Algorithm design for mixed-integer black-box optimization problems with uncertainty

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Chapter 1

Introduction

1.1 Background

The automotive industry is confronted with increasing competition, requiring the manufacturers to develop technologically advanced vehicles while meeting tighter schedules. As a solution approach to succeed in this highly competitive environment, the companies combine state-of-the-art simulation technologies with the growing availability of computing resources to improve product quality, accelerate time to market and optimize costs.

An important task in the automotive industry is designing the parameters of vehicle dynamics control systems. Traditionally, this process is carried out on test tracks with the physical vehicle and relies heavily on the expertise of the engineer. However, virtual simulation environments are being developed to pre-design the parameters of a control system virtually and create a preliminary parameter configuration that can serve as the basis for the final tuning on the test track. This is accomplished by modeling the complete vehicle and its control systems. By employing optimization algorithms, the virtual pre-design can be transformed into an automated, data-driven decision-making process. The aim thereby is to provide a scalable, efficient and robust method for the industry to cope with the increasing competition.

To fully utilize these advanced methodologies, numerous open questions and challenges need to be addressed in order to tailor the process for industrial application. This thesis concentrates on the following research questions (Section 1.2). An overview of the contributions and the structure of this thesis is presented in Section 1.3.

1.2 Research Questions

This thesis is centered around a primary research question (RQ):

How can an optimization algorithm be effectively and efficiently designed to solve computationally expensive real-world problems, such as the design of vehicle dynamics control system parameters?

To address this overarching question, the thesis will delve into seven sub-questions, which are presented as the main research questions below.

The basic prerequisite in applying an optimization algorithm is the availability of a formal definition of the objective function to be optimized. Thus, the first research question arises:

RQ 1: *How can the desired behavior of the control system and the vehicle be objectified to define the real-world problem mathematically by an objective function?*

Once the optimization problem is formulated, identifying a suitable class of optimization algorithms becomes possible based on the properties of the problem. Besides these properties, the performance of an optimization algorithm is influenced by its parameters, leading to the second and third research questions:

RQ 2: *How can an optimal parameter configuration of an optimization algorithm for a specific real-world problem be determined?*

RQ 3: *Does a single parameter configuration suffice for a class of related real-world problems, such as the design of vehicle dynamics control system parameters, or is each problem unique, necessitating a tailored parameter configuration?*

Considering that tuning the parameters of an optimization algorithm is an optimization task in itself, the fourth research question is posed:

RQ 4: *What methods can efficiently determine the optimal parameters of an optimization algorithm for solving a specific optimization problem?*

Many real-world problems, including vehicle dynamics design, involve discrete parameters. This leads to the fifth research question:

RQ 5: *How can the discretization of parameter values be handled within an optimization algorithm, and how does this affect the performance of an optimization algorithm?*

Finally, the variability of the objective function due to measurement errors, external disturbances or the stochastic nature of a system must be addressed, leading to the sixth and seventh research questions:

RQ 6: *How can the uncertainty inherent in the variability of an objective function be quantified?*

RQ 7: *Can this uncertainty quantification be incorporated into an optimization algorithm to reduce computational resources?*

1.3 Contribution and Structure of the Thesis

This thesis systematically addresses the seven research questions posed in Section 1.2. Chapter 2 lays the groundwork with a comprehensive overview of the theoretical underpinnings of optimization, the intricacies of algorithm tuning and the principles of uncertainty quantification.

Chapter 3 focuses on the design of vehicle dynamics control systems. The desired behavior of two vehicle dynamics control systems is objectified to define the engineering problems mathematically by objective functions. In addition, a comprehensive dataset is created to represent real-world optimization problems for five different vehicle settings (Section 3.4). This dataset removes the need to run extensive simulations and, thus, reduces the computational cost of evaluations from several minutes to milliseconds, enabling benchmarking and algorithm design directly on the five real-world problems.

In Chapter 4, the properties of the five different real-world problems derived from the created dataset (Chapter 3) and the performance impacts of different parameter configurations on the optimization algorithms are analyzed. A method for tuning the parameters of the optimization algorithm to computationally expensive problems is presented, in which surrogate problems are used that approximate the properties of the original optimization problem. The effectiveness of this method for tuning optimization algorithms for real-world applications is validated through extensive experiments. In addition, Section 4.6 provides a comparison of different optimization algorithms in the context of parameter tuning.

In Chapter 5, the effects of discretized parameter values on the performance of optimization algorithms are analyzed. A method for handling discretization is considered. In addition, recommendations are given for adjusting the parameters of the algorithm to handle discrete variables more efficiently.

Chapter 6 presents a novel methodology that combines uncertainty quantification with optimization algorithms. This method quantifies the uncertainty in order to reduce the number of evaluations required. The effectiveness of the methodology and its potential for saving evaluations are examined using a test function and the aforementioned dataset.

In Chapter 7, the thesis is concluded with a discussion of the results and implications. Moreover, directions for future research are given.

1.4 Publications

Portions of this thesis incorporate material previously published in manuscripts by the author and collaborators, as detailed in the list of contributions below. These publications focus on aspects of the development of the method for tuning the parameters of optimization algorithms (Chapter 4) for computationally expensive real-world problems (Chapter 3). The first publication quantifies and analyzes the landscape of the optimization problem using features. The second publication examines the effect of tuning the optimization algorithm parameters on solution quality or wall-clock time. The third publication analyzes the impact of parameter discretization (Chapter 5) on the performance of various optimization algorithms. The fourth publication deals with identifying similar problems for tuning optimization algorithms. The final publication compares different optimization algorithms for optimizing the optimization algorithm.

1) André Thomaser, Anna V. Kononova, Marc-Eric Vogt, and Thomas Bäck. One-Shot Optimization for Vehicle Dynamics Control Systems: Towards Benchmarking and Exploratory Landscape Analysis. In *Proceedings of the Genetic and Evolutionary Computation Conference Companion*, GECCO '22, pages 2036–2045, New York, NY, USA, 2022. Association for Computing Machinery

2) André Thomaser, Marc-Eric Vogt, Anna V. Kononova, and Thomas Bäck. Transfer of Multi-objectively Tuned CMA-ES Parameters to a Vehicle Dynamics Problem. In Michael Emmerich, André Deutz, Hao Wang, Anna V. Kononova, Boris Naujoks, Ke Li, Kaisa Miettinen, and Iryna Yevseyeva, editors, *Evolutionary Multi-Criterion Optimization*, pages 546–560, Cham, 2023. Springer Nature Switzerland

3) André Thomaser, Jacob de Nobel, Diederick Vermetten, Furong Ye, Thomas Bäck, and Anna V. Kononova. When to Be Discrete: Analyzing Algorithm Performance on Discretized Continuous Problems. In *Proceedings of the Genetic and Evolutionary Computation Conference*, GECCO '23, pages 856–863, New York, NY, USA, 2023. Association for Computing Machinery

4) André Thomaser, Marc-Eric Vogt, Thomas Bäck, and Anna V. Kononova. Real-World Optimization Benchmark from Vehicle Dynamics: Specification of Problems in 2D and Methodology for Transferring (Meta-)Optimized Algorithm Parameters. In *Proceedings of the 15th International Joint Conference on Computational Intelligence*, pages 31–40. SCITEPRESS - Science and Technology Publications, 2023 (best paper award)

5) André Thomaser, Marc-Eric Vogt, Thomas Bäck, and Anna V. Kononova. Optimizing CMA-ES with CMA-ES. In *Proceedings of the 15th International Joint Conference on Computational Intelligence*, pages 214–221. SCITEPRESS - Science and Technology Publications, 2023