Model-assisted robust optimization for continuous black-box problems

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CHAPTER 7

Conclusion and Outlook

In this thesis, several important aspects of robust optimization (Ben-Tal et al., 2009) are empirically investigated in depth. **Chapter 1** introduces the fundamental research questions of the thesis. The first three questions are related to each other, in that they deal with the applicability of surrogate modeling to find robust solution in an efficient manner, by taking into account a list of factors such as noise level, problem landscape, dimensionality, and design of experiment. Note that the notion of efficiency in this context is based on the utilization of computational resources.

We made two attempts to answer these questions in a comprehensive manner. The first one is based on "one-shot optimization" and described in detail in **Chapter 3**. The key findings from this investigation indicate the following points.

1. Kriging, Response Surface Models (Polynomials), and Support Vector Machines construct good quality surrogate models with linear sample sizes. These models can then be utilized to estimate robust solution. The robust solutions estimated with these models are very close to the baseline.

2. Dimensionality is a detrimental factor on the quality of the surrogate models, whereas the noise level does not play a significant role in this context.

Due to the significant impact of dimensionality on the quality of surrogate models, we devote the rest of **Chapter 3** to find dimensionality reduction techniques that can be utilized for efficient surrogate modeling. To this end, we empirically compare the performance of Principal Component Analysis, Kernel Principal Component Analysis, Autoencoders, and Variational Autoencoders. Following points summarize the key findings from this study.

1. Based on the criteria of modeling accuracy, Autoencoders are the most promising dimensionality reduction technique.
2. Based on the quality of optimal solutions obtained from low dimensional surrogate models, Principal Component Analysis perform superior to the other competitors.
3. The quality of the optimal solutions obtained after dimensionality reduction can be very low in some cases. Therefore, dimensionality reduction is not always feasible.

In **Chapter 4**, we attempt to answer the first and the third research questions of our thesis with “sequential model-based optimization” framework (Jones et al., 1998). We refer to it as the “Bayesian optimization” framework, since we always employ Kriging (or Gaussian process) as the modeling technique. Here, we also consider the impact of the acquisition function to find robust solution.

Following points summarize the applicability of the Bayesian optimization approach to find robust solution.

1. The Bayesian optimization algorithm is to be extended to account for parametric uncertainty in the search variables. The extended Bayesian optimization algorithm is computationally tractable, and able to find robust solutions efficiently as backed by the empirical investigation.
2. Dimensionality and computational budget play a significant role in the performance of our extended version.
3. Noise level does not directly affect the quality of the robust solution in an adverse manner.
4. “Expected Improvement” criterion and “Moment-Generating Function of the Improvement” prove to be excellent choices for the acquisition function, as opposed to the “Lower Confidence Bound”, which is affected adversely if the dimensionality increases.
5. The evaluation of the “Lower Confidence Bound” is also computationally costlier when compared with the other two sampling infill criteria.

Chapter 5 focuses on the fourth research question of our thesis – 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?

An empirical study (Ullah et al., 2022) is conducted to answer this questions. The major findings from this study are as follows.

1. In the situations where the designer cannot afford the computational budget beyond a certain threshold, “mini-max robustness”, “mini-max regret robustness”, “expectation-based robustness”, and “composite robustness” can be utilized to find robust solutions in an efficient manner.

2. On the other hand, if the designer cannot compromise on the quality of the solution, “mini-max robustness” is the most efficient robustness criterion to be employed.

3. The average cpu time per iteration of the Bayesian optimization algorithm is lowest when “mini-max robustness” is employed.

Chapter 6 emphasizes on benchmarking the surrogate modeling approaches, described earlier in the thesis, on a real-world engineering application. To this end, we emphasize on the design optimization of car hood frames, obtained from (Ramnath et al., 2019). Our findings from this case study validate some of our earlier results, and also provide a new perspective in the applicability of surrogate modeling. For instance, we observe that Kriging and Random Forest generally perform excellently in the context of “one-shot optimization”, and the sample size can be set linearly in terms of dimensionality. Furthermore, we note that “Moment-Generating Function of the Improvement” and “Lower Confidence Bound” perform competitively as the sampling infill criteria, and that dimensionality affects the quality of the optimal solutions in an adverse manner.

7.1 Challenges and Opportunities

Robust optimization (Ben-Tal et al., 2009) has received a lot of attention in the last two decades due to the advancements in several field of engineering. For instance, shortening the product-development cycle, reducing the resource consumption during the complete process, and creating more balanced and innovative products has become a desirable outcome in the field of product engineering. To achieve this, designers have to account for uncertainties and noise in an efficient manner. Therefore, a practical approach to robust optimization is necessitated.

When accounting for uncertainties and noise, we believe "environmental variables" (or operating conditions of the product) have been overlooked in the literature. As stated earlier, they can impact the quality of an optimal design in an adverse manner. Therefore, effectively modeling the uncertainties surrounding these "environmental variables" is of huge significance.

In the context of parametric uncertainties in the search variables, the choice of robustness criterion is very important due to three main reasons: "computational cost of robustness", "price of robustness", and "problem landscape induced by the robustness criterion". We believe all three of these aspects have been overlooked in the literature. The first one of these, namely the "computational cost of robustness" has been studied in an empirical fashion in **Chapter 5**, but the findings need to be validated with real-world engineering case studies. Furthermore, the "price of robustness": the aspect of compromising on the performance/optimality to achieve robustness/stability, also needs to be systematically studied. Lastly, it may be the case that the "problem landscape induced by the robustness criterion" encompasses certain attributes, making the robust counterpart easier or more difficult to solve. We believe this aspect of robustness criterion also needs to be systematically studied.

In practical scenarios, high dimensionality poses a major obstacle in the applicability of surrogate modeling. Albeit we discuss the issue of high dimensionality at great length in **Chapter 3**, further research is necessary to validate our findings for the robust scenario. In particular, answering the following is very important:

"In the face of high dimensionality, what can be done to find robust solutions in an efficient and effective manner via surrogate modeling? Which dimensionality reduction techniques are most suitable in this context? What factors influence the performance of the dimensionality reduction techniques in this context?"

When extending the Bayesian optimization algorithm to the robust scenario, certain practical compromises have to be made, in order to effectively model the true "robust" response of the function. For instance, we assumed in **Chapter 4** that the true "robust" response of the function can also be modeled according to a Gaussian process, similar to the nominal scenario. However, this approach is not entirely rigorous, as we are not estimating the true joint posterior distribution of all search points induced by the uncertainty. Estimating this posterior distribution would be a significant contribution to the literature, as it would enable us to extend the Bayesian optimization algorithm to the robust scenario in a seamless fashion (from the nominal case).

Benchmarking the empirical performance of the Bayesian optimization algorithm in robust optimization also entails an interesting opportunity for researchers. To this end, we made an attempt in **Chapter 4**, which includes the variability in problem landscape, dimensionality, noise level, robustness and sampling infill criteria. Note, however, that, further research is necessary to cover a broad spectrum of test scenarios.

Lastly, observing the synergies between surrogate modeling and machine learning, we note that "robustness" also needs to be incorporated in machine learning. This is due to the fact that learning and mining in the presence of uncertain (industrial) data poses additional challenges for the modeling techniques. Therefore, these modeling techniques need to be extended to care for "robustness", in order to effectively account for the uncertainties present in the training data. A major contribution in this direction is to extend the Support Vector Machines to the robust scenario, based on the conceptual framework proposed in (Ben-Tal et al., 2009). Similarly, the adaptation of the "Variational Recurrent Models" to account for irregular, highly-sporadic, and asynchronous sequential data is also an important contribution (Ullah et al., 2020b) in this direction.