Quantum machine learning: on the design, trainability and noise-robustness of near-term algorithms

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Abstract

The past decade has brought on tremendous progress in the quest to build a quantum computer, and cloud access to first devices is starting to get available. Although these devices are still very limited in terms of the number of qubits and coherence times, their emergence has focused attention on the question of how these near-term devices can be of value. A specific type of hybrid quantum-classical algorithms, namely variational quantum algorithms, has stood out as a candidate for providing value in these early stages of quantum computing. Machine learning is believed to be a field where variational quantum algorithms can be beneficial, and they have been studied in the context of various learning tasks. Theoretical guarantees are hard to obtain for these algorithms due to their heuristic nature, so progress in this field will heavily rely on empirical discovery and evaluation of algorithms. However, many fundamental questions about successfully running these types of algorithms are still open, like how to design individual components of the quantum circuits that are used, and how to avoid pitfalls in their training. In this thesis, we study various aspects of variational quantum algorithms for machine learning, with a focus on reinforcement learning. We study the steps of the whole pipeline in training a variational quantum machine learning model on near term devices, starting at the question of how to encode classical data and read out information from a quantum circuit, and how to design the circuit itself in a problem-tailored manner. We address the question of how the classical optimization routine in this model can be tailored to quantum-specific issues in optimization landscapes, as well as how various noise sources present on quantum hardware affect the training of these algorithms. With the above, this thesis aims at contributing to the knowledge of how to train variational quantum machine learning models, in order to foster further investigation of these types of algorithms once high-performance quantum hardware will become available.

Publications

This thesis is partially based on content that was previously published by the author and collaborators in the following manuscripts, with author contributions as listed below.

1. **Layerwise learning for quantum neural networks**
   Andrea Skolik, Jarrod R. McClean, Masoud Mohseni, Patrick van der Smagt, Martin Leib
   Quantum Machine Intelligence 3.1 (2021): 1-11

   AS conceived the idea for this work and the layerwise learning algorithm. AS and JRM performed the numerical simulations. JRM defined the cost model for measuring the performance of the studied models. AS and JRM wrote the first draft of the manuscript, all authors were involved in the final editing. MM, PS, and ML supervised the work.

2. **Quantum agents in the Gym: a variational quantum algorithm for deep Q-learning**
   Andrea Skolik, Sofiene Jerbi, Vedran Dunjko
   Quantum 6 (2022): 720

   AS and VD conceived the idea for this work. AS performed the numerical simulations, with the help of SJ. AS, SJ, and VD worked out theoretical separation between quantum and classical learners. AS wrote the manuscript, all authors were involved in the final editing. VD supervised the work.

3. **Equivariant quantum circuits for learning on weighted graphs**
Andrea Skolik, Michele Cattelan, Sheir Yarkoni, Thomas Bäck, Vedran Dunjko
npj Quantum Information 9 (1), 1-15

AS conceived the idea for this work. AS and VD conducted theoretical analysis of the proposed ansatz. AS and MC performed numerical simulations and the analysis of their results. SY created the data set used in this work. AS, MC and SY wrote the first draft of the manuscript; all authors contributed to editing the final manuscript. VD and TB supervised the project.

4. **Robustness of variational quantum reinforcement learning under hardware errors**
Andrea Skolik, Stefano Mangini, Thomas Bäck, Chiara Macchiavello, Vedran Dunjko
EPJ Quantum Technology 10 (1), 1-43

AS conceived the idea for this work and conducted the numerical experiments. SM performed analytical study on the effect of Gaussian noise and provided decoherence noise model. AS and VD proposed shot allocation algorithm. AS and SM wrote the first version of the manuscript, all authors contributed to the final editing.

The following publications were co-authored during the course of the PhD and are not included in this thesis.

5. **TensorFlow Quantum: A Software Framework for Quantum Machine Learning**
Michael Broughton, Guillaume Verdon, Trevor McCourt, Antonio J. Martinez, . . . , Andrea Skolik, . . . , Alan Ho, Hartmut Neven, Masoud Mohseni
arXiv preprint arXiv:2003.02989

6. **Quantum approximate optimization of non-planar graph problems on a planar superconducting processor**
Matthew P. Harrigan, Kevin J. Sung, Matthew Neeley, Kevin J. Satzinger, . . . , Andrea Skolik, . . . , Erik Lucero, Edward Farhi, Ryan Babbush
Nature Physics 17.3 (2021): 332-336

7. **Beating classical heuristics for the binary paint shop problem with the quantum approximate optimization algorithm**
Michael Streif, Sheir Yarkoni, Andrea Skolik, Florian Neukart, Martin Leib
Physical Review A 104.1 (2021): 012403

8. **Hyperparameter optimization of hybrid quantum neural networks for car classification**
Asel Sagingalieva, Andrii Kurkin, Artem Melnikov, Daniil Kuhmistrov, Michael Perelshtein, Alexey Melnikov, Andrea Skolik, David von Dollen
arXiv preprint arXiv:2205.04878

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