technical fellow at General Motors, has a 124-dimensional space with 68 nonlinear black box constraints which are the output of the crash simulation. In the ideal case the constraint functions can be computed 60 times a day in practice. It is desired to find a design with 10% to

20% reduced mass within one month which means the maximum number of function evaluations is limited to $60 \times 30 = 1800$. The second real-world COP used in this dissertation is an airfoil design problem aiming at minimizing the aerodynamic drag force subject to multiple equality and inequality constraints, as it is described in **Chapter 5**.

SACOBRA, standing for *self-adjusting constrained optimization by radial basis function interpolation*, is an efficient technique using RBF interpolations as surrogates for objective and constrained functions which is introduced in **Chapter 3** of this thesis. This optimization framework is able to automatically control some of its important hyperparameters without any prior information about the problems. SACOBRA is able to successfully solve about 80% of the G-problems with a fixed configuration and without any further parameter tuning. This being said, SACOBRA outperforms other state-of-the-art algorithms in optimizing MOPTA08 and G-problems. In **Chapter 4** the SACOBRA framework is extended to handle equality constraints as well as inequality constraints. Cubic radial basis function interpolation has shown strong performance as surrogate in the SACOBRA optimization framework. However, no theoretical or practical evidence suggested that cubic RBFs are the best choice. We have developed an online model selection procedure for SACOBRA to automatically choose the best type of radial basis function during the optimization procedure in **Chapter 8**. This approach boosts SACOBRA's performance by 10% on the whole set of 24 G-problems. The online model selection mechanism can be applied to any other sequential surrogate-assisted optimizer.

A second optimization approach, the so-called SOCU, is introduced in **Chapter 5**. The name SOCU stands for *surrogate-assisted optimization encompassing constraints and uncertainties*. SOCU which utilizes a probabilistic modeling technique (Kriging aka Gaussian Processes,) as surrogates, is an extension to the efficient global optimization algorithm [90] (EGO) for handling optimization problems with constraints. To our best knowledge it is the first time that an EGO-based optimizer is evaluated on the challenging G-problem-COPs. SOCU performs better than the Kriging-based constrained solvers of Schonlau [159] due to its plugin control ability. However, it could only compete with SACOBRA on the low-dimensional problems and early iterations.

RBF interpolation used in SACOBRA and **Kriging** used in SOCU are both common choices of modeling techniques for surrogate-assisted optimization frameworks. Although both methods come from very different origins, they have undeniable similarities. Some similarities and differences between RBF and Kriging are mentioned in **Chapter 7**. Kriging unlike the RBF interpolation, provides an uncertainty measure, indicating how uncertain the model at each point is. This property makes Kriging a popular choice for many optimizers, especially efficient unconstrained solvers like SOCU which employ probabilistic concepts. Although the RBF interpolation does not provide any uncertainty measure by its nature, we formulated an uncertainty measure for any arbitrary RBF kernel by means of analogy to Kriging in **Chapter 7**.

Providing a reasonably good surrogate model for functions with high-conditioning is a big challenge. Such functions have a high ratio of steepest slope in one direction to flattest slope in another direction. In **Chapter 9** we try to address the challenges that SACOBRA faces in solving optimization problems with high conditioning objective functions. We develop an online whitening approach (OW) for SACOBRA trying to transform the functions with high-conditioning to easier functions to model. SACOBRA with the online whitening approach (OW) is able to find solutions with significantly better optimization errors. Although a great number of function evaluations are imposed by the proposed OW mechanism, most of them are parallelizable. SACOBRA+OW outperforms SACOBRA in addressing the noiseless BBOB problems [58] with high-conditioning.