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Ph.D. Dissertation Defense

Candidate:	Mingsong Ye
Degree:	Doctor of Philosophy
School/Department.:	Interdisciplinary/Data Science
Date:	Tuesday, November 26, 2024
Time:	10:00 AM – 12:00 PM
Location:	Babbio 601
Title:	The use of Machine Learning and AI to Improve Computational Performance in Large-scale Optimization and Time Series Applications
Chairperson:	Dr. Edward Stohr, Information Systems, School of Business
Committee Members:	Dr. Choudur, Lakshminarayan, Analytics, School of Business
	Dr. Alkis Vazacopoulos, Analytics, School of Business
	Dr. Foad Pajouh, Analytics, School of Business
	Dr. Yue Ning, Computer Science, School of Engineering & Sciences

Abstract

The three essays in my dissertation proposal examine the use of machine learning and artificial intelligence (ML/AI) for performance improvement in large-scale combinatorial problems and time series forecasting.

The first essay, "*Using ML/AI to Improve Computational Performance in Large-scale Optimization Problems*" surveys recent research on the use of ML/AI techniques to improve computational performance in large-scale combinatorial optimization (CO) problems. These problems may be NP-hard or beyond. Exact and heuristic optimization algorithms have been designed to solve CO problems. However, many CO problems cannot be solved in a reasonable time by traditional approaches. I survey research on ML/AI approaches to this problem. I develop a framework for categorizing the various approaches based on whether they involve algorithm imitation or algorithm generation. The survey concludes that ML/AI approaches have promise but that a general approach to solving a broad class of CO problems has yet to be discovered.

The second essay, *"Configuring Optimization Solvers using Large Language Models."* Modern optimization solvers combine multiple algorithms to process a single optimization problem instance and have hundreds of parameters to force/disallow certain techniques and control the computation process. The chosen configuration can heavily impact optimization performance. Parameter tuning has been the subject of much previous research however the problem is difficult because of the complexity of CO problems and the weak transferability among problem instances. I examine the potential of large language model (LLM) integration to automatically set the parameters and determine the best configuration. My experimental results focusing on cutting-plane selection demonstrate the feasibility of applying LLM to parameter tuning.

The third essay, "*Uncertainty Quantification",* explores uncertainty quantification in Big Data. Uncertainty (variability) is composed of two sources: aleatoric uncertainty and epistemic uncertainty. The former is due to inherent randomness in the data, while the latter captures the uncertainty due to missing data and unmeasured confounders. We extend linear models to more complex systems to decompose uncertainty additively into epistemic and aleatoric components. Inspired by the two-sample test in statistics, we proposed a two-step learning algorithm to assess the epistemic uncertainty utilizing the reparameterization tricks in variational auto-encoder. Experimental analyses of the proposed approach are conducted for generated data and financial time series from the real world.