Optimizing solvers for real-world expensive black-box optimization with applications in vehicle design
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Summary

Optimally solving real-world expensive Black-Box Optimization (BBO) problems w.r.t. real-world constraints, such as wall-clock time and computational costs, is extremely difficult and tedious. While a variety of BBO algorithms have been introduced over the years, such as Covariance Matrix Adaptation Evolutionary Strategy (CMA-ES) and Differential Evolution (DE), a considerable function evaluation budget is usually necessary for an optimization convergence, which is less practical for real-world applications using expensive function evaluations. Automotive crashworthiness optimization using expensive Finite Element (FE) simulations in the automotive industry, for instance, is a representative example of real-world BBO problems, which is typically highly nonlinear, discontinuous, and high-dimensional. Due to the stricter regulations on road safety imposed by authorities and the fact that various features and functionalities must be integrated to better retain customer satisfaction, an efficient solving of vehicle design problems is critical, yet challenging. Meanwhile, state-of-the-art optimization approaches like Response Surface Method (RSM) and Successive Response Surface Method (SRSM) are gradually losing their effectiveness in solving the increasingly sophisticated vehicle design problems. Consequently, optimization approaches that can efficiently solve crashworthiness optimization problems have gained growing attention in the automotive industry.

Motivated to fill the gaps, we investigate an automated optimization approach for optimally solving real-world expensive BBO problems using a limited function evaluation budget within the scope of this thesis. Essentially, we aim to assist practitioners in automatically fine-tuning optimization configurations for optimally solving their applications w.r.t. real-world constraints. By exploiting some cheap-to-evaluate representative functions that belong to the same optimization problem classes as the BBO problems to-be-solved, nearly optimal optimization configurations can be identified at a relatively low computational expense, e.g., using Hyperparameter Optimization

(HPO), prior to the actual optimization runs using expensive function evaluations. Eventually, the expensive BBO problems can be efficiently solved using the fine-tuned optimization configurations.

To identify representative functions that belong to the same optimization problem classes, we consider quantifying the optimization landscape characteristics of BBO problems using Exploratory Landscape Analysis (ELA). Principally, BBO problems belong to the same optimization problem classes as test functions with similar ELA features. Based on our analysis on 20 automotive crash problem instances of different crash scenarios and problem dimensionalities, we show that the automotive crash problems belong to optimization problem classes that are different from the widely-used Black-Box Optimization Benchmarking (BBOB) functions. In other words, the BBOB functions are insufficiently representative for real-world automotive crash problems, and thus, they are inappropriate to serve as representative functions. On the other hand, the automotive crash problems are most similar to the optimization problem classes of Randomly Generated Function (RGF) created using a tree-based random function generator in terms of ELA features. In fact, we propose considering such RGFs as scalable and cheap-to-evaluate representative functions for real-world expensive BBO problems, e.g., for HPO purposes. Further investigations demonstrate that RGFs have promising potential in estimating the actual performance of different optimization configurations on unseen BBO problems. Put differently, well-performing optimization configurations for real-world expensive BBO problems can be indeed identified using RGFs as representative functions.

When evaluated on the BBOB suite, we can identify better performing optimization configurations than the default configuration using the proposed optimization approach, in line with our motivation. Remarkably, the optimal optimization configurations are even competitive against the Single Best Solver (SBS) on some BBOB functions. Here, a selection process of appropriate representative functions and a training-testing split during HPO are additionally implemented, to improve the overall robustness in fine-tuning optimization configurations. More importantly, the Bayesian Optimization (BO) configurations fine-tuned using our approach can outperform the BO default configuration and RSM for solving an automotive side crash problem in terms of the best-found-solution and convergence speed. Especially for solving complex crash functions using a limited function evaluation budget, such as a multi-pole impact problem, significantly better solutions can be found using our approach, e.g., compared to SRSM.

In conclusion, our results show that the proposed automated optimization pipeline

has an encouraging potential for an efficient solving of real-world expensive BBO problems, such as vehicle design problems. Since the proposed optimization approach can perform relatively well on the BBOB suite, covering a variety of optimization problem classes, we are confident that our approach can generalize well to other BBO domains that are sufficiently represented by the BBOB functions. With further modifications, we believe that our approach can be extended to efficiently solving other real-world expensive BBO problems, such as ship designs.