Quantum Computing

Variational Quantum Simulation

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*Negative Result

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INTRODUCTION

Variatonal Quantum Simulation

Variational Quantum Simulation involves simulating quantum processes on a quantum computer using parameterized trial states, and mapping the target problem onto a cost function which depends on the measurement outcomes of the quantum state.

The cost function is input into a classical optimizer which tweaks the values of the parameters and runs the circuit again with a new trial state. This process of optimization and running the circuit continues until a specified number of iterations or accuracy is reached.

The VQS method provides a quantum advantage since the preparation as well as measurement of quantum states is quite straightforward in a quantum computer, as opposed to classical simulations of quantum behavior. Further, the preparation of entangled states is easier on a quantum computer.

INTRODUCTION

Static Problem: Rayleigh-Ritz Method

The Rayleigh-Ritz method can be used to solve static problems involving calculation of the ground state energy E_0 of a Hamiltonian **H**. This energy E_0 can be given as:

$$E_0 = \min_{|\psi\rangle} \frac{\langle\psi| H |\psi\rangle}{\langle\psi|\psi\rangle} \quad \text{--(1)}$$

$$\langle A\rangle_\psi = \langle\psi|A|\psi\rangle$$

- Classical Case

The ansatz can be prepared as a linear combination of a few basis states to give

$$|\phi(\vec{a})\rangle = \sum_i a_i |\phi_i\rangle \quad \text{--(2)}$$

The minimum energy obtained from among these states would give an upper bound on the ground state energy (since the ground state energy would be the minimum among all possible states, and we are only considering a subset)

$$E_0 \leq E_0^{est} = \min_{\vec{a}} \frac{\langle\phi(\vec{a})| H |\phi(\vec{a})\rangle}{\langle\phi(\vec{a})|\phi(\vec{a})\rangle} = \min_{\vec{a}} \frac{\sum_{i,j} a_i^* a_j \langle\phi_i| H |\phi_j\rangle}{\sum_{i,j} a_i^* a_j \langle\phi_i|\phi_j\rangle} \quad \text{--(3)}$$

This minimization problem could be solved either analytically or numerically.

INTRODUCTION

Static Problem: Rayleigh-Ritz Method

• Quantum Case

The ansatz can be prepared using a sequence of parameterized quantum gates to yield

$$|\phi(\vec{\theta})\rangle = R_N(\theta_N)\dots R_k(\theta_k)\dots R_1(\theta_1)\,|\bar{0}\rangle \quad \text{--(4)}$$

The measurement is performed after applying the relevant circuitry, and the measurement outcomes are used to evaluate the cost function. This cost function is optimized classically, and the optimal values of the parameters $\boldsymbol{\theta_1}, \dots, \boldsymbol{\theta_N}$ are obtained.

Quantum Advantage: The preparation as well as the measurement of the ansatz is easier on a quantum computer as compared to a classical computer, since the quantum behavior which is inherent in a quantum computer is difficult to simulate on a classical computer.

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Variational Quantum Eigensolver

This is one of the implementations of the Rayleigh-Ritz method in quantum computing. Given a Hermitian matrix **H**, the VQE determines its minimum eigenvalue using an initial guess called an ansatz, and iteratively updating it until the desired accuracy is achieved.

The VQE utilizes the unitary operator **U3**, given as

$$U3(\theta, \phi, \lambda) = \begin{pmatrix} \cos(\frac{\theta}{2}) & -e^{i\lambda}\sin(\frac{\theta}{2}) \\ e^{i\phi}\sin(\frac{\theta}{2}) & e^{i\lambda+i\phi}\cos(\frac{\theta}{2}) \end{pmatrix} \quad \text{--(5)}$$

This gate inputs three parameters, $\boldsymbol{\theta}$, $\boldsymbol{\Phi}$, and $\boldsymbol{\lambda}$, and can be used to implement any possible single-qubit transformation up to a global phase. A combination of these **U3** gates, along with controlled gates for entanglement, can be used to generate our variational circuit (also known as the variational form).

The parameters are then optimized for a given cost function using a classical optimizer. Some classical optimizers commonly used in Qiskit for this purpose are SLSQP and COBYLA.

INTRODUCTION

Dynamic Problem (Closed System, Pure State Case)

The Schrödinger's equation can be given as

$$\frac{d\,|\psi(t)\rangle}{dt} = -iH\,|\psi(t)\rangle \qquad \text{--(6)}$$

We can approximate the differential as a difference to obtain

$$|\psi(t+\delta t)\rangle \approx |\phi(\vec{\theta}(t))\rangle - i\delta t H\,|\phi(\vec{\theta}(t))\rangle \qquad \text{--(7)}$$

The state $\boldsymbol{\psi}$ can be approximated by the trial state $\boldsymbol{\Phi}$ as

$$|\phi(\vec{\theta}(t+\delta t))\rangle \approx |\phi(\vec{\theta}(t))\rangle - i\delta t H\,|\phi(\vec{\theta}(t))\rangle \qquad \text{--(8)}$$

Using Taylor's theorem, we can obtain

$$|\phi(\vec{\theta}(t+\delta t))\rangle \approx |\phi(\vec{\theta}(t))\rangle + \sum_j \frac{\partial\,|\phi(\vec{\theta}(t))\rangle}{\partial\theta_j}\delta\theta_j \qquad \text{--(9)}$$

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Dynamic Problem (Closed System, Pure State Case)

Hence, from equations **(8)** and **(9)**, the simulation of the Schrödinger's equation can be approximated by

$$\sum_j \frac{\partial \left|\phi(\vec{\theta}(t))\right\rangle}{\partial \theta_j} \delta\theta_j \approx -i\delta t H \left|\phi(\vec{\theta}(t))\right\rangle \quad \text{--(10)}$$

From **(8)**, the RHS can be interpreted as the evolution of the state according to the Schrödinger's equation. The LHS denotes the change in the trial state caused by a small change in the time-dependent parameters. Hence, this equation can be used to map the evolution of the state onto the time evolution of the parameters. Using different variational principles, we aim to select time-dependent parameters that minimize the difference between the LHS and the RHS of **(10)** for a more accurate approximation.

Different variational principles use different ways to utilize equation **(10)**

- Dirac-Frenkel → Projects the equation onto the tangent subspace $\{\frac{\partial|\phi(\vec{\theta}(t))\rangle}{\partial\theta_j}\}$ --(11)
- McLachlan's → Minimizes the 'distance' between the LHS and the RHS $\delta\|(d/dt + iH)\left|\phi(\vec{\theta}(t))\right\rangle\| = 0$ --(12)
- Time-dependent → Uses the Euler-Lagrange equation

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Dirac-Frenkel Variational Principle

As we have seen **(6)(8)(9)**, the Schrödinger's equation can be written as

$$\frac{d\left|\phi(\vec{\theta}(t))\right\rangle}{dt} = \sum_i \frac{\partial\left|\phi(\vec{\theta}(t))\right\rangle}{\partial\theta_i}\dot{\theta}_i = -iH\left|\phi(\vec{\theta}(t))\right\rangle \quad \text{--(13)}$$

We can construct a projector **P** to project the RHS of equation **(13)** onto the tangent subspace **(11)**. The projector can be given as

$$P = \sum_i \frac{\partial\left|\phi(\vec{\theta}(t))\right\rangle}{\partial\theta_i}\frac{\partial\left\langle\phi(\vec{\theta}(t))\right|}{\partial\theta_i} \quad \text{--(14)}$$

Pre-multiplying the LHS and RHS of **(13)** with **P**, we get

$$P\sum_j \frac{\partial\left|\phi(\vec{\theta}(t))\right\rangle}{\partial\theta_j}\dot{\theta}_j = -iPH\left|\phi(\vec{\theta}(t))\right\rangle \quad \text{--(15)}$$

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Dirac-Frenkel Variational Principle

Expanding **P** from **(15)**, we get

$$i\sum_i \frac{\partial |\phi(\vec{\theta}(t))\rangle}{\partial\theta_i}\frac{\partial \langle\phi(\vec{\theta}(t))|}{\partial\theta_i}\sum_j \frac{\partial |\phi(\vec{\theta}(t))\rangle}{\partial\theta_j}\dot{\theta}_j = -i\sum_i \frac{\partial |\phi(\vec{\theta}(t))\rangle}{\partial\theta_i}\frac{\partial \langle\phi(\vec{\theta}(t))|}{\partial\theta_i}H|\phi(\vec{\theta}(t))\rangle \quad \text{--(16)}$$

Equating the coefficients of $\frac{\partial|\phi(\vec{\theta}(t))\rangle}{\partial\theta_i}$ in **(16)**, we get

$$\sum_j \frac{\partial \langle\phi(\vec{\theta}(t))|}{\partial\theta_i}\frac{\partial |\phi(\vec{\theta}(t))\rangle}{\partial\theta_j}\dot{\theta}_j = -i\frac{\partial \langle\phi(\vec{\theta}(t))|}{\partial\theta_i}H|\phi(\vec{\theta}(t))\rangle \quad \text{--(17)}$$

We can express **(17)** more succinctly by constructing matrices **A** and **C** from **(17)**.

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Dirac-Frenkel Variational Principle

The matrices **A** and **C** can be given as

$$A_{i,j} = \frac{\partial \langle \phi(\vec{\theta}(t)) |}{\partial \theta_i} \frac{\partial | \phi(\vec{\theta}(t)) \rangle}{\partial \theta_j} \quad \text{--(18)}$$

$$C_i = \frac{\partial \langle \phi(\vec{\theta}(t)) |}{\partial \theta_i} H | \phi(\vec{\theta}(t)) \rangle \quad \text{--(19)}$$

Using these matrices, we can express **(17)** as

$$\sum_j A_{i,j} \dot{\theta}_j = -iC_i \quad \text{--(20)}$$

Using **(20)**, we can calculate the time evolution of the parameters $\boldsymbol{\theta}_j$ given **A** and **C**.

VARIATIONAL QUANTUM EIGENSOLVER

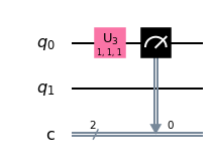
VQE

We have designed a VQE program to calculate an eigenvector of a 2x2 unitary matrix. The implementation makes use of the property that the eigenvalues of a unitary matrix lie on a unit circle, and that the measurement probabilities for a quantum state are independent of a global phase. Next we describe the process we used, and the results.

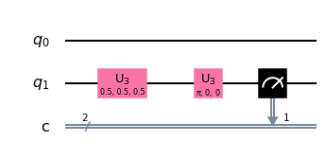
Problem Statement - Given a 2x2 unitary matrix **A**, calculate one of its eigenvectors

Circuit

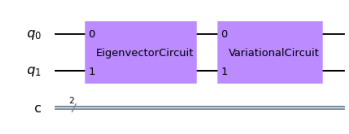
Implementation 1



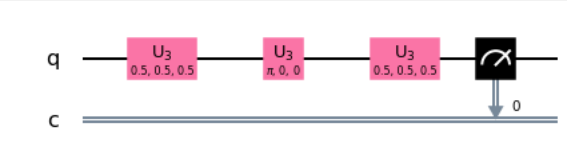
EigenvectorCircuit



VariationalCircuit



Implementation 2



VQE

Implementation 1

The eigenvector circuit uses a **U3** gate to take the initial state to a state in our trial space. The measurement output of this circuit yields the output of the measurement on the trial state, $\mathbf{\Phi}$.

The same **U3** gate is applied to the initial state in our variational circuit, followed by another **U3** gate that applies the unitary **A** to the trial state. The measurement output of this circuit yields the output of $\mathbf{A\Phi}$.

When $\mathbf{\Phi}$ is an eigenvector of **A** the output of the variational circuit must be $\mathbf{e^{i\theta}\Phi}$ since **A** is a unitary matrix. This means that when $\mathbf{\Phi}$ is an eigenvector of **A**, the measurement outcomes of the eigenvector circuit and the variational circuit must be the same. This is used as a cost function to optimize the circuit parameters.

Implementation 2

It is similar to implementation 1. Initially, a **U3** gate is applied to the initial state, followed by the **U3** representing **A**. A replica of the first **U3** gate is then applied, and the output is measured. When the state $\mathbf{\Phi}$ generated by the first **U3** gate is an eigenvector of **A**, the output of the second **U3** would be $\mathbf{e^{i\theta}\Phi}$. Since $\mathbf{\Phi}$ remains the same up to a global phase, another application of the first unitary **U3** gate would revert the state $\mathbf{e^{i\theta}\Phi}$ to $\mathbf{e^{i\theta}|0\rangle}$. Measurement of this state must yield 0. The ratio of the number of 0s obtained is used as a cost function here.

VQE

Results

Both the implementations were tested on the Pauli matrices. The results obtained were inconsistent, i.e., sometimes the results would agree with our expectations, while at other times they would be somewhat off from the expected values.

The rationale behind the algorithm seems quite right. In implementation 2, the process of equating two qubits by comparing their measurement outcomes was replaced by inversion of the output **AΦ** so that when the output is the same as our trial state, the measurement state becomes **|0⟩**. This did not improve the results by much.

Another possible way to improve the algorithm was to use the **|+⟩** state as the initial state rather than **|0⟩**, since using **|0⟩** only utilizes two parameters out of the three provided to the **U3** gate. However, even using this modification does not improve the performance by much.

This example was included just to illustrate the flow of a VQS algorithm.

REFERENCES

[1] https://arxiv.org/abs/1812.08767
[2] Simulating Molecules using VQE (qiskit.org)

THANKS