Variational Quantum Eigensolver

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1. Abstract

The variational quantum eigensolver (VQE) is a hybrid classical-quantum algorithm to calculate the ground state energy level of a particle. VQE's approach utilizes quantum computation to develop states, which are then optimized by varying circuit parameters via classical methods. Compared to other proposals to find the ground state VQE is computationally less expensive, and has practical applications/tests.

2. Objectives

Our objective for the VQE algorithm is to represent a molecule by its wavefunction, which is the mathematical representation of the molecule's quantum state. The goal is to find the ground state energy level, or the lowest possible energy level that the particle can occupy.

3. Background

In order to simulate molecules, quantum computers can be utilized to accurately predict their chemical interactions. To this end, scientists hope to use this technology to simulate chemical reactions that will help us engineer better medicines and materials. Using a quantum computer's ability to solve complex eigenvalue problems is one of the main challenges in achieving accurate predictions of molecules. In 2014, Peruzzo and McLean [1] developed the variational quantum eigensolver (VQE), which utilizes both quantum and classical computing. The quantum portion of the algorithm tests varying wavefunctions and finds its lowest energy level by calculating the

eigenvector with the lowest eigenvalue of the Hamiltonian. The trial wavefunctions are often referred to as “ansatz states” because each wavefunction is essentially a trial-and-error approach. The classical part of the algorithm optimizes the ansatz state by varying the parameters of the circuit so that the new ansatz state has a smaller expectation value than before. A brute force approach to find the ground state of the particle can be thought of as trying every state within the Bloch Sphere, but changing the parameters of the state reduces the number of states to a portion of the Bloch Sphere. The optimization process is boiled down to updating the state in an attempt to improve the ground state measurement. If the ground state doesn’t improve due to the changes, the parameters are reversed [2]. Some optimization methods employ classical machine learning algorithms to improve the change of parameters of the quantum state.

Before VQE was developed, the first idea proposed to find the ground state energy level of a particle was by using quantum phase estimation (QPE) and the inverse quantum Fourier transform (IQFT). The main drawback of this method is the need for “millions of qubits and gates even for relatively small systems, a requirement far beyond the capabilities of present NISQ (Noisy Intermediate-Scale Quantum Devices) hardware.” [3] The NISQ era of quantum computing that we are in today means that the qubits we work with are not isolated enough from their physical environments, so there is a lot of room for noise to interfere with the qubits and introduce errors to the computation. VQE is useful because it uses small circuit depth, or gates, to reduce the computation time and therefore the errors.

4. Methods

The first stage of our VQE algorithm involves mapping the ansatz states to the qubit by means of the Hamiltonian. We express the Hamiltonian as the sum of the tensor products of Pauli

operators, and initialize the Hamiltonian by randomly generating the coefficients of each Pauli term. We initialize our qubit to the |0> state, and then use two gates that correspond to rotations about the x and y axes, to transform the state into any point on the Bloch Sphere. The parameters of these gates are controlled by the classical optimization method and are the foundation for creating the ansatz states. These parameters are also used to prepare the circuits that act on each Pauli term.

Our program then calculates the expectation value of each term. To prepare for measurement in the Z basis, we apply the Hadamard and Y gate to the wavefunction in order to make the probability of each basis state outcome equivalent regardless of the basis. The circuit is run on each term and the expectation value for each term is summed up.

Finally, the optimization part of our code changes the parameters for the next ansatz state and circuit to be created. This allows for a minimized expectation value that, when converged, gives the ground state energy level. To compare our quantum results with a value that is known to be correct, we use Qiskit's NumpyEigensolver class to classically compute the smallest eigenvalue of the given Hamiltonian.

5. Discussion

In this approach to a VQE algorithm, we ran into many issues with the qiskit library. The main submodule that we utilized in our implementation is qiskit.aqua, which was deprecated in 2021, and is no longer recognized by Python. The migration guide for aqua is outdated and many of the replacement modules, such as Opflow and QuantumInstance, have also been deprecated. Because of this, we could not use the WeightedPauliOperator or NumPyEigensolver functions. We attempted a new approach that did not require aqua, but new errors came up for the

BasicAer/ Aer module and the quantum_info module. Due to all of these relatively recent changes to the qiskit library, there was a lack of current online resources and many tutorials and code samples were outdated. Without these library errors, we expect that our VQE algorithm would effectively find the ground state energy level for a randomly generated molecule.

One area of interest is how our algorithm would be implemented for multiple qubits, which would require using the tensor products of Pauli operators, such as XY. We would then take the expectation value of the tensor products. Additional gates would also need to be applied to each additional qubit. The general process of computation would remain the same. Each additional qubit would double the linearly independent basis states as well as the gates needed, so the computational expense will double. Another issue with simulating multiple qubits is the large error rate of multi-qubit gates [3].

6. Conclusions

In this project, we implemented a variational quantum eigensolver algorithm that utilizes a hybrid classical-quantum approach to find the ground state energy level of a particle. This is a common goal in quantum chemistry where simulating particles would be especially useful for engineering new materials and medicines. The VQE algorithm iterates over trial wavefunctions and finds the minimum expectation value of the Hamiltonian. Classical methods optimize the wavefunction by changing the parameters of the circuits on each iteration. This algorithm is a huge improvement over algorithms like Quantum Phase Estimation (QPE) which also finds the ground state energy level. This is because of the small circuit depth of VQE which reduces the time for noise to interfere with the system. In our implementation, we represent the Hamiltonian as the sum of Pauli terms, and prepare a quantum circuit on each term. The Hadamard gate is

used to make the measurement outcomes equal in all three measurement bases, and then the expectation values are calculated. Finally, the expectation value is optimized by changing the parameters of the circuit. The results of this implementation are unclear due to issues within the qiskit library. If the code was to be altered to accommodate multiple qubits, we would use Pauli tensor products instead of single Pauli operators, and an additional gate for each additional qubit. The computational cost should double with each added qubit.

7. References

[1] A. Peruzzo et al., Nature Communications, "A variational eigenvalue solver on a photonic quantum processor" (2014).

[2] Michał Stęchły, "Variational Quantum Eigensolver explained".

[3] Dmitry A. Federov, VQE: A Short Survey and Recent Developments