Model-assisted robust optimization for continuous black-box problems

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CHAPTER 1

Introduction

Solving a real-world optimization problem entails dealing with uncertainties and noise within the system, or a model of the system, for which optima are sought. Due to various reasons, various types of uncertainties and noise can emerge in optimization problems. These uncertainties and noise can alter the problem landscape, and affect the practical applicability of the optimal solutions found by the algorithms. Hence, for practical scenarios, optimization methods are needed which can deal with these uncertainties, and solutions have to be found which take into account the impact of the unexpected drifts and changes in the optimization setup. The practice of optimization that accounts for uncertainties and noise is referred to as *robust optimization* (Ben-Tal et al., 2009).

In real-world engineering applications, e.g., automobile manufacturing, building construction, and steel production, finding a robust solution, i.e., a solution whose performance is not greatly affected by the uncertainties in the optimization setup, is crucial due to the potentially serious impact in case of a failure. Despite the significance, however, achieving robustness in modern engineering applications is quite challenging. Some of the most important reasons for that include the variety of problem landscapes, high dimensionality, the type and structure of the uncertainty, and the robustness formulation or criterion among others (Gabrel et al., 2014). In practice, the optimization scenarios in these applications are treated as *black-box problems*, which need to be efficiently solved in the face of uncertainty and noise.

Most of the approaches to efficiently solve black-box problems fall under the category of *direct-search methods* (Lewis et al., 2000), such as *evolutionary algorithms* (EAs) (Bäck and Schwefel, 1993), and *surrogate-assisted optimization* (SAO) (Forrester et al., 2008). This thesis emphasizes on SAO to efficiently solve numerical black-box problems, subject to uncertainty and noise. Note that SAO refers to the utilization of statistical models while solving expensive to evaluate black-box problems. These statistical models are referred to as the *surrogate models* or the *meta-models* (Keane et al., 2008). The basic idea behind SAO is to replace the actual (expensive) function evaluations by the predictions of these statistical models, which is desirable if the optimization problem under consideration is hard to solve directly. The abstraction provided by the surrogate models is useful in multiple situations. For instance, it can simplify the task to a great extent in simulation based modeling and optimization, i.e., where a non-deterministic simulator replaces the actual (physical) system (Sóbester et al., 2014). Surrogate models can also provide practically useful insights about the *search space*, e.g., space visualization and comprehension (Forrester et al., 2008).

It is worthwhile to note that SAO was initially utilized to find the nominal solution of an optimization problem (Schmit Jr and Farshi, 1974; Barthelemy and Haftka, 1993), without taking into account the unexpected drifts and changes in the optimization setup. However, this is problematic for many real-world scenarios, since uncertainty can alter the practical applicability of the optimal solutions. Therefore, a natural question arises on the suitability of SAO to find optimal solutions which are still useful in the face of uncertainty and noise. This thesis focuses on the applicability of SAO in this context. The most important research questions that we address in this thesis are:

1. Is surrogate modeling suitable to find robust solutions efficiently[1]?
2. How can one select the modeling approach and the sampling plan to find robust solutions via surrogate modeling?
3. What is the impact of external factors, such as the noise level – the scale of the uncertainty, the problem landscape, and the dimensionality, on the applicability of surrogate modeling in this context?
4. What is the impact of robustness formulation/criterion in efficiently solving black-box problems subject to uncertainty and noise, and which robustness formulations are recommended to practitioners with regards to computational efficiency?

[1] The notion of efficiency is based on the utilization of computational resources, and would be further discussed in Chapter 2.

1.1 Robust Optimization

In the first half of the twentieth century, Sir Ronald A. Fisher made efforts to grow larger crops in the face of varying weather and soil conditions (Fisher, 1936). His work comprised the basic techniques of *design of experiments* (DoE) and *analysis of variance* (ANOVA), which were later enhanced by several statisticians (Plackett and Burman, 1946; Rao, 1946; Cox and Cochran, 1957). The Japanese engineer Taguchi employed similar techniques for quality improvement of industrial products and processes in 1950s and 1960s. Taguchi's work, referred to as *robust design*, was virtually unknown outside Japan until the 1980s when he traveled to the United States and introduced his concept, which became popular afterwards (Taguchi and Phadke, 1989; Parr, 1989).

In Taguchi's framework of robust design, three different types of parameters can be distinguished. The first type of parameters are referred to as the controllable parameters, since they can be chosen or controlled by the designer during the process of optimization. The second category of parameters are known as the noise parameters, which serve as the source of variation in system's performance. Note, however, that, while the variation in these parameters is beyond the designer's control, they can be known or describable in the form of probability density functions. The third category of parameters are known as the system constants. The overall goal of the robust design in Taguchi's methods is to determine the optimal settings of the control parameters, such that the resulting process or product performance is insensitive to the variations originating from the noise parameters (Taguchi, 1995).

This manifestation of robust design was based on classic DoE techniques, where all control variables were altered according to an orthogonal array (Rao, 1946), which was referred to as the *inner array.* At each control variable setting, the noise variables were altered according to a second orthogonal array, which was referred to as the *outer array.* Based on the combinations of the inner and the outer arrays, the response data was used to estimate the process mean and variance. Both of these statistics, namely the mean and the variance, were then combined to give rise to a single quantitative measure, which was referred to as the *signal-to-noise-ratio* (SNR) (Johnson, 2006). SNR was further used to perform a standard ANOVA, and those control variable settings were identified which yielded the most stable performance. Taguchi's work started a process which made aware the importance of parameters variations to engineers and designers. His work has been reviewed, criticized, and enhanced throughout the years (Pignatiello Jr, 1988; Pignatiello Jr and Ramberg, 1991; Goh, 1993).

Different from Taguchi's work, the problem of dealing with uncertainties and noise consisted of a number of variants in *operations research*. Studies that considered uncertainty in the optimization model date back to the work of Dantzig in 1955 (Dantzig, 1955), and Wets in 1966 (Wets, 1966). Today, approaches dealing with uncertainties can be found in various settings in the scope of *mathematical programming*, such as in the form of stochastic programming (Kall et al., 1994), under the term robust optimization (Mulvey et al., 1995; Ben-Tal et al., 2004; Bertsimas et al., 2011), and in the scope of fuzzy programming (Bellman and Zadeh, 1970), which includes the two types of flexible programming (Zimmermann, 1975; Tanaka et al., 1973), and possibilistic programming (Tanaka and Asai, 1984). A survey of different mathematical programming classes in the context of robust optimization is provided by Sahinidis (Sahinidis, 2004).

Within the scope of numerical black-box optimization, and particularly in the field of surrogate modeling, there has been an increasing interest for methods that deal with uncertainty and noise. Earlier work by Jurecka (Jurecka, 2007) focused on the application of surrogate modeling for structural optimization problems, whereas the work of Rehman (Rehman, 2016) emphasized on the application of integrated electronics. Both of these works contributed extending the *Bayesian optimization* approach (Jones et al., 1998) to the robust scenario with a particular focus on computational efficiency. Some of the most important challenges and opportunities highlighted in the literature (Rehman, 2016; Jurecka, 2007; Beyer and Sendhoff, 2007; Kruisselbrink, 2012) form the starting point of this thesis. Our research questions, introduced earlier, are based on these points. These points are summarised in the following.

- Surrogate modeling was initially utilized to find the nominal solution of a black-box problem. Its validity to find a robust solution needs further empirical evidence. In particular, the impact of some of the most important factors, e.g., the type, structure, and the scale of uncertainty, the corresponding robustness formulation, the choice of the modeling technique, the dimensionality, and the problem landscape, should be considered (Jurecka, 2007; Rehman, 2016).

- Regarding the computational tractability of surrogate modeling to find robust solutions, empirical evidence on some of the most important details, e.g., the sample size, and the appropriate computational budget, is lacking (Jurecka, 2007).

- Solving high dimensional black-box problems with surrogate modeling is quite challenging due to the computational complexity involved (Shan and Wang, 2010).

- Bayesian optimization is a global-search strategy designed for expensive to evaluate black-box problems, and has been extended to the robust scenario. Within the scope of *robust Bayesian optimization*, an important contribution in the literature would be to propose, evaluate, and compare the sampling plans to sequentially update the surrogate model in a region of interest based on different robustness formulations/criteria (ur Rehman et al., 2014).

- Finding a robust solution requires additional computational resources as opposed to finding a nominal solution, since the optimizer has to take into account the impact of uncertainty and noise as well. This need for additional computational resources is referred to as the "computational cost of robustness" (CCoR) in this thesis. CCoR depends on the formulation of the robustness, and could be an important factor in efficiently solving the problem. Ranking and evaluating some of the widely applied robustness formulations based on CCoR would be a nice contribution to the literature, as it would help practitioners choose a suitable robustness criterion with regards to computational efficiency.

1.2 Organization and Contributions

The organization of this thesis is as follows. The motivation, research questions, and major contributions of each chapter are briefly introduced, followed by a list of publications resulting from this research.

Chapter 2 provides the technical background and context for robust optimization. Starting with black-box optimization and related material in Section 2.1, we provide a concise overview on uncertainty and noise in Section 2.2. Next, surrogate modeling is defined in Section 2.3.

Chapter 3 deals with the applicability of surrogate modeling to find robust solutions with the help of a "one-shot optimization" strategy. In this chapter, Section 3.1 answers the question regarding the training sample size, modeling techniques, effect of the type and structure of the uncertainty, and quality of the robust solution. In the following section, we discuss how to alleviate the "Curse of Dimensionality" in surrogate modeling. To answer our questions in this chapter, two empirical studies are conducted and presented. The results of these studies are published as:

Ullah, S., H. Wang, S. Menzel, B. Sendhoff, and T. Bäck (2019). An Empirical Comparison of Meta-Modeling Techniques for Robust Design Optimization. In *2019 IEEE Symposium Series on Computational Intelligence* (SSCI), 2019, pp. 819-828.

Ullah, S., D. Anh Nguyen, H. Wang, S. Menzel, B. Sendhoff, and T. Bäck (2020). Exploring Dimensionality Reduction Techniques for Efficient Surrogate-Assisted optimization. In *2020 IEEE Symposium Series on Computational Intelligence* (SSCI), 2020, pp. 2965-2974.

Chapter 4 deals with the applicability of the Bayesian optimization algorithm to the robust scenario. In particular, Section 4.1 provides an overview of the existing literature for BO and the so-called infill criteria. Section 4.3 empirically compares the performance of the so-called *Moment-Generating Function of the Improvement*, which is an infill criterion extended to the robust scenario. For the baseline, the so-called *Expected Improvement* criterion is chosen, which has already been extended to find robust solutions. The publication reports the results in this chapter:

Ullah, S., H. Wang, S. Menzel, B. Sendhoff, and T. Bäck (2021). A New Acquisition Function for Robust Bayesian Optimization of Unconstrained Problems. In *2021 Genetic and Evolutionary Computation Conference Companion* (GECCO 21 Companion), New York, NY, USA, pp. 1344-1345.

Chapter 5 provides a novel perspective on the computational cost for achieving robustness. Note that it has been observed in the literature that finding a robust solution is computationally more expensive than finding a nominal solution. The needs for additional computational resources are determined by the robustness formulation/criterion among others. Because of this, Section 5.2 conducts an empirical study which measures the running (cpu) time for some of the widely adopted robustness formulations on a wide range of test scenarios. Based on the findings in this section, these robustness formulations are ranked with respect to each other. These rankings provide a new perspective to practitioners for choosing the robustness formulations in practical scenarios with regards to computational efficiency. The results of this investigation have been published as:

> Ullah, S., H. Wang, S. Menzel, B. Sendhoff, and T. Bäck (2022). A Systematic Approach to Analyze the Computational Cost of Robustness in Model-Assisted Robust Optimization. In *Seventeenth International Conference on Parallel Problem Solving from Nature* (PPSN 2022), pp. 63-75.

Chapter 6 focuses on benchmarking the performance of the surrogate modeling techniques, introduced earlier in the thesis, on a real-world engineering case study. To this end, a case study focusing on the optimization of car hood designs is investigated for both the “one-shot optimization” strategy and the Bayesian optimization algorithm. The results from this case study validate some of the earlier findings in the thesis and provide a novel perspective regarding the applicability of surrogate modeling in robust optimization.

Chapter 7 provides the overall summary of the thesis, alongside major challenges and opportunities pertaining to robust optimization.