Evolution strategies for robust optimization

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Chapter 1

Introduction

When solving real-world optimization problems a frequently encountered difficulty is the presence of uncertainties and noise within the system for which optima are sought. Due to various reasons, various types of uncertainties and noise can arise in optimization problems. Hence, for real-world scenarios, optimization methods are needed that can deal with these uncertainties and solutions ought to be found that are not only optimal in the theoretical sense, but that are also practical in real life. The practice of optimization that accounts for uncertainties and noise is often referred to as *robust optimization*.

Evolutionary Algorithms (EAs) form a class of optimization algorithms that use the principle of evolution to find good solutions to optimization problems. The paradigm of *evolutionary computation* is simple and effective; take a population of candidate solutions for the optimization problem and simulate the process of evolution to evolve the population toward better solutions. With applications in various real-world settings, Evolutionary Algorithms are well-established and have proven to be powerful for optimization, especially for complex problems that are difficult or impossible to solve analytically.

Evolutionary Algorithms are originally proposed for solving optimization problems that are not affected by uncertainties and noise. However, natural evolution seems to be inherently robust when viewing it as an optimization process, because uncertainty and noise are indispensable parts of nature. Being inspired by evolution in nature, one question is therefore to what extent the natural mechanisms adopted by Evolutionary Algorithms make them robust against uncertainties and noise. Additionally, when acknowledging the limited precision of natural evolution, the challenge is to make Evolutionary Algorithms even more effective in the scope of robust optimization.

In this work we will study the application of Evolutionary Algorithms, and in particular *Evolution Strategies*, in the context of robust optimization. The main questions that we will try to answer are: What is robust optimization and how does it relate to the traditional view on optimization? In what ways can noise and uncertainties emerge within an optimization model? To what extent are Evolutionary Algorithms indeed robust against uncertainties and noise in the optimization model? What can be done to fix or improve the behavior of Evolutionary Algorithms when dealing with uncertainties and noise?

1.1 A Brief History

The concept of robust (design) optimization originated from the concept of *robust design* in industrial engineering. The introduction, or better, popularization of this concept is generally attributed to Taguchi [Tag78, Tag86, Tag89]. Taguchi stated that for product design engineering, a product should be designed not only for optimal performance, but also as to make the performance as insensitive as possible to variations that are beyond the designer's control. He proposed a method based on simple experimental designs and *loss functions* to incorporate the notion of quality or performance robustness into the process of design engineering. Taguchi bundled his ideas in a design method called the *Taguchi method* (see e.g., [Pha89]). Although the methodologies proposed by Taguchi have received much criticism [BST$^+$88, AMB$^+$92] and are considered to be outdated [CWZ99], the impact of the robust design philosophy cannot be neglected. The general aim of trying to take uncertainty and noise into account within the scope of product development has become a standard part of modern engineering [Par07].

In modern engineering, the increasing use of computer models to virtually test (parts of) designs has also led to increased interest in computational optimization techniques to aid the design process [EH02]. However, classical optimization methods focus mainly on finding optimal solutions for exact, noise-free systems. Due to the frequently noisy and uncertain nature of real life, the increased application of optimization techniques for real-world applications led to the awareness that there are a number of problems that require ways of incorporating the notion of robustness in the measures of solution quality (which is the leading principle of robust design) in optimization techniques [Tro97, TAW03].

As noted by Trosset [Tro97], robust optimization is only a part of the broader concept of robust design. The general aim of obtaining high quality products often involves *design of experiments* methods and *sensitivity analysis* where the optimization is performed manually by means of statistical analysis. Only in some cases automated optimization is used to aid the design process, and robust optimization methods can be applied to find robust solutions.

However, the inverse can also be said to be true; although the concept of robust optimization seems to borrow its right of existence directly from the concept of robust design, its context is much broader than only finding solutions which are stable under varying conditions. Beyer and Sendhoff [BS07] consider in their overview paper not only the robustness of the designs (or, in the scope of optimization, the robustness of optimal solutions), but also the robustness of the optimization process itself. Hence, robust optimization also deals with uncertainties of the optimization model, such as noisy output, and uncertainty within the optimization model, such as aiming to find robust optima. Also other studies, such as [SJ08] and [JB05], consider a broader view of uncertainties and noise in the complete optimization model. The work of

[SJ08] is particularly worthwhile mentioning as it presents a large number of applications of robust optimization techniques within the field of mechanical engineering.

In Operations Research, the problem of dealing with uncertainties and noise comprises a number of variants. Studies that consider uncertainty in the optimization model date back to the work of Dantzig [Dan55] in 1955 and Wets [Wet66] in 1966. Today, approaches dealing with uncertainties can be found in various settings in the scope of mathematical programming; in the form of *stochastic programming* (e.g., [KW94]), under the term *robust optimization* [MVZ95, BTGGN04, BBC11], and in the scope of *fuzzy programming* [BZ70, IR00] which knows the two types of *flexible programming* [TOA74, Zim76] and *possibilistic programming* [TA84]. In [Sah04], an overview can be found of the different mathematical programming classes that deal with uncertainty and noise, and the way in which these are modeled into optimization problems.

Also in the scope of *black-box optimization*, and particularly in the field of evolutionary computation, there is an increasing interest for methods that deal with uncertainty and noise. A summary of the way in which such optimization problems are approached within this field, and references to approaches proposed in literature can be found in [JB05].

Finally, some of the challenges and opportunities stated by Sahinidis [Sah04] in an overview of robust optimization using mathematical programming techniques also hold for the broader scope of optimization under uncertainty and noise. The following list of challenges, based on those stated by Sahinidis, forms the starting point of this thesis:

- An effort should be made to construct a unified framework which combines the different philosophies of modeling uncertainty and noise within optimization problems.

- Many approaches focus solely on one particular type of uncertainty and noise, whereas real-world optimization problems can exhibit multiple types. Hybrid approaches that can deal with various types of uncertainties and noise simultaneously can be the next step of robust optimization.

- Non-standard search spaces have received limited attention within the scope of optimization under uncertainty and noise. Extending the modeling framework and also the optimization approaches such that they also allow for optimization under uncertainty and noise in other domains (e.g., graph-like spaces) is a challenging next step.

- Accounting for uncertainty and noise will lead to higher computational demands in order to obtain solutions of reasonable quality. There is an ongoing need of smart sampling and search methods that further limit the computational effort (e.g., the number of function evaluations) for solving optimization problems that are subject to uncertainty and noise.

1.2 Aim and Objectives

The first objective of the current work is to obtain a clear formulation of robust optimization. The term *robustness* is in itself a very general term, obtaining a clear view on the scope and goals of robust optimization is therefore essential. An objective emerging from this is to provide guidelines for systematic classification of various types of robust optimization problems.

The second objective is to bridge the gap from the formulation of robust optimization to the practice of robust optimization. The aim is to exemplify how to approach robust optimization problems. Moreover, we aim to study the behavior of Evolution Strategies on such problems and find how they should be adapted in order to better deal with such problems. For this, approaches from the literature and newly proposed ideas will be compared conceptually and empirically using two Evolution Strategy variants as algorithmic cores.

The third objective is to provide a framework for empirical comparison for the two robust optimization scenarios considered in this work. This is done by providing a small, focused set of benchmark problems and empirical results that can, in term, be used as benchmarks.

1.3 Overview of this Thesis

This work consists of two parts. In the first part, the aim is to form an exact conceptual picture of what robust optimization is, how it relates to traditional non-robust optimization, and what the implications are for solving real-world optimization problems. The second part of this work focuses on the application of Evolution Strategies (ES) targeted on solving real-parameter robust optimization problems. In particular two main scenarios of robust optimization are considered: *optimization of noisy objective functions* and *finding robust optima*. These are considered as frequently occurring and representative scenarios of robust optimization. For these two scenarios, the performance and possible ways of improvement of two particular Evolution Strategy instances, namely the $(5/2_{DI}, 35)$-σSA-ES and the CMA-ES, are studied.

Chapter 2 lays out the background by providing an overview on the classical view on optimization, together with frequently used terms and concepts. This chapter forms the backbone of this work.

Chapter 3 extends the classical view on optimization to a framework and definition of robust optimization. It provides a taxonomy of the different ways in which uncertainties and noise can arise within optimization problems and a unified and concise framework for their systematic classification. This chapter is partially based on insights and results previously published in [KBIvdH08, KAE$^+$09, KEB$^+$09b].

Chapter 4 introduces Evolutionary Algorithms and Evolution Strategies, therewith forming the bridge between the (robust) optimization problem specification and the practice of solving optimization problems.

Chapter 5 discusses the application of Evolution Strategies to noisy objective functions. In this chapter, the negative effects of noise on Evolution Strategies are studied and techniques to counter the effects of noise in the objective function are compared conceptually. In Section 5.4.6 an alternative type of uncertainty quantification is proposed and discussed. This chapter uses results and insights that have been published partly in [KEB09a, KRD$^+$11].

Chapter 6 focuses on a particular class of noise handling techniques, namely adaptive averaging techniques. For these techniques the main question is how these compare to straightforward ways of dealing with noisy objective functions. This chapter presents new results on accuracy limits for adaptive noise handling in Evolution Strategies with the theoretical results presented in Section 6.1 and the empirical comparisons of different noise handling schemes.

Chapter 7 focuses on the scenario of finding robust optima in anticipation of uncertainties/noise in the design variables. The goal of finding robust optima is explicitly stated and formulated in the light of the framework of robust optimization. Different techniques that are proposed for finding robust optima are reviewed and compared conceptually. This chapter merges the individual results on algorithmic schemes of [KEDB10a, KEB10, KEDB10b, KRD$^+$11] with each other and puts them into a global scope of existing studies.

Chapter 8 presents an empirical comparison of different strategies for finding robust optima. This chapter presents new results with an empirical comparison of different techniques for finding robust optima, amongst which are the algorithms presented in [KEDB10a, KEB10, KEDB10b, KRD$^+$11].

Chapter 9 closes with a summary and an outlook.

Last, but not least, **Appendix A** and **Appendix B** contain collections of benchmark problems that can be used for empirical comparison of optimization algorithms for robust optimization scenarios. Appendix A provides descriptions of benchmark problems for optimization of noisy objective functions and Appendix B provides descriptions of benchmark problems for finding robust optima. These benchmark sets are used in the empirical studies of Chapter 6 and Chapter 8, respectively. **Appendix C** provides a brief description of Kriging, which is used as metamodeling technique in algorithmic approaches considered in Chapter 7 and Chapter 8.