Quantum algorithms for Hamiltonian learning problems

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by

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to

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Certificate of Original Authorship

I, Youle Wang, declare that this thesis is submitted in fulfilment of the requirements for the award of Doctor of Philosophy, in the School of Computer Science, Faculty of Engineering and Information Technology at the University of Technology Sydney.

This thesis is wholly my own work unless otherwise referenced or acknowledged. In addition, I certify that all information sources and literature used are indicated in the thesis.

This document has not been submitted for qualifications at any other academic institution.

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Abstract

Learning the dynamic Hamiltonian of a quantum system is a fundamental task in studying condensed matter physics and verifying quantum technologies. Many protocols have been proposed for Hamiltonian learning. Still, many of them require the ability to prepare quantum Gibbs states and estimate entropies of quantum states, which are not easy for classical computers. Recent experimental progress of quantum hardware has drawn much attention, motivating us to investigate the application of near-term quantum computers in Hamiltonian learning. In this dissertation, we study the Hamiltonian learning problems and propose algorithms to recover interaction coefficients of a Hamiltonian, prepare quantum Gibbs states, and estimate the quantum entropies of quantum states. We employ quantum circuits that are expected to be implementable in the near-to-intermediate future.

First, we use the variational quantum algorithms to enable a hybrid quantum-classical algorithmic scheme to tackle the Hamiltonian learning problem. By transforming the Hamiltonian learning problem to an optimization problem using the Jaynes' principle, we employ a gradient-descent method to give the solution and could reveal the interaction coefficients from the system's Gibbs state measurement results. In particular, the computation of the gradients relies on the Hamiltonian spectrum and the log-partition function. Hence, as the main subroutine, we develop a variational quantum algorithm to extract the Hamiltonian spectrum and utilize convex optimization to compute the log-partition function. We also apply the importance sampling technique to circumvent the resource requirements for large-scale Hamiltonians.

Second, we propose variational quantum algorithms for quantum Gibbs state preparation. First, we take the loss function as the system's free energy and estimate it by a truncated version. Then we train a parameterized quantum circuit to optimize the loss function so that it can learn the desired quantum Gibbs state. Notably, our algorithms can be implemented on near-term quantum computers. Furthermore, by performing numerical experiments, we show that shallow parameterized circuits with only one additional qubit can be trained to prepare the Ising chain and spin chain Gibbs states with a fidelity higher than 95%. In particular, for the Ising chain model, we find that a simplified circuit ansatz with only one parameter and one additional qubit can be trained to realize a 99% fidelity in Gibbs state preparation at inverse temperatures larger than 2.

Third, we propose quantum algorithms to estimate the von Neumann and quantum α-Rényi entropies of an n-qubit quantum state ρ using independent copies of the input state. We show how to efficiently construct the quantum circuits of both methods using primitive single/two-qubit gates. We prove that the number of required copies scales polynomially in $1/\epsilon$ and $1/\Lambda$, where ϵ denotes the additive precision and Λ denotes the lower bound on all non-zero eigenvalues. Notably, our method outperforms previous methods in the aspect of practicality since it does not require any quantum query oracles, which are usually necessary for previous methods. Furthermore, we conduct experiments to show the efficacy of our algorithms to single-qubit states and study the noise robustness.

Dedication

To my family.

Statement of authorship and publications

The dissertation is based on the following articles:

- Youle Wang, Guangxi Li, and Xin Wang. A hybrid quantum-classical Hamiltonian learning algorithm. Sci. China Inf. Sci. 66, 129502 (2023). `https://doi.org/10.1007/s11432-021-3382-2`
- Youle Wang, Guangxi Li, and Xin Wang. (2020). Variational quantum Gibbs state preparation with a truncated Taylor series. Physical Review Applied, 16(5), 054035. `https://doi.org/10.1103/PhysRevApplied.16.054035`
- Youle Wang, Benchi Zhao, and Xin Wang. (2022). Quantum algorithms for estimating quantum entropies. `http://arxiv.org/abs/2203.02386`

The first work above has been published in Science China Information Sciences and was also accepted as a short talk at the 21st Asian Quantum Information Science Conference, AQIS 2021. The second work has been published in Physical Review Applied. The third work is available online. In addition, I have co-authored the following articles that are not included in this dissertation. In the first work below, the authors are listed in alphabetical order.

- Xin Wang, Youle Wang, Zhan Yu, and Lei Zhang. Quantum Phase Processing: Transform and Extract Eigen-Information of Quantum Systems. `http://arxiv.org/abs/2209.14278`
- Xin Wang, Zhixin Song, and Youle Wang. (2021). Variational Quantum Singular Value Decomposition. Quantum, 5(1), 483. `https://doi.org/10.22331/q-2021-06-29-483`
- Guangxi Li, Youle Wang, Yu Luo, Yuan Feng, Quantum data fitting algorithm for non-sparse matrices. `http://arxiv.org/abs/1907.06949`

All my publications are available on arXiv and Google Scholar.

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