Efficient VQE Ansatz Design by Conditional Reinforcement Learning

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Abstract

This study proposes the use of conditional Reinforcement Learning to address the optimization challenges in the Variational Quantum Eigensolver (VQE). While VQE is recognized highly as a promising algorithm, it faces the issues to re-optimize and redesign the ansatz structure whenever a new Hamiltonian is introduced. This paper aims to overcome this problem by employing conditional Reinforcement Learning (RL) techniques. The proposed approach seeks to automatically learn the optimal ansatz and optimization strategies for various Hamiltonians, significantly enhancing the applicability and efficiency of VQE.

Keywords— Reinforcement Learning, Variational Quantum Eigensolver

The Variational Quantum Eigensolver (VQE) [1] is a promising algorithm in quantum computing for finding ground state energies of quantum systems. However, a significant challenge arises when a new Hamiltonian is introduced: the optimization process and the ansatz structure must be reconfigured, which is both time consuming and computationally demanding. This paper aims to overcome this challenge by employing a conditional-continuous-discrete hybrid Reinforcement Learning approach.

We utilize the Soft Actor-Critic (SAC) [2] algorithm in our study. In this hybrid RL framework, the continuous actions represent the angles of the quantum gates, while the discrete actions correspond to the types of gates used. The electron integral values of the training Hamiltonians are considered as conditions for the actor and Q networks, i.e. $\pi(s) \rightarrow \pi(s,c)$, $Q(s) \rightarrow Q(s,c)$. Here, s and c denote state and condition, respectively, which represents the electron integral values. Our algorithm is trained to effectively generalize and adapt to new Hamiltonians.

Our method requires conditioning the RL agent on specific Hamiltonian parameters, enabling it to learn the optimal ansatz and corresponding parameters. This approach automates the VQE process, significantly reducing the computational overhead associated with manual optimization trials, and enhancing the algorithm efficiency.

We tested our algorithm on several molecules, using electron integral values at various bond lengths as our dataset for training and test. Fig.1 provides a brief overview of our algorithm, while Fig.2 illustrates the learning progress and results for H_2 molecule. The results highlight the potential of conditional continuous-discrete hybrid RL that can improve the scalability and applicability of VQE in quantum chemistry and physics. The results of this research offer novel solutions to the everlasting challenge of ansatz optimization in VQE, paving the way for more efficient quantum computations.

Acknowledgments

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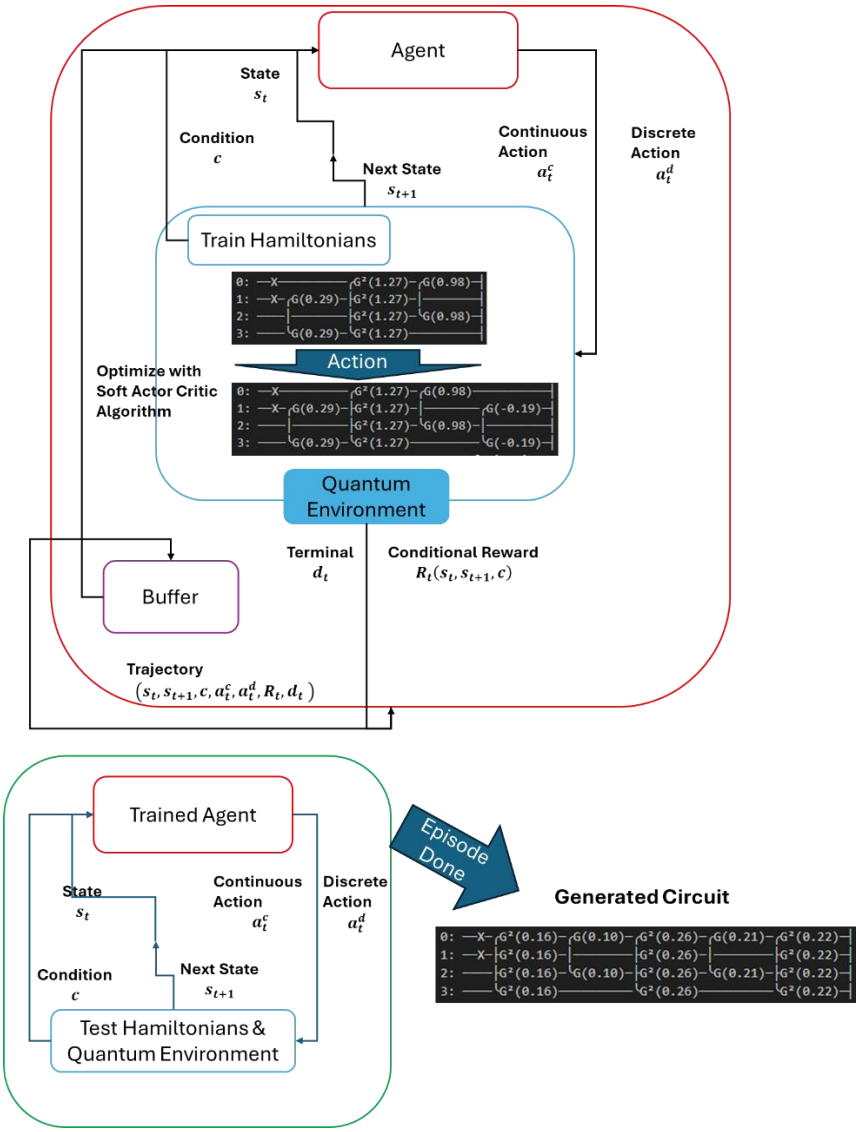

Figure 1: The training part involves the agent interacting with the environment using train electron integral values as conditions to perform reinforcement learning. In the Test part, the trained agent's actor is used to generate ansatz for test conditions and evaluate them.

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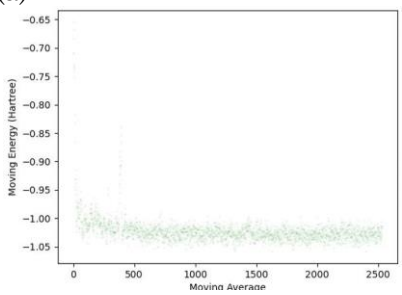

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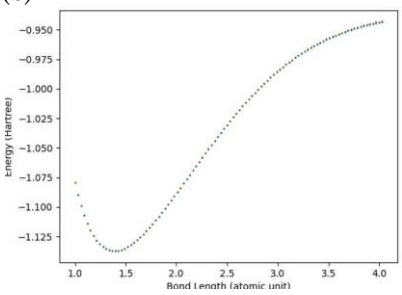

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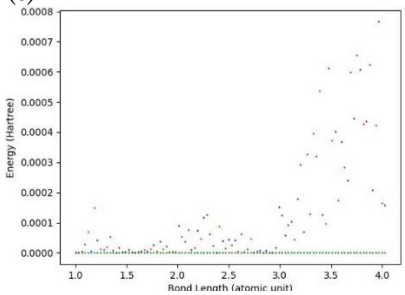

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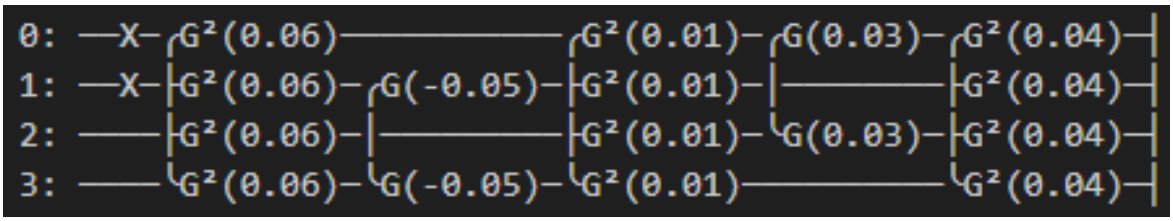

Figure 2: Results from performing the algorithm on the H_2 molecule (Jordan-Wigner transform, STO-3G basis) with 50 training points and 50 test points.
(a) The x-axis represents the moving average of episode, and the y-axis represents the moving average of energy from the ansatz generated by the actor with condition as electron integrals of training Hamiltonians and measure by such Hamiltonians.
(b) The x-axis represents bond length, while the y-axis represents energy. The green line indicates the true ground energy. The red dots represent the energy from the ansatz generated by the agent conditioned on the training bond length electron integrals, and similarly, the blue dots represent the energy from the ansatz generated by the agent conditioned on the test bond length electron integrals.
(c) The x-axis represents bond length, while the y-axis represents the energy gap between the true ground energy and the energy generated by the agent, showing error less than chemical accuracy requirement of 0.0017 Hartree. Red dots are from training conditions, and blue dots are from test conditions.
(d) An example of circuits generated by the agent at a bond length of 4.0 atomic unit. $G(\cdot)$ and $G^2(\cdot)$ denote single and double excitation gates, respectively. [3]