VQE

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2025

Abstract

Motivation

The Variational Quantum Eigensolver uses the variational principle to compute the ground state energy of a Hamiltonian, which is the first step in computing the energetic properties of a molecule. The potential of VQE can be used for drug discovery, material science, chemical engineering.

Abstract

Advantage

An array of qubits obeys the laws of quantum mechanics, which allows for the simulation of electronic wavefunctions. Encoding the wavefunctions of a molecule on conventional computers is exponentially costly, while it only requires a linear growing number of qubits on a quantum computer. The VQE allows for the probabilistic measurement of the observable over certain classes of parameterized approximate wavefunctions, which can neither be sampled from nor have their properties computed efficiently (in polynomial time) on conventional devices as system size increases.

Abstract

Ground State Energy

A ground state is a state in which atom, molecule, or ion has the lowest possible energy, and all its atoms, molecules, or ions are in their most stable arrangement. The ground state is the starting point for all chemical reactions, and it is the state in which most molecules exist under normal conditions. The reactants then absorb energy to transition to a higher energy state before reacting.

Components

- **Hamiltonian**: the matrix that describes the energy of a system. It can be written as a sum of Pauli operators. The number of terms increases with the system size relatively slowly.
- **Ansatz**: It needs to be expressive enough to represent the ground state of the Hamiltonian, but also simple enough to be efficiently optimized.
- **Optimizer**: The optimizer significantly impacts the convergence rate of VQE optimization and the overall cost of the algorithm.

Obstacles

Measurement

Despite scaling polynomially, the number of measurements needed will grow rapidly along with the system's size. We need a more efficient measurement method. In order to achieve precision with ϵ error of the expecation value of an operator, we are required to perform $O(1/\epsilon^2)$ measurements.

The Barren Plateau

The barren plateau is a phenomenon that occurs in the optimization of quantum circuits, where the gradients of the cost function become exponentially small as the number of qubits increases. This makes it difficult to find the optimal parameters for the ansatz.

Formal Definition

Given a Hamiltonian $\hat{H}$, and a trial wavefunction $|\varphi\rangle$, the ground state energy E_0 of the Hamiltonian ,is bouned by:

$$E_0 \leq \frac{\langle\varphi|\,\hat{H}\,|\varphi\rangle}{\langle\varphi|\varphi\rangle} \tag{1}$$

VQE's job is to find a parameterization of $|\varphi(\vec{\theta})\rangle$, such that the expectation value of the Hamiltonian is minimized.

The Hamiltonian

The Hamiltonian that describes the energy of Hydrogen molecule is:

$$H = g_0\mathbb{I} + g_1 Z_0 + g_2 Z_1 + g_3 Z_0 Z_1 + g_4 Y_0 Y_1 + g_5 X_0 X_1 \tag{2}$$

Where the coefficients g_i will be dependent on the distance between atoms.

The Ansatz

Using the UCC Theory to construct the ansatz:

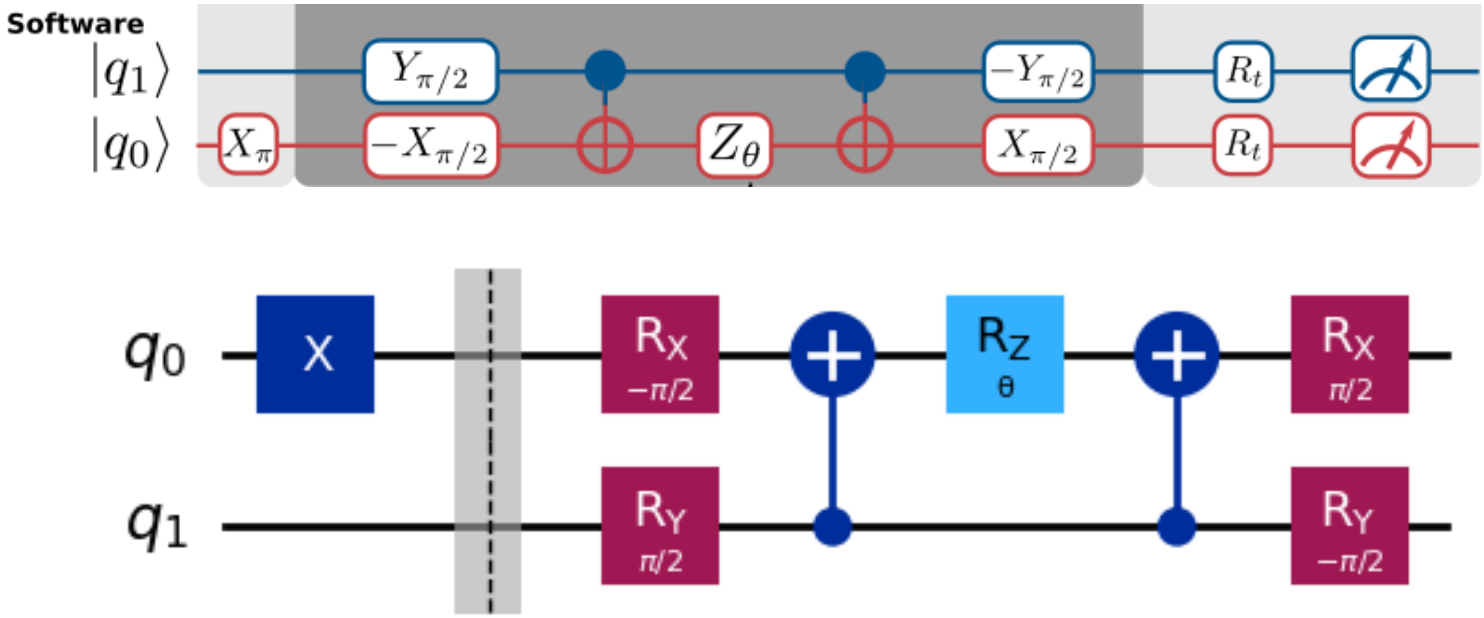
$$|\varphi(\vec{\theta})\rangle = U(\vec{\theta})\,|\varphi\rangle = e^{T(\vec{\theta}) - T(\vec{\theta})^{\dagger}}\,|\phi\rangle \tag{3}$$

Where $|\phi\rangle$ is the reference Hatree Fock state. According to the UCC theory, the ground state of equation (2) can be expressed as:

$$|\varphi(\theta)\rangle = e^{-i\theta X_0 Y_1}\,|01\rangle \tag{4}$$

where $|\phi\rangle = |01\rangle$.

The Circuit Visualization



The Cost Function

The trial wavefunction is produced by a variational quantum circuit (ansatz) $U(\vec{\theta})$ acting on $|0\rangle^{\otimes N}$,written as $|\mathbf{0}\rangle$ for simplicity, where N is the number of qubits. $\vec{\theta}$ denoting the sets of parameters taking values in $(-\pi, \pi]$, the VQE optimzation problem can be written as:

$$E(\vec{\theta}) = \langle \mathbf{0} | U^{\dagger}(\vec{\theta}) \hat{H} U(\vec{\theta}) | \mathbf{0} \rangle \tag{5}$$

More specifically, from the Hamiltonian in equation (2), we can see that the cost function is a linear combination of the expectation values of the Pauli operators:

$$E(\vec{\theta}) = \sum_{\gamma} g_{\gamma} \langle \mathbf{0} | U^{\dagger}(\vec{\theta}) \hat{H}_{\gamma} U(\vec{\theta}) | \mathbf{0} \rangle \tag{6}$$

Where $\hat{H}_{\gamma}$ is the Pauli operator in the Hamiltonian.

The Optimizer

The optimization of the VQE is NP-hard (nondeterministic polynomial-time hard). It means that there exist at least some problems in which finding an exact solution is computationally infeasible.

Obstacles

- Samping noise and gate noise on NISQ devices.
- The number of shots for measurment is limited, which affects the precision of the optimization.
- The above mentioned barren plateau phenomenon.

References

- A Review of Barren Plateaus in Variational Quantum Computing
- The Variational Quantum Eigensolver: a review of methods and best practices
- Scalable Quantum Simulation of Molecular Energies