Hybrid quantum-classical metaheuristics for automated machine learning applications

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Summary

This thesis explores emerging and intersecting areas of research in machine learning, optimization, and quantum computing. Despite being in its nascent stages, quantum computing promises substantial theoretical and practical advances in processing power and efficiency for certain classes of problems. We start with a foundational understanding of quantum mechanics and its application to quantum computing, discussing quantum logic gates, circuits, and quantum annealing in Chapter 2. In this chapter, we also provide an overview of machine learning methods, as well as some discussion on the bias-variance trade off and the no-free-lunch theorems and their implications for machine learning and optimization.

The thesis also delves into quantum machine learning, a fast-moving research area that investigates learning tasks for which a quantum computer may prove beneficial. Chapter 3 studies how quantum annealing systems may be used to enhance feature selection towards optimization of machine learning pipelines, showing a real-world application in feature selection for vehicle price prediction to demonstrate the practical benefits of these quantum-enhanced methods.

In Chapters 4 and 5 we introduce a new method of quantum-enhanced selection for evolutionary algorithms via quadratic unconstrained binary optimization and hybrid quantum-classical solvers, illustrating their effectiveness in finding optima across various objective functions. These quantum-enhanced evolutionary algorithms are employed as metaheuristics toward hyperparameter optimization and finding optimal configurations for deep neural networks for supervised learning tasks across 34 real-world datasets. These chapters also explore how these metaheuristics may be applied towards neuroevolution of neural networks for learning control policies of reinforcement learning algorithms.

In chapter 6, the focus of the study shifts to kernel approximation methods and the role of quantum data in quantum machine learning. Characterization and com-

parison between quantum feature maps and traditional kernel methods underscore the potential of quantum kernel methods to enhance data analysis and model training processes. The exploration of sparse QUBO and quantum-enhanced estimators for Bayesian optimization highlights the practical implications of quantum advances in tackling real-world machine learning challenges, such as hyperparameter optimization of deep learning models.

Throughout the thesis, it is evident that while quantum computing offers exciting prospects for machine learning, the technology is still in its early stages, with several constraints and challenges. These include issues related to the scalability, degree of connectivity, and coherence of quantum systems. However, the ongoing improvements in quantum hardware and the novel approaches to hybridizing quantum and classical techniques suggest a promising future where these challenges may be overcome, enhancing the capabilities and efficiency of machine learning systems.

Overall, the thesis aims to demonstrate the potential intersections of quantum computing and machine learning, offering insights into how quantum and quantum-inspired technologies can be incorporated to advance the field of automated machine learning, despite the current limitations and early stage of quantum technology.