

Optimization Analysis for the Variational Quantum EigenSolver

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Abstract

The Variational Quantum EigenSolver (VQE) is a groundbreaking approach to tackle complex quantum problems. Its implementation shines the light on a promising future where scientists can utilize for new drug discovery, material science innovations, and machine learning acceleration. This paper delves into the underlying machine learning approach, variational method implementation, eigensolver enforcement, and a detailed explanation for the different steps to implement the VQE.

Furthermore, this paper analyzes the selection and impact of optimizers within the algorithm. Different studies were conducted such as an evaluation of how algorithm's performance evolves with increasing iterations, how different optimizers compare and contrast to VQE performance, and an assessment on the optimal number of iterations for energy estimations in the context of molecular simulation.

1. Introduction

The Variational Quantum Eigensolver (VQE) is a hybrid algorithm that integrates both classical and quantum computing. It is designed to address optimization problems through predefined sets of parameters. By leveraging the power of a quantum computer and accuracy of classical computing, it is showing to be a promising algorithm to replace full classical algorithms.

The objective of optimization algorithms is to identify the lowest cost within a given parameter space. Consequently, the underlying graph representing this parameter space is not directly visible or easily accessible. Therefore, it becomes difficult to find the global minimum space within the entire graph. In machine learning, the technique of gradient descent is employed to guide its algorithm by calculating the cost function of each parameter value. As a result, it directs its algorithm to a reaching point where the gradient is zero indicating a minimum. Complications arise when the algorithm “thinks” it has found the minimum of the entire space when in fact it has just found a local minimum.

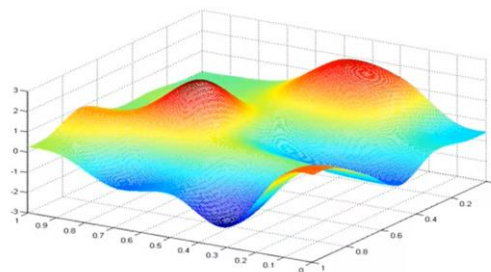


Figure 1. 3-D parameter space wave function graph.

2. Background

Current classical algorithms are not only computationally expensive but also not as accurate especially when its system begins to scale. Therefore, the main motivation behind the development of the VQE was to find a way to solve the electronic structure problem in quantum chemistry [1]. The electronic structure problem is finding the ground state energy of a given system. Therefore, the VQE was first developed by Peruzzo et al (2014) and has been proposed as an alternative to fully quantum algorithms such as the Quantum Phase Estimation (QPE) [2]. This means that the VQE was made as a work around to use the power of a quantum computer without relying too much on the quantum computer's accuracy.

3. Algorithm Name

The name of the VQE encapsulates three pivotal components which sum up the heart of the algorithm. The term “Variational” signifies the adaptation of the variational method used in quantum mechanics. It states that, “For a given Hermitian matrix H , its expectation value must always be equal to or greater than the lowest possible eigenvalue” [3]. As a result, by minimizing the expectation value, you can only get closer to the minimum eigenvalue but never below it.

The second crucial component “Quantum” represents the involvement of a quantum computer. Unlike classical computers, quantum computers leverage the principles of superposition, entanglement, and interference which enables them to perform calculations in parallel across a multitude of possibilities simultaneously. This hardware

design allows the ability to transform certain exponentially complex algorithms into polynomial time.

Finally, the term “EigenSolver” denotes the capability of an algorithm to calculate the minimum eigenvalue of a Hamiltonian matrix. Eigenvalues are scalar values associated with linear transformation. In molecular simulation, eigenvalues correspond to different energy levels of the molecule. Furthermore, eigenvectors represent a vector associated to an eigenvalue. In Schrödinger's time-independent equation $\hat{H}\psi = E\psi$ (Eq 1), \hat{H} is the molecular Hamiltonian operator, E is the eigenvalue representing the energy association with the system, and ψ is the eigenvector that is associated with the wavefunction of the molecule.

4. VQE Steps

When implementing the Variational Quantum EigenSolver for molecular simulation, there are multiple steps in the classical side of the algorithm which prepare the quantum circuit to execute the minimum eigenvalue. Then the classical computer aids the quantum circuit by updating the results and feeding it back into the quantum circuit until the answer starts converging. Figure 2 highlights the classical implementation in green and the quantum circuit in blue.

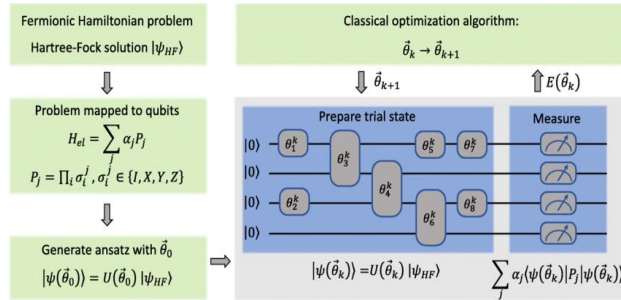


Figure 2. Diagram of VQE implementation [2]

The experimental environment consisted of using the IBM Quantum Lab which uses a software development kit for programming quantum computers called Qiskit. The code crafted for this experiment uses Qiskit version 0.46 and Python version 3.10.8. The code repository hosting the implemented algorithms is accessible via [4] on GitHub.

4.1. Map Hamiltonian

The Hamiltonian serves as a matrix that describes the total energy levels of a certain system, with the focus here being a molecule. Determining the total energy involves computing both the kinetic and potential energy of the molecule (Eq 2).

$$H_{\text{operator}} = \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \quad \text{Eq 2}$$

Hamiltonian Operator
Operator for Kinetic Energy
Potential Energy

To leverage the Hamiltonian in a quantum computer, it is essential to transform the molecular Hamiltonian into a qubit Hamiltonian. This means mapping the electron orbital interactions inside the molecules onto our qubits to be able to perform calculations. Due to the nature of quantum gates being represented as matrices as well, the encoding process consists of breaking down the Hamiltonian matrix into a series of rotational quantum gates.

4.2. Prepare Ansatz

In preparation for the VQE, it requires an initial estimate for the optimization process to converge effectively towards the minimum energy. The term Ansatz is German which means “beginning” or “approach”. Classical approximation methods such as the Hartree-Fock play a crucial role in generating an Ansatz which serves as an educated guess for the initial trial wavefunction. These are the parameters given to the VQE representing the parameter space where the minimum energy may exist at.

4.3. Quantum Circuit

Now that the information has successfully been mapped to work on a quantum computer, the variational method is implemented using a series of rotational gates that represent segments of the trial wave function. Additionally, CNOT gates are employed to enforce entanglement. This causes the qubits to now become connected as if they are one which establishes a collective representation of the molecular system. The quantum circuit in Figure 3 is a representation of the variational method being constructed in linear entanglement. With linear entanglement, the qubits are entangled in a sequential matter. This creates a linear chain which reduces the number of quantum gates needed. As a result, we are able to implement larger problems without it becoming computationally expensive.

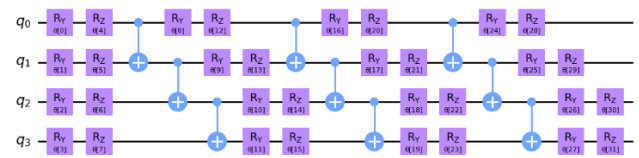


Figure 3. 4-qubit linear entanglement variational quantum circuit. [4]

4.4. Classical Optimizer

The last and important part of the VQE is the optimizer which is run by a classical computer. Once the quantum circuit result gets measured, it has essentially found the minimum eigenvalue from its given parameters. Just like how gradient descent updates its parameters to direct its algorithm to the local minimum, the same is needed for the VQE which is what the optimizer is for. As the output of the quantum circuit is fed into the optimizer, it updates the parameters of the quantum circuit which is the wave function. As a result, once all parameters are updated, the algorithm starts again with the quantum circuit.

There are many different types of optimizers that updates the parameters for the VQE which are:

- Sequential Least Squares Programming optimizer (SLSQP)
- Constrained Optimization By Linear Approximation optimizer (COBYLA)
- Conjugate Gradient optimizer (CG)
- Limited-Memory BFGS Bound optimizer (L_BFGS_B)

SLSQP is designed to minimize a multivariate function by considering a mix of bounds, equality, and inequality constraints. COBYLA serves as a numerical optimization method tailored for constrained problems where the derivative of the objective function is unknown. CG operates as an iterative algorithm because it uses an initial guess to generate a series of improving approximations to the problem, where each approximation is derived from the previous ones. Lastly, L_BFGS_B minimizes the value of the differentiable scalar function. [5]

4.5. Output

The output of the VQE will be a negative decimal number representing the minimum energy. Figure 4 shows the different energy levels a molecule experiences the further apart the atoms inside begin to separate. As soon as all atoms are no longer touching, their energy state is considered as zero. As you begin separating them more, it starts losing its potential energy and eventually hits an equilibrium where the molecule energy is at a minimum. However, as you continue to increase the interatomic distance beyond the minimum energy configuration, the potential energy starts to increase due to attractive forces weakening causing repulsive forces to become dominant again. This is why it's important to test the minimum energy of a molecule at various interatomic distances to find the true minimum energy state.

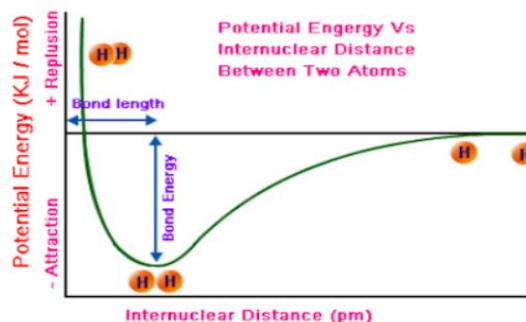


Figure 4. Graph representation of molecular energies. [6]

5. Research Analysis

Since current quantum computers are affected highly with noise which leads to inaccurate results, the following experiments were conducted on a quantum simulator which are essentially classical computers simulating quantum behavior. These simulators are used to put theory into practice to verify our circuit achieves the expected output. In the near future when quantum computers become more accurate, quantum algorithms reach their full potential by being able to execute their algorithms in polynomial time.

We extended the algorithm design to simulate different molecules. We noticed a trend when it came to the number of iterations needed through the optimizer to find the exact minimum energy. In the case of Dihydrogen (H₂), a mere 4 iterations through the SLSQP optimizer proved sufficient to achieve the exact minimum energy. However, the simulation of Lithium Hydride (LiH) exhibited a different behavior. It started converging around the 5th iteration and reached the exact minimum energy on the 8th iteration as seen in Figure 5.

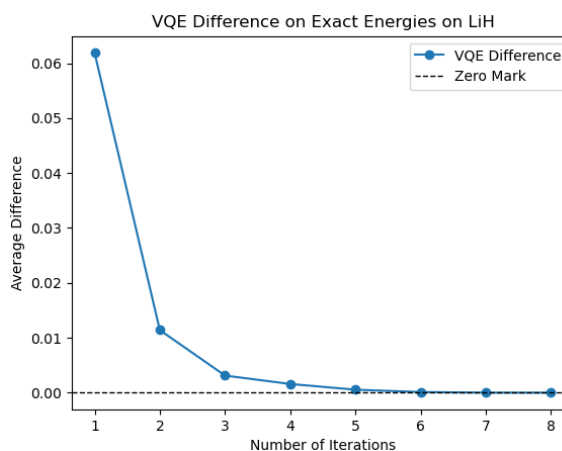


Figure 5. Difference in VQE and exact energies from LiH

With this in mind. We came up with a hypothesis that there must be a correlation between an increase of electrons a molecule has, with more iterations needed to be

able to achieve more accurate results. Part of the encoding process essentially makes the quantum circuit implement a qubit per electron (Jordan-Wigner Representation) [7]. Since each orbital can have 2 electrons, a qubit can be initialized as $|1\rangle$ if an electron is present or $|0\rangle$ otherwise. Our analysis confirmed that as the molecule begins to scale in number of electrons, so does the quantum circuit resulting in more gates being used to try to represent a bigger parameter space.

5.1. Local Minima Results

When simulating molecules of various sizes, an observation was first made on Beryllium Hydride (BeH_2). When increasing the number of iterations, the results got closer to the exact result. However, a plateau was eventually reached where further increases in the number of iterations did not change the results. As seen in figure 6, the VQE energies aren't on the exact energy especially when the interatomic distance is small.

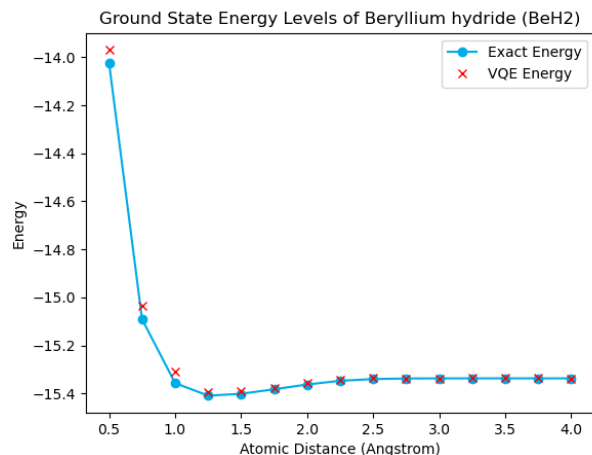


Figure 6. VQE output compared to exact energies.

This behavior can be attributed to the VQE converging to a local minimum instead of the global minimum. As discussed in section 1. of the paper, optimization algorithms have the potential to become “trapped” in a local minimum, incorrectly assuming it to be the global minimum. In the context of the VQE, a local minimum occurs when the initialization of the algorithm fails to span the global minimum. This observation implies that the Hartree-Fock initialization may not sufficiently explore the entire parameter space correctly.

5.2. Different Optimizer Comparison

When analyzing how the different optimizers influenced the results of the VQE, we noticed a shift in results amongst the 4 optimizers mentioned in section 4.4.

Our experiment set up was to simulate the different optimizers on Lithium Hydride with two iterations. The reason why two iterations were chosen was because as seen in Figure 5 with the SLSQP optimizer, it couldn't find the exact energy level at that state. Therefore, there is still room for improvement. We could have chosen one iteration, but we wanted the optimizer to have a chance to update its parameters from not only the first output of the quantum circuit, but also update the parameters on the suggestions it made through the first iteration. These are the two different parts an optimizer goes through before it just keeps on repeating upon itself.

Figure 7 shows the results of our experiment with optimizers CG and L-BFGS-B demonstrating notable effectiveness in assisting the VQE in converging to the minimum energy. The y-axis represents the difference of VQE energy from the exact energy. Meanwhile, the x-axis is the different interatomic distance the ground state energy was measured on.

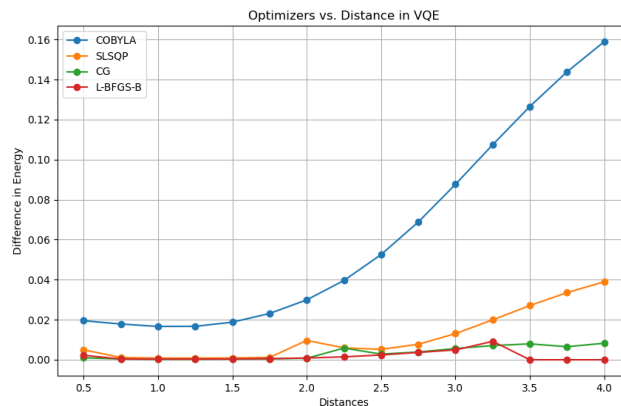


Figure 7. Optimizer comparison on LiH with 2 iterations.

From the results, it appears that COBYLA encounters difficulty in updating parameters and becomes less accurate as the interatomic distance increases. SLSQP does hold itself to be a good optimizer. Although runtime is not a part of the experiment, CG and L-BFGS-B did take a noticeable longer time to finish executing compared to the other two optimizers but were by far the best ones.

With this observation, we ran the same experiment but with modelling bigger molecules such as Water (H_2O). As mentioned earlier, bigger molecules are more complex and therefore require more iterations to find where the minimum energy begins to converge. When comparing the results of all four optimizers, they were all noticeably the **same**. Based on our results, it doesn't really matter which optimizer you use, especially when modelling bigger molecules. However, in the future when the VQE can run on an actual quantum computer, further testing should be done on larger molecules to see if it exhibits a different shift with the results.

5.3. Iteration Correlation

The last experiment we conducted was to see how many iterations it takes for the VQE to achieve maximum accuracy in getting to the exact energy level for any molecule. We simulated the molecules from 0.25 - 2.00 angstroms as this is the range where the minimum energy lies. Any further distances would have just been irrelevant (refer to Figure 4).

Table 1 is our experimental results in which we modelled Dihydrogen, Lithium Hydride, Beryllium Hydride, and Water. These were the only molecules we could model as current simulators cannot simulate any bigger molecules. This is due to the main difficulty in the state preparation where it's expressible and scalable Ansatz becomes highly complex and has a long decomposition into quantum gates [8].

Table 1. Experiment results.

Molecule	# Electrons	# Iterations
H2	2	4
LiH	4	8
BeH2	6	27
H2O	10	86

As a result, when modelling molecules with more electrons, there needs to be more iterations to get it closer to the exact energy. It's important to remember that the VQE is an approximation algorithm and therefore does not find the exact energy. Although with this current data, these results show that if you count the number of electrons in a molecule and square it, that number will be around the number of iterations required for maximum accuracy.

6. Conclusion

The contribution from this analysis provides an insight on how the different optimizers influence the VQE in a practical setting of simulating molecules. From the experiments, COBYLA performed the worst when simulating molecules with smaller number of electrons. However, as electrons increase, they all performed noticeably the same. Also, when trying to find the number of iterations required for maximum accuracy, there seemed to be a correlation in squaring the number of electrons being modelled with the number of iterations, as the exact energy approaches. With more computing resources, the molecules could be scaled larger to further investigate that the trends we found continue to be valid.

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