Scalable Primal Heuristics Using Graph Neural Networks for Combinatorial Optimization (Abstract Reprint)

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Abstract

By examining the patterns of solutions obtained for various instances, one can gain insights into the structure and behavior of combinatorial optimization (CO) problems and develop efficient algorithms for solving them. Machine learning techniques, especially Graph Neural Networks (GNNs), have shown promise in parametrizing and automating this laborious design process. The inductive bias of GNNs allows for learning solutions to mixed-integer programming (MIP) formulations of constrained CO problems with a relational representation of decision variables and constraints. The trained GNNs can be leveraged with primal heuristics to construct high-quality feasible solutions to CO problems quickly. However, current GNN-based end-to-end learning approaches have limitations for scalable training and generalization on larger-scale instances; therefore, they have been mostly evaluated over small-scale instances. Addressing this issue, our study builds on supervised learning of optimal solutions to the downscaled instances of given large-scale CO problems. We introduce several improvements on a recent GNN model for CO to generalize on instances of a larger scale than those used in training. We also propose a two-stage primal heuristic strategy based on uncertainty-quantification to automatically configure how solution search relies on the predicted decision values. Our models can generalize on 16x upscaled instances of commonly benchmarked five CO problems. Unlike the regressive performance of existing GNN-based CO approaches as the scale of problems increases, the CO pipelines using our models offer an incremental performance improvement relative to CPLEX. The proposed uncertainty-based primal heuristics provide 6-75% better optimality gap values and 45-99% better primal gap values for the 16x upscaled instances and brings immense speedup to obtain high-quality solutions. All these gains are achieved through a computationally efficient modeling approach without sacrificing solution quality.

References

[Cantürk *et al.*, 2024] Furkan Cantürk, Taha Varol, Reyhan Aydoğan, and Okan Örsan Özener. Scalable primal heuristics using graph neural networks for combinatorial optimization. *J. Artif. Int. Res.*, 80, September 2024.