

Self-adaptive strategies for the large-scale Gray Box optimization

Despite a tremendous progress in solution techniques for large-scale problems, the demands of practical applications significantly surpass the algorithms' capabilities. Further progress is highly desired here for discrete and mixed integer linear optimization with black-box items in constraints and/or objective function. The present challenge aims to highlight a promising and demanded directions of research in this area. Advanced applications often consider systems that involve components that cannot be easily modeled using conventional algebraic expressions suitable for in-depth analysis or general-purpose solvers, like GUROBI, CPLEX or LocalSolver. These components of the system can be represented by a black-box function that must be invoked to evaluate the viability or quality of a candidate solution. Simulation models can be design for it by experts but, as a rule, spend a lot of efforts for calculations. From a practical point of view, a model incorporating black-box components as part of its design is significantly more flexible. These black-box components can be substituted for alternative ones, enabling a wide range of potential applications for the model, while preserving its overall structure and, consequently, a set of tools dealing with it. The current literature on discrete optimization models with black-box terms is scarce due to the fact that this research topic is on its very beginning [1].

Dramatic increase in the dimensions of the problems to solve provide an additional challenge. One of the most promising direction here is the development of new decompositions strategies that allow to disassemble the problem into smaller components, that can be tackled relatively independently. Due to the black box nature, the decomposition methodology, the number of components and their interdependencies are unknown and can be an area of research.

Recent advancements show the effectiveness of self-adaptation and self-tuning procedures in state of the art approaches, that allow to adapt to instances of a different nature without the help of a developer.

In its scope, the list of promising directions of work could include but not limited to:

1. Literature review on large scale optimization models with black-box terms in objective function and/or the chance constraints. All aspects related to algorithms and computational complexity are interesting and important including optimization models with deterministic or stochastic simulation models for black-box terms.
2. Development of optimization algorithms for the discrete and mixed-integer models with black-box terms. Exact methods, approximate algorithms and metaheuristics, including hybrids with classical mathematical optimization methods, are highly desirable. A posteriori upper and lower bounds for the optimal solution, if they exist, can be studied for the large-scale models.
3. Efficient decomposition strategies, that allow to seek for independent components of the problem. To be able to tackle high-dimensional problems, the efficient decomposition seems to be unavoidable. Any suggestions on methods and approaches to divide the set of variables into disjoint subsets would be of a great value.
4. Self-adaptive strategies, including, but not limited to fine tuning of numerical parameter, configuration of hyperparameters, adaptation of the search strategy, etc., are of a great interest again. Recent works show that implementation of ML\RL components into well-known heuristic schemes lead to sufficient rise in efficiency [2]. Another example of successful application of self-adaptive strategies can be found in [3] where a double-adaptive VNS approach for classical TSP is proposed.

References

1. Panos M. Pardalos, Varvara Rasskazova, Michael N. Vrahatis, Black Box Optimization, Machine Learning, and No-Free Lunch Theorems, Springer Cham, 2021
2. Yi, Wenjie and Rong Qu. "Automated design of search algorithms based on reinforcement learning." *Inf. Sci.* 649 (2023): 119639.
3. Panagiotis Karakostas, Angelo Sifaleras, A Double-Adaptive General Variable Neighborhood Search algorithm for the solution of the Traveling Salesman Problem, Applied Soft Computing, Volume 121, 2022.