

Quantum Imaginary Time Evolution

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The goal of many quantum algorithms is to accurately estimate the ground state and ground energy of a Hamiltonian. The ground energy is the smallest eigenvalue and its corresponding eigenvector is the ground state, and being able to solve this problem for a given Hamiltonian is important in physics and chemistry. In this paper, we will follow [1] and see how to solve this problem on a quantum computer using imaginary time evolution.

1 Imaginary Time Evolution

Recall that the evolution of a quantum system is dictated by the Schrodinger equation

$$\frac{d}{dt}|\psi\rangle = -iH|\psi\rangle. \quad (1)$$

Given an initial state $|\psi(0)\rangle$, we can solve the Schrodinger equation to obtain the unitary evolution $|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$. Suppose that we apply a change of variables $\tau = it$, which is called a Wick rotation. The chain rule says

$$\frac{d}{dt} = \frac{d}{d\tau} \frac{d\tau}{dt} = i \frac{d}{d\tau},$$

so (1) becomes

$$\frac{d}{d\tau}|\psi\rangle = -H|\psi\rangle. \quad (2)$$

When we solve equation (2) to calculate $|\psi(t)\rangle$ from an initial state $|\psi(0)\rangle$, the evolution operator becomes $e^{-H\tau}$. Notice that when τ is real, the evolution dictated by equation (2) is no longer unitary. Instead, applying the operator $e^{-H\tau}$ has the effect of exponential decay on the initial $|\psi(0)\rangle$.

Since (2) looks like exponential decay, what happens if we start with an initial state $|\psi(0)\rangle$ and let $\tau \rightarrow \infty$? Since $e^{-\tau H}|\psi(0)\rangle$ will not have norm 1, we will normalize the resulting state and consider the limit for large τ . We will show that

$$\lim_{\tau \rightarrow \infty} \frac{e^{-\tau H}|\psi(0)\rangle}{\|e^{-\tau H}|\psi(0)\rangle\|} = \lim_{\tau \rightarrow \infty} \frac{|\psi(\tau)\rangle}{\|\psi(\tau)\rangle\|} = |\phi_0\rangle,$$

where $|\phi_0\rangle$ is the ground state of the Hamiltonian H . To see why this is true, let λ_i and $|\phi_i\rangle$ be the orthonormal eigenvectors of H , with $\lambda_0 \leq \lambda_1 \leq \dots$ and express the initial state as

$$|\psi(0)\rangle = \sum_{j=0}^{N-1} c_j |\phi_j\rangle.$$

Then we can compute the normalized, time evolved state as follows. First we will apply $e^{-\tau H}$ to $|\psi(0)\rangle$ which scales the coefficients, since $e^{-\tau H}$ is diagonal. Then we will factor out the coefficient attached to the ground energy on the numerator and denominator, which leaves the ground state as the only

non-decaying term. Explicitly,

$$\begin{aligned}
\frac{|\psi(\tau)\rangle}{\| |\psi(\tau)\rangle \|} &= \frac{\sum_{j=0}^{N-1} e^{-\tau\lambda_j} c_j |\phi_j\rangle}{\| \sum_{j=0}^{N-1} e^{-\tau\lambda_j} c_j |\phi_j\rangle \|} \\
&= \frac{e^{-\tau\lambda_0} c_0 |\phi_0\rangle + \sum_{j=1}^{N-1} e^{-\tau\lambda_j} c_j |\phi_j\rangle}{\| e^{-\tau\lambda_0} c_0 |\phi_0\rangle + \sum_{j=1}^{N-1} e^{-\tau\lambda_j} c_j |\phi_j\rangle \|} \\
&= \frac{e^{-\tau\lambda_0} c_0}{\| e^{-\tau\lambda_0} c_0 \|} \left(\frac{|\phi_0\rangle + \sum_{j=1}^{N-1} e^{-\tau(\lambda_j - \lambda_0)} c_j |\phi_j\rangle}{\| |\phi_0\rangle + \sum_{j=1}^{N-1} e^{-\tau(\lambda_j - \lambda_0)} c_j |\phi_j\rangle \|} \right) \\
&= \frac{|\phi_0\rangle + \mathcal{O}(e^{-\tau(\lambda_1 - \lambda_0)})}{\| |\phi_0\rangle + \mathcal{O}(e^{-\tau(\lambda_1 - \lambda_0)}) \|} \\
&\xrightarrow{\tau \rightarrow \infty} |\phi_0\rangle,
\end{aligned}$$

where we ignore a global phase in the second to last line.

From this calculation we have three key takeaways. The first is that we are using the fact that $c_0 = \langle \phi_0 | \psi(0) \rangle \neq 0$ so the **initial state must overlap with the ground state of the Hamiltonian**. The second takeaway is that the **speed of convergence is dependent on the spectral gap** $\lambda_1 - \lambda_0$, the gap between the first excited state and the ground state. The third takeaway is that given $c_0 \neq 0$, imaginary time evolution **guarantees convergence to the ground state**.

When H is expressed as the sum of local Hamiltonians $\sum_{j=1}^m H_j$, we estimate the evolution with the Trotter product formula

$$e^{-\tau H} \approx \left(e^{-\Delta\tau H_1} \dots e^{-\Delta\tau H_m} \right)^n$$

where $\frac{\tau}{n} = \Delta\tau$. While this method works well on paper, it can be difficult to calculate $e^{-\Delta\tau H_j}$ due to the large dimension of the state space. This motivated the development of the quantum imaginary time evolution (QITE) algorithm, which uses a quantum computer to carry out the imaginary time evolution of and find the ground state.

2 Quantum Imaginary Time Evolution Algorithm

The difficulty in carrying out imaginary time evolution on a quantum computer is that the evolution is non-unitary. In fact, there is a more general notion of quantum processes called quantum channels, and imaginary time evolution is not even a quantum channel since it does not preserve trace. At step j of Trotter, we apply $e^{-\Delta\tau H_j}$ to the current state $|\psi\rangle$. Since we wish to simulate this on a quantum computer, we normalize this evolved state to have norm 1. Then the goal of the algorithm is to use a quantum computer to approximate the evolution

$$|\psi\rangle \mapsto \frac{|\psi(\Delta\tau)\rangle}{\| |\psi(\Delta\tau)\rangle \|} = \frac{e^{-\Delta\tau H_j} |\psi\rangle}{\| e^{-\Delta\tau H_j} |\psi\rangle \|}$$

with a unitary transformation $e^{-iA_j\Delta\tau}$. Label the evolved and normalized state $|\psi'\rangle$, then at each Trotter step we have the approximation

$$|\psi\rangle \mapsto |\psi'\rangle \approx e^{-iA_j\Delta\tau} |\psi\rangle \quad (3)$$

If we can an appropriate A_j , then we can successfully implement imaginary time evolution on a quantum computer.

Recall that H_j is local, and here local means that H_j acts non-trivially on a site of k neighboring qubits with respect to some topology. We will call the site where H_j acts non-trivially its support. Since A_j is derived from H_j , we would like to construct A_j with the same locality as H_j . However, the non-linear renormalization step in (3) does not allow this. To understand why, consider the following example.

Let $H = |0\rangle\langle 0| \otimes I$, which acts non-trivially on the first qubit. Then the evolution $e^{-\tau H}$, along with renormalization, transforms a bell state as

$$\frac{|00\rangle + |11\rangle}{\sqrt{2}} \xrightarrow{e^{-\tau H}} \frac{c|00\rangle + |11\rangle}{\sqrt{2}} \xrightarrow{\text{renormalize}} \frac{c|00\rangle + |11\rangle}{\sqrt{c+1}}$$

for some $c = e^{-\tau}$. Notice that even though H acted only on qubit 1, at the end of the process the state of qubit 2 is changed, no longer in an even superposition of $|0\rangle$ and $|1\rangle$. From this example we can see that in general, **the operator A_j cannot be local on the same site as H_j** , we must expand the support of A_j to a larger neighborhood encompassing the support of H_j . One special case is when $|\psi\rangle$ is a product state. In this case when we renormalize after applying $e^{-\tau H_j}$, we can keep the coefficients with the qubits on which H_j acts, and the locality is preserved.

In general, to answer the question of how large the neighborhood on which A_j acts should be, we introduce the notion of a correlation length. A state $|\psi\rangle$ has finite correlation length if for observables A and B which act on qubits i and j , the correlation shrinks exponentially as the distance $|i - j|$ increases. If the state $|\psi\rangle$ has a finite correlation length, then a consequence of a result called Uhlmann's theorem states that we can construct A_j in a neighborhood around the support of H_j , the size of which is bounded by the correlation length.

After determining the support of A_j , we must calculate A_j . We can express A_j as a linear combination

$$A_j = \sum_I a_I \sigma_I$$

where σ_I is a Pauli string and the sum is over all such Pauli strings with the same support as A_j . Then the task is to optimize the coefficients a_I . If we use a first order approximation $e^{-i\Delta\tau A_j}|\psi\rangle \approx |\psi\rangle - i\Delta\tau A_j|\psi\rangle$, then obtaining a good approximation means minimizing

$$\| |\psi'\rangle - (|\psi\rangle - i\Delta\tau \sum_I a_I \sigma_I) \|^2$$

over all a_I . If we expand out this inner product and simplify notation with $|\psi'\rangle - |\psi\rangle = |D\rangle$, we are minimizing

$$\begin{aligned} & \langle D|D\rangle + i\Delta\tau \sum_J a_J \langle D|\sigma_J|\psi\rangle - i\Delta\tau \sum_I a_I \langle \psi|\sigma_I^\dagger|D\rangle + \sum_{I,J} a_I a_J \Delta\tau^2 \langle \psi|\sigma_I^\dagger \sigma_J|\psi\rangle \\ &= \langle D|D\rangle + \Delta\tau \sum_I a_I (i\langle D|\sigma_I|\psi\rangle - i\langle \psi|\sigma_I^\dagger|D\rangle) + \sum_{I,J} a_I a_J \Delta\tau^2 \langle \psi|\sigma_I^\dagger \sigma_J|\psi\rangle. \end{aligned}$$

Simplifying the notation, we wish to minimize the function

$$f(\mathbf{a}) = \sum_I b_I a_I + \sum_{I,J} a_I a_J S_{IJ} = \mathbf{b}^T \mathbf{a} + \mathbf{a}^T \mathbf{S} \mathbf{a}$$

where $b_I = i\langle D|\sigma_I|\psi\rangle - i\langle \psi|\sigma_I^\dagger|D\rangle$ and $S_{IJ} = \langle \psi|\sigma_I^\dagger \sigma_J|\psi\rangle$. If we compute the gradient of f and set it equal to zero, we find the minimum is achieved when \mathbf{a} solves the system

$$(\mathbf{S} + \mathbf{S}^T) \mathbf{a} = -\mathbf{b}.$$

With this, we can solve the least squares problem and calculate A_j , completing the description of the QITE algorithm.

3 Discussion

The QITE algorithm provides a way to calculate the ground state of a Hamiltonian H , with guaranteed convergence if the initial state has nonzero overlap. Compared with the variational quantum eigensolver (VQE) algorithm, a big advantage for QITE is that there is no need to choose an ansatz. The main drawbacks of QITE are that QITE can require deeper circuits than VQE, and QITE requires an initial state with good overlap with the ground state.

References

- [1] M. Motta, C. Sun, A. T. K. Tan, M. J. O'Rourke, E. Ye, A. J. Minnich, F. G. S. L. Brandão, and G. K.-L. Chan, "Determining eigenstates and thermal states on a quantum computer using quantum imaginary time evolution," *Nature Physics*, vol. 16, p. 205–210, Nov. 2019.