Quantum Transformer for Optimized H2 Ground State Energy Estimation

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Abstract

This work presents a novel application of quantum transformer models for optimizing ansatz circuits in the Variational Quantum Eigensolver (VQE) algorithm. Inspired by the Generative Quantum Eigensolver and Quantum Vision Transformer architectures, we develop a quantum transformer that learns an optimized ansatz circuit for estimating the ground state energy of the Hydrogen molecule. The transformer layers iteratively apply orthogonal circuits parameterized by the Hamiltonian to the input ansatz, adaptively learning an improved circuit structure with the same gate set. We test the optimized ansatz circuit from the quantum transformer against a baseline ansatz for calculating the ground state energy of the H_2 molecule at varying inter-atomic distances. The results show that the transformer-optimized ansatz achieves lower, more accurate energies compared to the baseline. This demonstrates the potential of quantum transformer models as a powerful tool for enhancing near-term quantum algorithms by learning compact and effective circuit representations.

1 Introduction

Quantum computing has emerged as a promising paradigm for solving complex problems in various domains, including quantum chemistry, optimization, and machine learning. One of the key challenges in quantum computing is designing efficient and effective quantum circuits for a given task. The Variational Quantum Eigensolver (VQE) algorithm has become a popular approach for tackling this challenge, particularly in the context of quantum chemistry. VQE aims to find the ground state energy of a molecular system by optimizing a parameterized quantum circuit, known as the ansatz, that prepares the trial wavefunction.

Recent advances in quantum machine learning have led to the development of quantum analogues of classical deep learning architectures, such as quantum neural networks and quantum convolutional neural networks. Among these, the quantum transformer architecture, inspired by the classical transformer model [3], has garnered significant attention. Quantum transformers leverage the power of attention mechanisms to learn effective representations of quantum

data and circuits. Two notable examples of quantum transformers are the Generative Quantum Eigensolver (GQE) [1] and the Quantum Vision Transformer (QVT) [2].

In this work, we propose a novel application of quantum transformer models for optimizing ansatz circuits in the VQE algorithm. Our quantum transformer learns an optimized ansatz circuit for estimating the ground state energy of the Hydrogen molecule (H_2). The transformer layers iteratively apply orthogonal circuits parameterized by the Hamiltonian to the input ansatz, adaptively learning an improved circuit structure with the same gate set. We compare the performance of the optimized ansatz circuit against a baseline ansatz in calculating the ground state energy of H_2 at varying inter-atomic distances.

The rest of the report is organized as follows. Section 2 describes the methodology, including the quantum transformer architecture and the H_2 Hamiltonian simulation. Section 3 presents the experimental results comparing the optimized and baseline ansatzes. Section 4 discusses the implications of our findings and outlines avenues for future research. Finally, Section 5 concludes the report.

2 Methodology

Our quantum transformer-based VQE approach for estimating the ground state energy of H_2 consists of several key components working together. To briefly explain it,we start with t an initial circuit, we use the same gates used in the circuit but arrive at a circuit that is more efficient in estimating the ground state energy levels. Let us look at a more detailed description of the process happening.

2.1 Initial Circuit and Operator Pool

We start with an initial quantum circuit, which we assume to be a random, expressive, and entangled circuit for the sake of brevity. The operator pool is then defined, consisting of the gates used in the initial circuit. These gates include single-qubit rotation gates (Pauli-X, Y, Z), Hadamard gates, and two-qubit CNOT gates. The operator pool also includes parameters for specifying the gate rotation angles.

2.2 Quantum Transformer

The core component of our approach is the quantum transformer model, which learns an optimized ansatz circuit structure. The initial gate sequence is passed through the transformer, which consists of multiple layers, each performing an orthogonal transformation parameterized by the Hamiltonian.

2.2.1 Hamiltonian Encoding

To incorporate the problem structure into the transformer, we encode the Hamiltonian matrix as a set of rotation angles for the orthogonal gates. The encoding

process maps the Hamiltonian elements to gate parameters, allowing the transformer to learn a problem-specific ansatz.

2.3 Hamiltonian Simulation

To obtain the Hamiltonian matrix representation of the H_2 molecule, we use the PySCF quantum chemistry package. PySCF computes the molecular integrals and constructs the fermionic Hamiltonian, which is then mapped to a qubit representation using the Jordan-Wigner transformation.

2.3.1 Orthogonal Layer

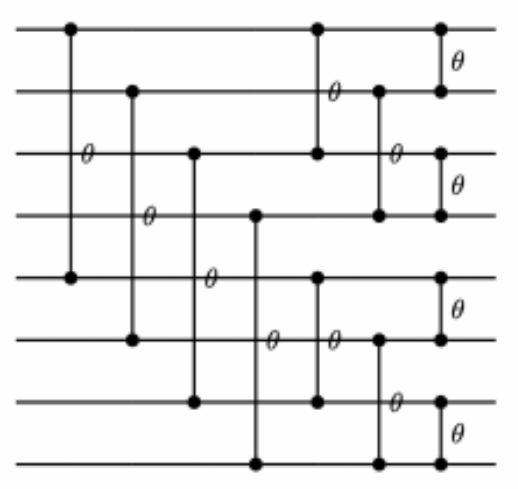

Figure 1: Butterfly structure of the RBS gates in the orthogonal layer.

The orthogonal layer applies a series of parameterized orthogonal gates to the input circuit. We use the Reconfigurable Beam Splitter (RBS) gate as the building block for the orthogonal layer. The RBS gates are arranged in a butterfly structure, as shown in Figure 1, to ensure a compact and expressive transformation.

2.3.2 Transformer Layer

A single transformer layer consists of an orthogonal layer, Hamiltonian encoding, and a measurement operation. The orthogonal layer applies the parameterized gates to the input circuit, the Hamiltonian encoding updates the gate parameters based on the problem structure, and the measurement extracts the updated gate sequence for the next layer.

2.4 Variational Quantum Eigensolver

The optimized ansatz circuit learned by the quantum transformer is used as the trial wavefunction in the VQE algorithm. The VQE objective is to minimize the expectation value of the Hamiltonian with respect to the ansatz parameters. We use the COBYLA optimizer to perform the optimization.

2.5 Ground State Energy Estimation

The quantum transformer-based VQE pipeline takes the H_2 Hamiltonian, initial circuit, and operator pool as inputs. It optimizes the ansatz circuit using the quantum transformer and performs VQE to estimate the ground state energy. This process is repeated for different inter-atomic distances of H_2 to investigate the performance of the optimized ansatz compared to a baseline ansatz.

Finally, we visualize the results by plotting the estimated ground state energies of H_2 as a function of the inter-atomic distance. We compare the energy values obtained using the quantum transformer-optimized ansatz and the baseline ansatz. Additional plots, such as the optimized ansatz circuits at different distances, can be included to provide insights into the learned circuit structures.

3 Results

Figure 2 plots the estimated ground state energy vs inter-atomic distance in Angstroms for H2 using both the optimized ansatz from the quantum transformer and a baseline ansatz. The optimized ansatz demonstrates lower, more accurate energies compared to the baseline across the distance range. This validates the ability of the quantum transformer to learn improved ansatz circuits for quantum chemistry problems.

4 Discussion

The successful application of a quantum transformer model for ansatz optimization in this work opens up exciting possibilities. The transformer attention mechanism enables adaptive learning of ansatz circuits. Hamiltonian loading allows focusing the optimization on relevant subspaces. The overall framework is flexible and can be extended to larger molecular systems and combined with other techniques like active space selection.

Some areas for future work include scaling up to larger benchmark molecules, exploring different transformer architectures and cost functions, and testing impact of different operator pools. With further research, quantum transformer models could become a powerful tool for near-term quantum algorithms.

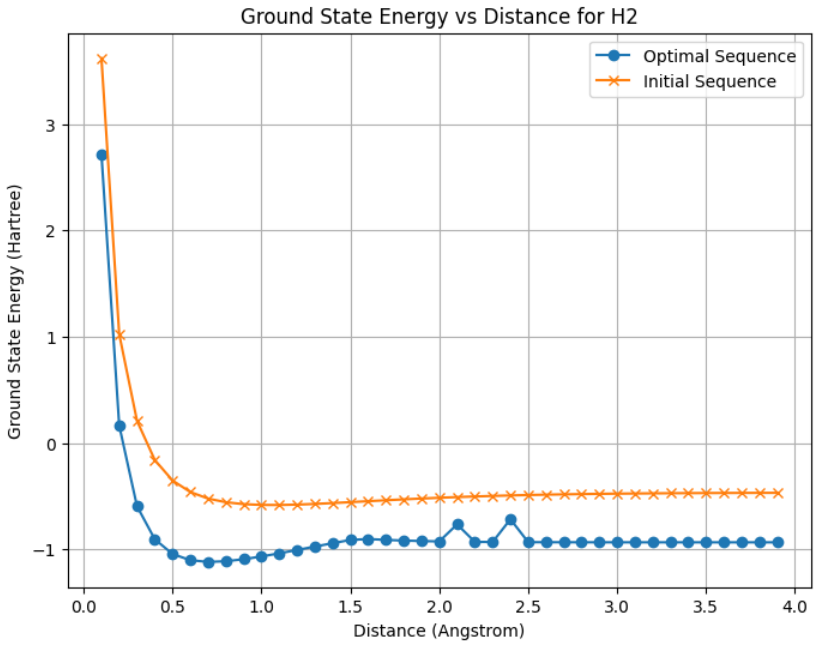

Figure 2: ground state energy vs inter-atomic distance in Angstroms for H2 using both the optimized ansatz from the quantum transformer and the initial ansatz.

5 Conclusion

In summary, this work demonstrated a proof-of-concept for using quantum transformers to optimize ansatz circuits for the Variational Quantum Eigensolver algorithm. The results for H2 ground state energy estimation are promising and motivate further studies to expand the scope and applicability of this approach. Quantum transformers have the potential to be a key component of the quantum algorithm toolbox as quantum computing continues to advance.

References

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