2022开源之夏MindSpore项目结项报告

一、项目基本信息

- 项目名称：基于昇思MindQuantum，实现量子虚时演化算法
- 项目编号：221cb0176
- 项目主导师：谢晴兴 634436649@qq.com (mailto:634436649@qq.com)
- 项目承接人：储贻达 chu_yi_da@163.com (mailto:chu_yi_da@163.com)
- 项目难度：进阶
- 项目要求：1. 实现变分线路参数的量子虚时演化算法，用于求解分子体系的基态能 2. 探索其它形式的量子虚时演化算法 3. 实现相关功能，相关评估指标符合要求，代码合入社区。
- 项目技术要求：深度学习，python，量子计算，MindSpore
- 方案描述：在本次项目中，我们将运用MindSpore quantum框架在量子线路上完成虚时演化算法的实现，并运用算法程序解决一些量子多体系统的基态能求解问题。
- 时间规划：

时间	内容	预期目标
6月15日-7月15日	前期调研，阅读文献	详细阅读相关文献
7月15日-8月1日	基本实现算法框架	实现基于Mindquantum的核心函数构建
8月1日-9月1日	完成整体算法并测试算法	实现基本算法的分子基态能求解问题
9月1日-9月30日	探索算法更多可能性	基于Mindquantum探究噪声对算法的影响

二、项目进展

1. 已完成工作

1.1 项目基本原理

(1). 摘要

Imaginary time evolution is a powerful tool for studying quantum systems. While it is possible to simulate with a classical computer,the time and memory requirements generally scale exponentially with the system size. Conversely, quantum computers can efficiently simulate quantum systems, but not non-unitary imaginary time evolution. So in this year's Open Source Promotion Plan, we think about wheter this imaginary time evolution algorithm can be accomplished by quantum computer. In fact, there have been some studies in this area that have given some solutions. For example, in this artical [Motta, Mario, et al.Nature Physics 16.2 (2020): 205-210], an algorithm is proposed to make this non-unitary evolution possible in quantum circuits, which is called the QITE(Qauntum Imaginary Time Evolution) algorithm. In addition to this, other methods are also proposed in another article [McArdle, Sam, et al.npj Quantum Information 5.1 (2019): 1-6.]. Different from the former approach, McArdle, Sam, et al. pointed out that a variational algorithm enables quantum circuits to simulate the process of imagnary time evolution, which is called the VITE(Variational quantum Imaginary Time Evolution)

algorithm. And the effect of the algorithm on solving the ground state energy of the molecular system is shown in the article. In addition, we also found that the VITE algorithm is very suitable to be implemented with the Mindspore quantum[] library. Therefore, in this Open Source Promotion Plan project, we refer to the principle of this article, and think about how to use the MindSpore quantum library to complete this VITE algorithm and verify its effectiveness. And on this basis, the algorithm program is used to solve the ground state energy of some more complex molecular systems. Finally, we also explore the performance of this algorithm in the presence of quantum noise.

(2). 理论概述

In a quantum many-body systems that are described by Hamiltonian H, if given an initial state $|\psi\rangle$, the normalised imaginary time evolution is defined by

$$|\psi(\tau)\rangle = A(\tau)e^{-H\tau}|\psi(0)\rangle$$

where the $A(\tau) = 1/\sqrt{\langle\psi(0)|e^{-2H\tau}|\psi(0)\rangle}$ is a normalisation factor. And when the initial state has a non-zero overlap with the ground state, the state at $\tau \to \infty$ is the ground state of H. It is precisely because this principle that we can choose the appropriate initial state to obtain the ground state of a quantum system by imaginary time evolution.

In variational method, we can approximate the evolution state using a parametrised trial state $|\phi(\vec{\theta}(\tau))\rangle$, with $\vec{\theta}(\tau) = (\theta_1(\tau), \theta_2(\tau), \dots, \theta_N(\tau))$. And using the quantum circuit, we can prepare the trial state $|\phi(\vec{\theta})\rangle$ by applying a sequence of parametrised unitary gates,

$$V(\vec{\theta}) = U_N(\theta_N)\dots U_k(\theta_k)\dots U_1(\theta_1)$$

to the initial state $|\bar{0}\rangle$. We express this as $|\phi(\vec{\theta})\rangle = V(\vec{\theta})|\bar{0}\rangle$ and remark that $V(\vec{\theta})$ is also referred to as the ansatz.

And in this artical it's pointed that we can use the McLachlan's variational principle to simulate the imaginary time evolution of the trial state:

$$\delta||\left(\partial/\partial\tau + H - E_\tau\right)|\psi(\tau)\rangle|| = 0$$

where the $||\rho|| = Tr\left[\sqrt{\rho\rho^\dagger}\right]$ denotes the trace norm of a state and $E_\tau = \langle\psi\tau|H|\psi\tau\rangle$. So we can use this variational principle by replacing the $|\psi(\tau)\rangle$ with $|\phi(\tau)\rangle = |\phi(\vec{\theta}(\tau))$.

So we can get

$$\begin{aligned}
||\partial/\partial\tau + H - E_\tau|\psi(\tau)\rangle|| &= \left((\partial/\partial\tau + H - E_\tau)|\psi(\tau)\rangle\right)^\dagger \left((\partial/\partial\tau + H - E_\tau)|\psi(\tau)\rangle\right) \\
&= \sum_{i,j}\frac{\partial\langle\phi(\tau)|}{\partial\theta_i}\frac{\partial|\phi(\tau)\rangle}{\partial\theta_j}\dot{\theta}_i\dot{\theta}_j + \sum_i\frac{\partial\langle\phi(\tau)|}{\partial\theta_i}(H - E_\tau)|\phi(\tau)\rangle\dot{\theta}_i \\
&= \sum_i\langle\phi(\tau)|(H - E_\tau)\frac{\partial|\phi(\tau)\rangle}{\partial\theta_i}\dot{\theta}_i + \langle\phi(\tau)|(H - E_\tau)^2|\phi(\tau)\rangle.
\end{aligned}$$

Focusing on $\dot{\theta}_i$, we obtain

$$\begin{aligned}
\frac{(\partial||\partial/\partial\tau + H - E_\tau)|\phi(\tau)\rangle||}{\partial\dot{\theta}_i} = &\sum_j\left(\frac{\partial\langle\phi(\tau)|}{\partial\theta_i}\frac{\partial|\phi(\tau)\rangle}{\partial\theta_j} + \frac{\partial\langle\phi(\tau)|}{\partial\theta_j}\frac{\partial|\phi(\tau)\rangle}{\partial\theta_i}\right)\dot{\theta}_j \\
&+ \frac{\partial\langle\phi(\tau)|}{\partial\theta_i}(H - E_\tau)|\phi(\tau)\rangle + \langle\phi(\tau)|(H - E_\tau)\frac{\partial\phi(\tau)\rangle}{\partial\theta_i}
\end{aligned}$$

Considering the normalisation condition for the trial state $|\phi(\tau)\rangle$,

$$\langle\phi(\tau)|\phi(\tau)\rangle = 1,$$

we have

$$E_\tau \frac{\partial\langle\phi(\tau)|\phi(\tau)\rangle}{\partial\theta_i} = E_\tau\left(\frac{\partial\langle\phi(\tau)|}{\partial\theta_i}|\phi(\tau)\rangle + \langle\phi(\tau)|\frac{\partial|\phi(\tau)\rangle}{\partial\theta_i}\right) = 0$$

and the derivative is simplified to

$$\frac{\partial||(\partial/\partial\tau + H - E_\tau)|\phi(\tau)\rangle||}{\partial\dot{\theta}_i} = \sum_j A_{ij}\dot{\theta}_j - C_i.$$

Where

$$A_{ij} = \Re\left(\frac{\partial\phi(\tau)|}{\partial\theta_i}\frac{\partial|\phi(\tau)\rangle}{\partial\theta_j}\right),$$
$$C_i = -\Re\left(\frac{\partial\langle\phi(\tau)|}{\partial\theta_i}H|\phi(\tau)\rangle\right).$$

McLachlan's variational principle requires

$$\frac{\partial||(\partial/\partial\tau + H - E_\tau)|\phi(\tau)\rangle||}{\partial\dot{\theta}_j} = 0,$$

which is equivalent to the differential equation of the parameters

$$\sum_j A_{ij}\dot{\theta}_j = C_i$$

So far, we use the parameterized ansatz circuit to encode trial quantum state, with the help of the MaLachlan's variational principle, the imaginary time evolution of state can be transformed into the special parameter update method which given in the above formula.

(3).算法初步实现-基于MindSpore quantum

Through the above analysis, we know that for a given quantum many-body system, the core part of implementation of the VITE algorithm is the calculation of the A_ij matrix and C_i vector. And the Mindquantum library of version 0.7.0 provides such a port mindquantum.core.circuit.partial_psi_partial_psi(circuit, backend) for Quantum Fisher Information calculation. But we found that this function is equal the calculation of A_{ij} matrix, so it's convenient to get the A matrix. And we can follow the method and idea of this function to create a function to calculate the C vector. We can use these two main functions --partial_psi_partial_psi() and get_ci_matrix() -- to get the A_{ij} and C_i. Then we need to calculate the inverse of A_{ij} to update the parameters of ansatz circuit. But the A_{ij} is not always an invertible matrix, so here we use the SVD decomposition to approximate the inverse matrix of A_{ij} in this case.

(4). 初步验证算法有效性

At first, we use the VITE method to find the groud-state energy of the H_2 molecules in their minimal spin-orbital bais set.

After some approximation, the qubit Hamiltonian of H_2 molecules can be representation by:

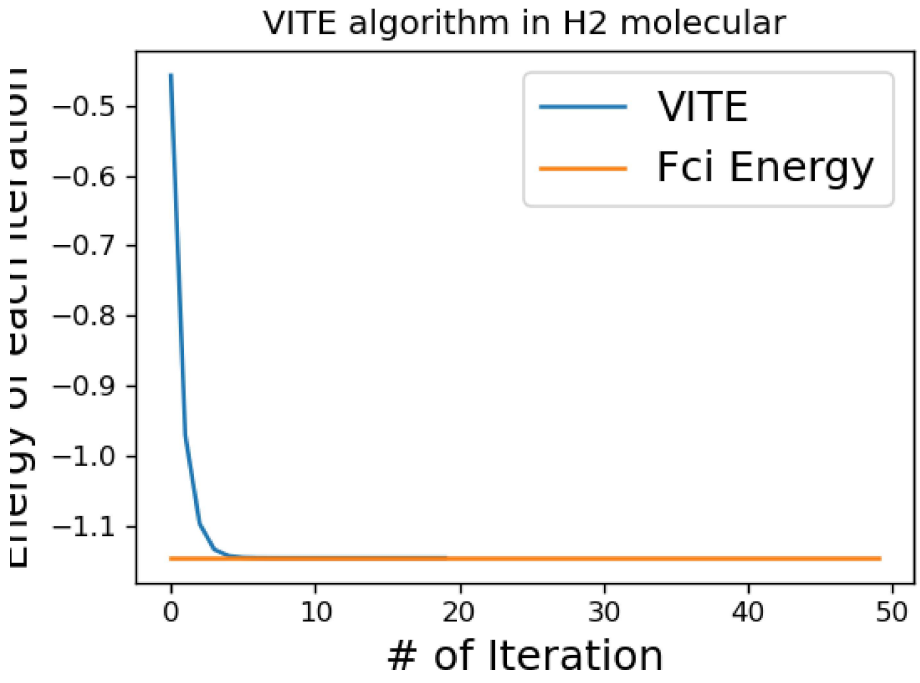
$$H = g_0 I + g_1 Z_0 + g_2 Z_1 + g_3 Z_0 Z_1 + g_4 Y_0 Y_1 + g_5 X_0 X_1$$

And we make use of the universal ansatz, then call the previous function to complete the demonstration of this VITE algorithm.

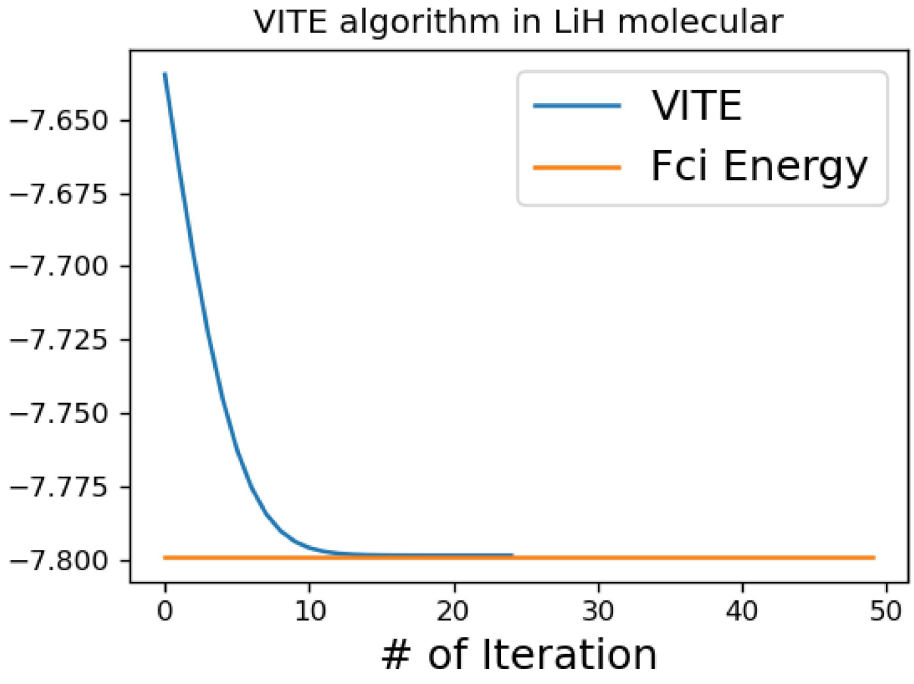
(5). 进一步运用在更复杂的分子体系上

After preliminarily verifying the effectiveness of the algorithm on hydrogen molecules, we further thought about whether we could use the VITE algorithm on more complex LiH molecules.

1.2 结果展示与分析



As the results show, our algorithm based on mindqunatum is indeed effective. For hydrogen molecules, it only takes a few steps of iteration to quickly converge to the ground state energy. This also basically verifies the effectiveness of the VITE algorithm.



When we apply the algorithm to more complex molecular systems and deeper quantum circuits, we find that as the complexity of the system increases, the computational difficulty and iteration times required by the algorithm also increase, but the algorithm can still solve the ground state energy!

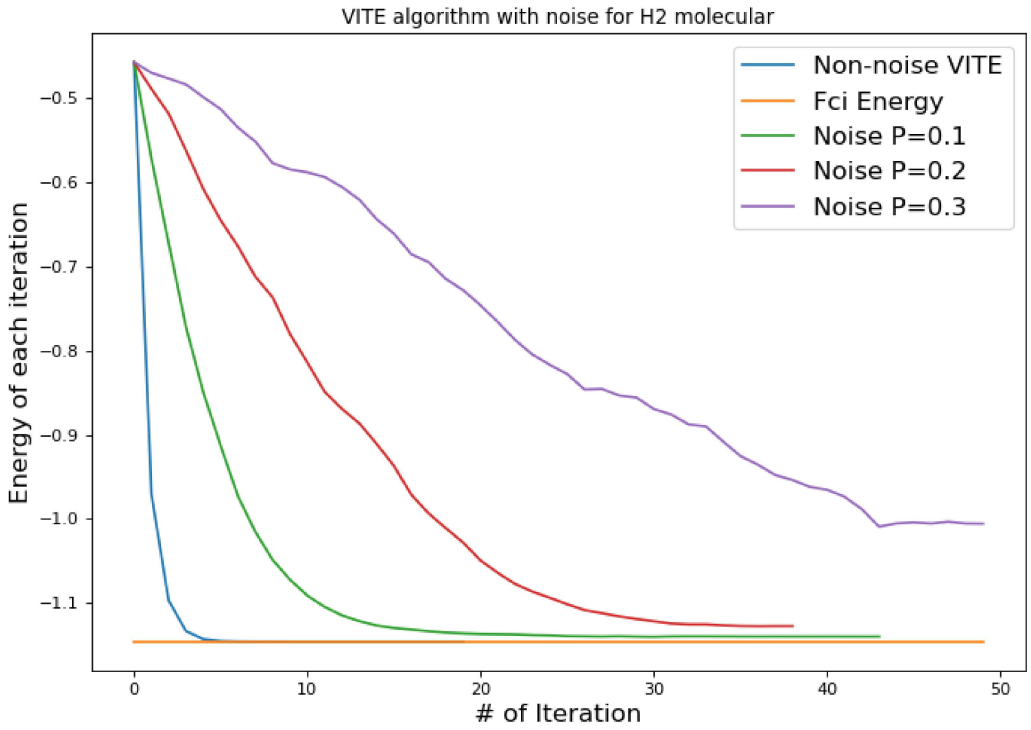
1.3 进一步分析噪声对算法带来的影响

So far, we have basically completed the basic goals required by the project. But we didn't stop there, we continued to think about whether quantum noise will have a huge impact on the convergence of the algorithm, because the inverse of the A_{ij} matrix is required.

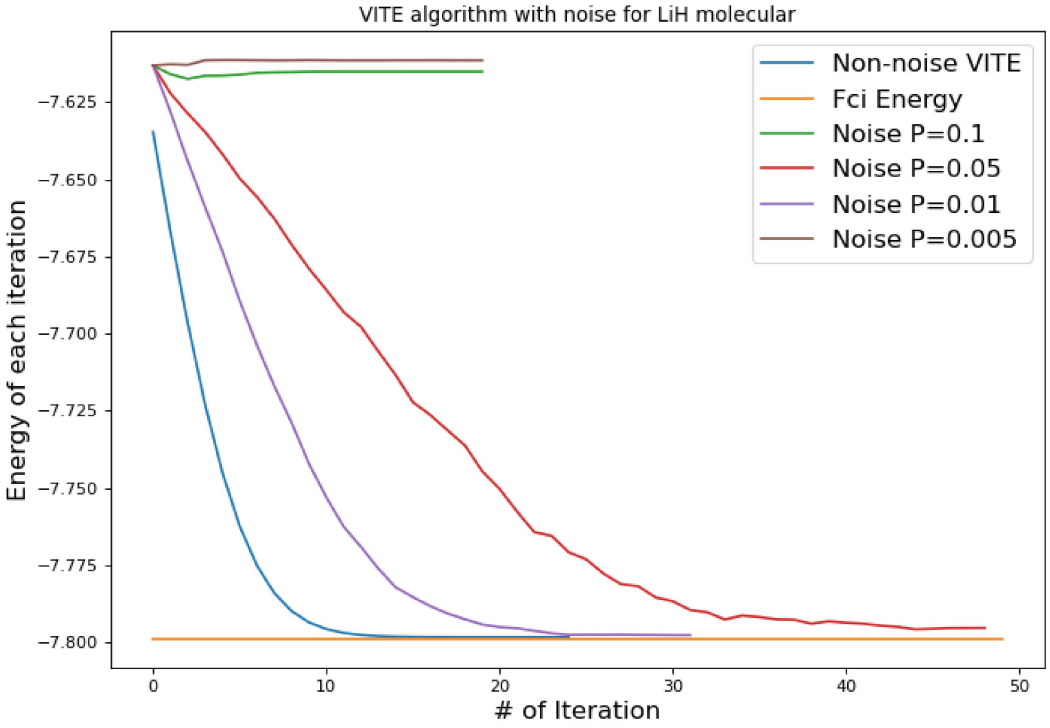
Here we first consider the impact of circuit noise on the algorithm implement. There is a kind of noise that affects the quantum circuit. After a certain quantum operation, the circuit is likely to be affected by an additional pauli gate, which is called a pauli channel. And if the X, Y, Z gates split equally, it is called a depolarization channel. This channel is often used to describe the noise generated by gate operation in real quantum hardware. And it's described by,

$$\epsilon_{DF}(\rho) = (1-p)\rho + \frac{p}{3}(X\rho X + Y\rho Y + Z\rho Z)$$

But the problem we face is how to introduce the noise on the quantum circuit. Due to the characteristics of the Mindqauntum library, if we use the noise port provided by itself to simulate the noise, then the previous function cannot be used to obtain the gradient of quantum state. So this requires us to construct the noise-containing circuit and design an algorithm to simulate the effect. What we adopt is a method based on Monte Carlo idea to introduce random numbers to randomize a large number of samples, and then take the mean value, so as to approximate the real moise circuit.



As shown in the result figure, when the quantum circuit noise is introduced, the stability of the algorithm will be affected and its convergence speed will be greatly slowed down. Even when the noise gradually increases, we find that the algorithm will fail and cannot converge to the ground state energy. But this is only the effect of hydrogen molecules on a shallow circuit. So we thought about whether the effect of noise would be different for more complex molecules on deeper circuit. So next, we still select LiH molecule to explore the impact of noise on the VITE algorithm。



The results in the figure once again verify our conjecture that for deeper lines, the implementation of the VITE algorithm will be more vulnerable to noise.

2. 遇到的问题及解决方案

- 如何在量子线路完成虚时演化算法?

> 解决方案：阅读文献，对比不同算法的原理。并最终确定关注于variational imaginary time evolution(VITE)算法。

- 如何基于MindSpore quantum程序库去实现VITE算法所需的核心函数?

> 解决方案：首先基于线路自己实现求梯度方案，但发现效率并不高。无法支持算法的验证工作。于是借助mindquantum已有的quantum fisher information板块来实现计算，并且基于其实现原理，自己搭建其他所需函数。

- 如何基于算法完成复杂分子体系的基态能求解?

> 解决方案：学习有关量子化学相关知识，并且运用约化密度矩阵分析来简化分子体系的Hamiltonian，使其能够在有限计算资源情况下任然能够运用算法程序完成所需计算。

- 如何运用Mindquantum框架引入噪声?

> 解决方案：阅读量子噪声有有关资料和mindquantum自带的噪声板块函数。

- 如何在Mindquantum实现的噪声量子线路上实现梯度计算?

> 解决方案：因为mindquantum限制了含噪声线路的梯度计算。于是借助Monte Carlo思想，自己构建算法来模拟含噪声线路的梯度计算，并验证噪声对于VITE算法的影响。

3. 后续思考和安排

基于本次开源之夏项目的开发，思考能否将VITE算法运用到更多的量子多体体系上并探究其效果差异；思考VITE算法与传统的GD等梯度算法在对于分子体系基态能求解上表现的不同；思考其他类型噪声对于算法的影响。

4.主要参考文献

[1] McArdle, Sam, et al. "Quantum computational chemistry." Reviews of Modern Physics 92.1 (2020): 015003.

[2] McArdle, Sam, et al. "Variational ansatz-based quantum simulation of imaginary time evolution." npj Quantum Information 5.1 (2019): 1-6.

[3] Li, Ying, and Simon C. Benjamin. "Efficient variational quantum simulator incorporating active error minimization." Physical Review X 7.2 (2017): 021050.

[4] Motta, Mario, et al. "Determining eigenstates and thermal states on a quantum computer using quantum imaginary time evolution." Nature Physics 16.2 (2020): 205-210.

[5] Seeley, Jacob T., Martin J. Richard, and Peter J. Love. "The Bravyi-Kitaev transformation for quantum computation of electronic structure." The Journal of chemical physics 137.22 (2012): 224109.

[6] Li, Yifan, et al. "Variational quantum simulation for quantum chemistry." Advanced Theory and Simulations 2.4 (2019): 1800182.