Model-assisted robust optimization for continuous black-box problems

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Abstract

Uncertainty and noise are frequently-encountered obstacles in real-world applications of numerical optimization, e.g., mechanics, engineering, economics and finance. 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. The practice of optimization that deals with uncertainties and noise is commonly referred to as robust optimization. This thesis concentrates on robust optimization with respect to the parametric uncertainties in the search variables. These parametric uncertainties are assumed to be structurally symmetric, additive in nature, and can be modeled in a deterministic or a probabilistic fashion.

Despite its significance, achieving robustness in real-world applications is quite challenging. One of the major reasons is the computational cost involved to find the robust solution. The computational cost mainly depends on problem landscape, dimensionality, type and structure of the uncertainty, and the robustness formulation or criterion among others. To achieve robustness in an efficient manner, this thesis utilizes surrogate modeling. For this purpose, several attempts are made to implement and apply surrogate modeling in robust optimization. One research stream (Chapter 3) focuses on the fundamental research questions with the help of a "one-shot optimization" strategy based on surrogate modeling. The main questions targeted in this research stream deal with the impact of factors, such as sample size, modeling technique, design of experiments, data pre-processing, structure and scale/severity of the uncertainty, robustness aim/criterion, dimensionality, and problem landscape among others. By and large, this research stream targets the practical applicability of surrogate modeling to find robust solutions

and the related difficulties thereof. To be able to answer these questions in a comprehensive manner, two empirical studies are designed.

The key findings from these studies reveal the promising nature of Kriging, Polynomials, and Support Vector Machines to construct a good quality surrogate model based on a reasonable sample size. Moreover, it is found that in the majority of the cases, surrogate modeling yields a reasonably good solution, which is very close to the baseline. Another observation from the empirical results in this context affirms the suitability of Principal Component Analysis and Autoencoders to perform dimensionality reduction in the case of high dimensional problems, albeit with some performance deterioration.

The second research stream (Chapters 4 and 5) targets more advanced research questions, such as the practicality of the Bayesian optimization approach to find robust solutions, as well as how to choose the robustness criterion/merit in practical scenarios. To investigate the applicability of the Bayesian optimization approach in this context, it is extended to account for parametric uncertainties in the search variables. Moreover, the validity of the Bayesian optimization approach to find robust solutions is investigated.

The key findings from this investigation indicate the suitability of the extended Bayesian optimization algorithm to find robust solutions in an efficient manner. Furthermore, it is found that dimensionality, and consequently the computational budget, plays a significant role in determining the performance of our approach. Lastly, we find that the "Expected Improvement" criterion and the "Moment-Generating Function of Improvement" prove to be excellent choices as the sampling infill criterion for robust optimization.

As part of the second research stream (Chapters 5), an attempt is made to answer a crucial yet unanswered question, namely how to select a robustness criterion/merit in practical scenarios with regards to computational efficiency? Another empirical investigation is carried out to answer this question in a comprehensive manner. This empirical investigation computes the running cpu time of the Bayesian optimization algorithm for five of the most common robustness criteria. The key findings from this investigation indicate the promising nature and practical applicability of "mini-max robustness" to find solutions under uncertainty with regards to computational efficiency.

The last part of the thesis (Chapter 6) deals with benchmarking the performance of the surrogate modeling approaches, 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 in detail for both, the "one-shot optimization" strategy and the Bayesian optimization algorithm. The results from this case study indicate the promising nature of Kriging and Ensemble methods, e.g., Random Forest, to effectively model the objective function in practical scenarios. Furthermore, it is found that the "Moment-Generating Function of Improvement" and the "Lower Confidence Bound" are excellent choices for the sampling infill criterion in Bayesian optimization. A short summary of the major contributions in the thesis is provided in Chapter 7, which also encompasses the list of major challenges and opportunities pertaining to robust optimization.

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