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PhD Thesis Review Report

Faculty:	Institute of Theoretical and Applied Informatics, Polish Academy of Sciences
Student:	mgr Akash Kundu
Supervisor:	dr hab. Jaroslaw Miszack
Title:	Reinforcement Learning-Assisted Quantum Architecture Search for Variational Quantum Algorithms
Reviewer:	dr Valeria Bartsch

Akash Kundu has published 7 articles in the field of quantum computing and 7 articles in the field of cosmology and optomechanical systems. He is first author in 3 publications and second author in another 3 publications in the field of quantum computing. He has published in high-ranking journals such as Physical Review A (impact factor: 2.9), New Journal of Physics (impact factor: 3.3) and Quantum Science and Technology (impact factor: 6.7).

The thesis studies the use of reinforcement learning to derive quantum computing circuits for variational algorithms. Some topics of the thesis (variational quantum state diagonalization (VQSD) and variational verification of quantum channels via VQSD) have been discussed in the publications. In addition, the code base has been published. Thus, important concepts described in the thesis have already been reviewed and positively evaluated by renowned experts in the field and opened to a broader community.

The thesis is divided into six chapters. After an introduction, the second chapter discusses variational quantum algorithms and the basics of reinforcement learning in detail and introduces how reinforcement learning will be setup to synthesis quantum computing circuits. The following chapters present the results obtained during the Ph.D. thesis. The third chapter discusses the usage of reinforcement learning to compile an efficient circuit for VQSD and presents results on it. Chapter 4 discusses the ansatz synthesis of the VQE algorithm. Chapter 5 discusses the variational certification of quantum channels with VQSD. Chapter 6 is a short discussion of the main results of the thesis. The thesis ends with the conclusion in chapter 7. Though the chapters are well structured it could have made sense to put the chapter on the circuit synthesis for the VQSD and the variational certification of the quantum channels behind each other to strengthen the thematic closeness of the topics. But this is a minor comment on the structure of the thesis.

Reinforcement learning based synthesis approaches are relevant to any variational algorithms. To utilize the expensive and scarce quantum computing resources to the best extent possible it is important to compact the quantum computing circuits as much as possible. The author introduces a framework for quantum architecture search that can be adapted to address a wide range of variational algorithms in deploying quantum architecture search methods that work in absence and presence of real device noise. Though reinforcement learning for quantum architecture search has already been implemented in other approaches (such as quantumDARTS or RL-VQE) several features have been added to the proposed framework that genuinely enhance the framework:

- The author contributed to the topic by providing a binary depth-based encoding scheme for the ansatz that can be easily modified and adapted to any quantum architecture search method.
- To reduce the training time of the reinforcement learning algorithm a method to avoid illegal actions has been added to the framework.
- A random halting scheme has been added which accelerates the discovery of an efficient ansatz and reduces the training time. The random halting scheme varies the number of time steps in an episode leading to a faster convergence of the variational algorithm.
- To avoid setting a threshold value for the cost function, curriculum reinforcement learning has been used. In the curriculum reinforcement algorithm, the threshold value is shifted after each episode so that the agent can find the ground state energy without prior knowledge of the ground state energy.

The source code for the variational fidelity estimation for quantum channels and for the VQE have been published in github and – in case of the VQSD - added to Qiskit which allows a broad use of the method.

One comment about the methodology: It would be helpful to compare reinforcement learning based quantum architecture search algorithms with other methods such as gradient based methods and genetic methods especially concerning their efficiency. The latter methods are known to outperform classical topology search algorithms in neural network design when parallelized. Parallelization could be an avenue for future research.

Two main use cases for the proposed quantum architecture search have been identified: the usage of an ansatz for VQE and VQSD. VQSD has several applications, including quantum state fidelity estimation, device certification, Hamiltonian diagonalization, and as a method to extract entanglement properties of a system. VQE is the state-of-the-art method for atomistic simulations for quantum chemistry. It is likely that quantum advantage will be seen in quantum chemistry algorithms which in turn will have a significant impact on the chemical industry.

Concerning the ansatz for VQE there are typically two possible approaches: a physics-inspired approach such as UCCSD (Unitary Coupled Cluster Single Double Excitation) and a hardware efficient approach. While the physics inspired CCSD approach is well tested in ab initio methods on classical devices and is a gold standard, the quantum equivalent UCCSD typically requires a high number of CX gates and a high circuit depth. The hardware-efficient approach is optimized for the quantum hardware, but often lacks a proper representation of the physical properties of the molecule to be simulated. Akash presents an approach based on reinforcement learning and evaluates it concerning the size of the quantum circuit proposed as well as the quality of the result with UCCSD methods. It turns out that the reinforcement-based method can deliver results with a similar quality as the UCCSD method with a smaller and shorter circuit. Any software improvements on the VQE algorithm are important in order not to only depend on the maturing of the hardware technology to reach quantum advantage. Thus, the thesis addresses relevant topics in quantum computing.

For VQSD the author proposes a new encoding scheme, the tensor-based binary encoding scheme for quantum circuits which scales polynomial with the number of qubits which is efficient for the purpose of reinforcement learning approaches. Comparing the reinforcement learning approach RL-VQSD to other approaches to solve VQSD Akash shows that the RL-VQSD outperforms existing algorithms. The RL-VQSD method is used to certify quantum channels. Quantum state tomography is the standard approach for such a certification, however due to the quadratic scaling of dimensions with the number of qubits full tomography can be prohibitively expensive. Thus, novel approaches such as the variational quantum state fidelity (VQSF) algorithm are investigated. Akash traces the VQSF algorithm using RL-VQSD which gives a compact ansatz. It can be shown noise has little effect on the performance of the algorithm.

Concerning suggestions for future research, I believe that it is important to test the method until it breaks down to check for the limiting factors of the methods. I would recommend benchmark the scaling behavior of the method (e.g. for the VQE algorithm to scale to larger molecules) and to compare the methods to current state-of-the-art methods (such as comparing the VQSD method to the state tomography method). To allow future users of such methods to evaluate their advantages and disadvantages better, it would be also good to analyze the runtimes. These suggestions go beyond the scope of the PhD thesis.

It has been very helpful that the main points and innovations have been clearly highlighted in the thesis. The dissertation testifies the author’s knowledge in quantum computing and a very detailed knowledge in the field of the thesis. Significant weaknesses of the presented thesis are not identified, and my comments raise follow-up research questions.

In my opinion, the presented material meets all the requirements for an PhD thesis. The author has published several high-quality papers and continues to be scientifically very active. His contribution to the field is highlighted by high-profile publications.

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