Variational Quantum Algorithms

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Outline

Introduction

Variational Quantum Algorithms

Variational Quantum Algorithms (VQA) are a class of *hybrid* Quantum and Classical algorithms that are designed to take advantage of the computational power of Quantum Algorithms and using Classical algorithms for optimization.

Why Use VQA

NISQ

VQA are particularly well suited for Noisy Intermediate-Scale Quantum (NISQ) devices. This is due to

- iterative nature
- short depth quantum circuits

We can reduce both the *shot noise* and *statistical error* by more measurements. While we reduce the NISQ error by *error mitigation*

How do these work

Implementation

- A parameterized circuit $\mathcal{U}(\theta)$ is used for preparing,

$$|\Psi(\theta)\rangle = \mathcal{U}(\theta)\,|0\rangle$$

- This is used to measure the expectation value of an **observable** O

$$\mathcal{L}(\theta) = \langle\psi(\theta)|\,O\,|\psi(\theta)\rangle$$

How do these work

Implementation

- The classical optimizer updates θ to *minimize the objective function*
- Because we are using a *finite number of measurements* (N) to estimate the expectation value

$$\mathcal{L}(\theta) \approx \frac{1}{N} \sum_{i=1}^{N} \langle \psi(\theta) | \, |x_i\rangle \, \langle x_i | \, O \, |\psi(\theta)\rangle$$

$$= \frac{1}{N} \sum_{i=1}^{N} |\langle x_i | \psi(\theta) \rangle|^2 \frac{\langle x_i | \, O \, |\psi(\theta)\rangle}{\langle x_i | \psi(\theta) \rangle}$$

How do these work

Errors

- The measurement can be made to an arbitrary error probability ϵ after $N \sim 1/\epsilon^2$ measurements. This is due to the *central limit theorem*
- Another error is the *approximation error* this is due to the approximation of the parameters and the optimization step aims to reduce this. We can reduce this error by using a more expressive *ansatz*

Variational Quantum Eigensolver (VQE)

Motivation

This is a method to compute the ground state energy of quantum systems. This uses the fact that for any trail state $|\psi(\theta)\rangle$ the expectation value of the Hamiltonian $\hat{H}$ can be used to upper bound the ground state energy. We optimize the value of θ iteratively to approximate the ground state.

Variational Quantum Eigensolver (VQE)

Ansatz

The efficiency of the algorithm depends a lot on the choice of the **ansatz**. There are two broad categories

- *Hardware Efficient:* These are tailored to the native gate set and connectivity of the quantum hardware
- *Physically Motivated:* These are created based on the specific physical specifications of the problem

Variational Quantum Eigensolver (VQE)

Parameter Otimization

The parameters are optimized using the following method

$$\theta^{(k+1)} = \theta^{(k)} - \eta \nabla E(\theta^{(k)})$$

- η is the learning rate
- $\nabla E(\theta^{(k)})$ is the gradient of the enery w.r.t. the parameters

Variational Quantum Eigensolver (VQE)

Parameter Otimization

To calculate the gradient we use method of *parameter-shift*

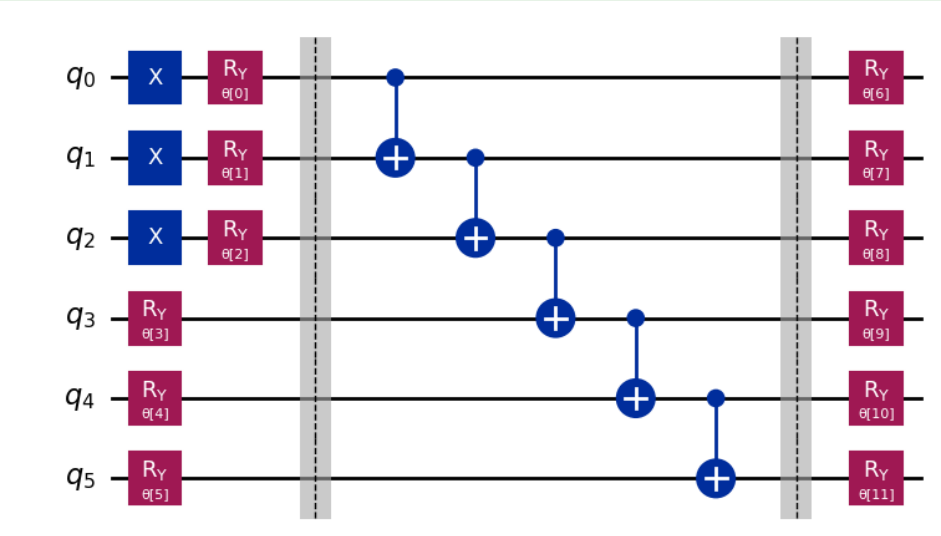
$$\frac{\partial E}{\partial \theta} = \frac{1}{2}\left[E(\theta + \frac{\pi}{2}) - [E(\theta - \frac{\pi}{2})\right]$$

The difference in not a small quantity due to the dependence of the ansatz on trignometric functions

Variational Quantum Eigensolver (VQE)

H-H Dissociation

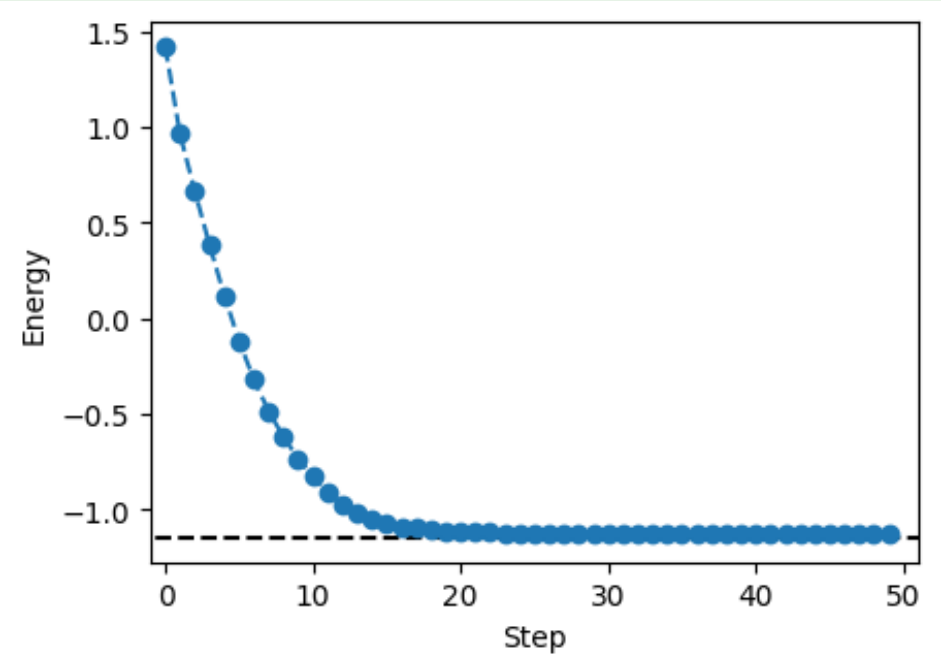
The H_2 dissociation process can be simulated using a quantum computer. Here is a version using a **6 qubit ansatz**



Variational Quantum Eigensolver (VQE)

H-H Dissociation

The optimization process can be represented as the value of energy as the number of iteration increases

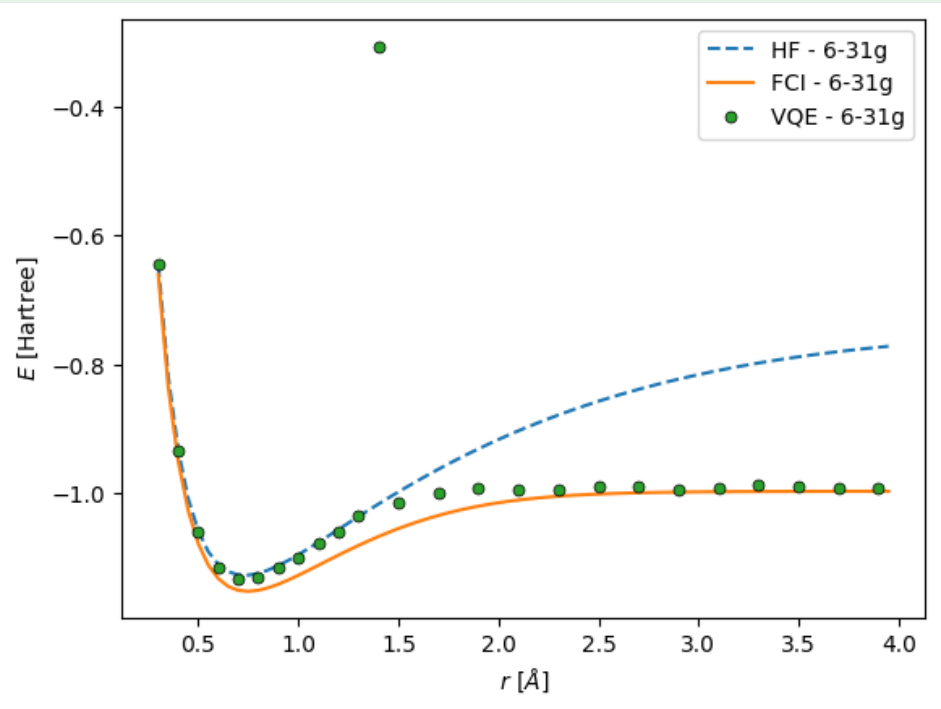


Variational Quantum Eigensolver (VQE)

H-H Dissociation

The following is a graph obtained from three different simulation methods.

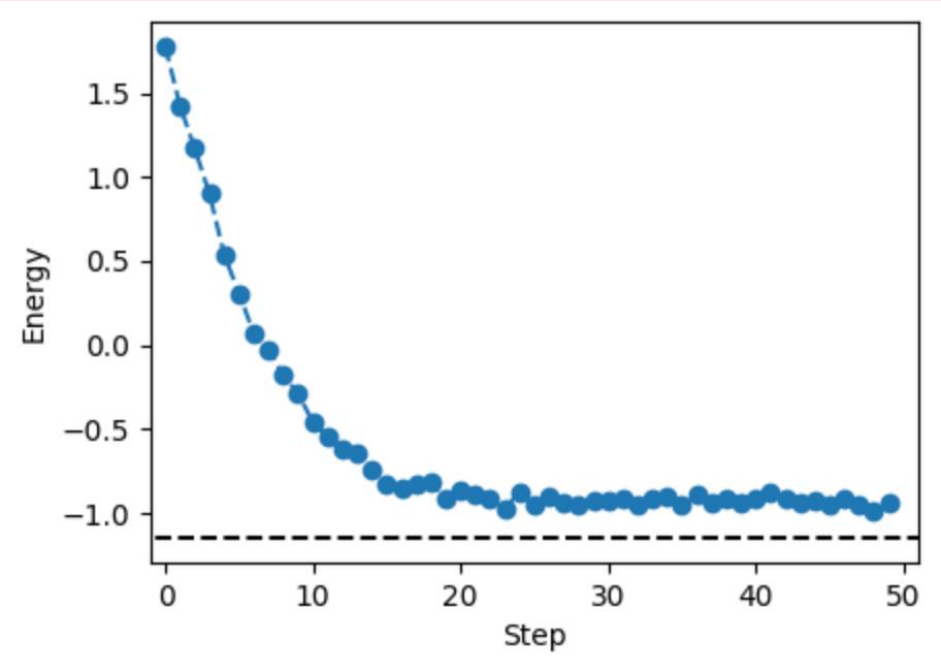
- Hartree-Fock (HF)
- Full Configuration Interaction (FCI)
- VQE



Variational Quantum Eigensolver (VQE)

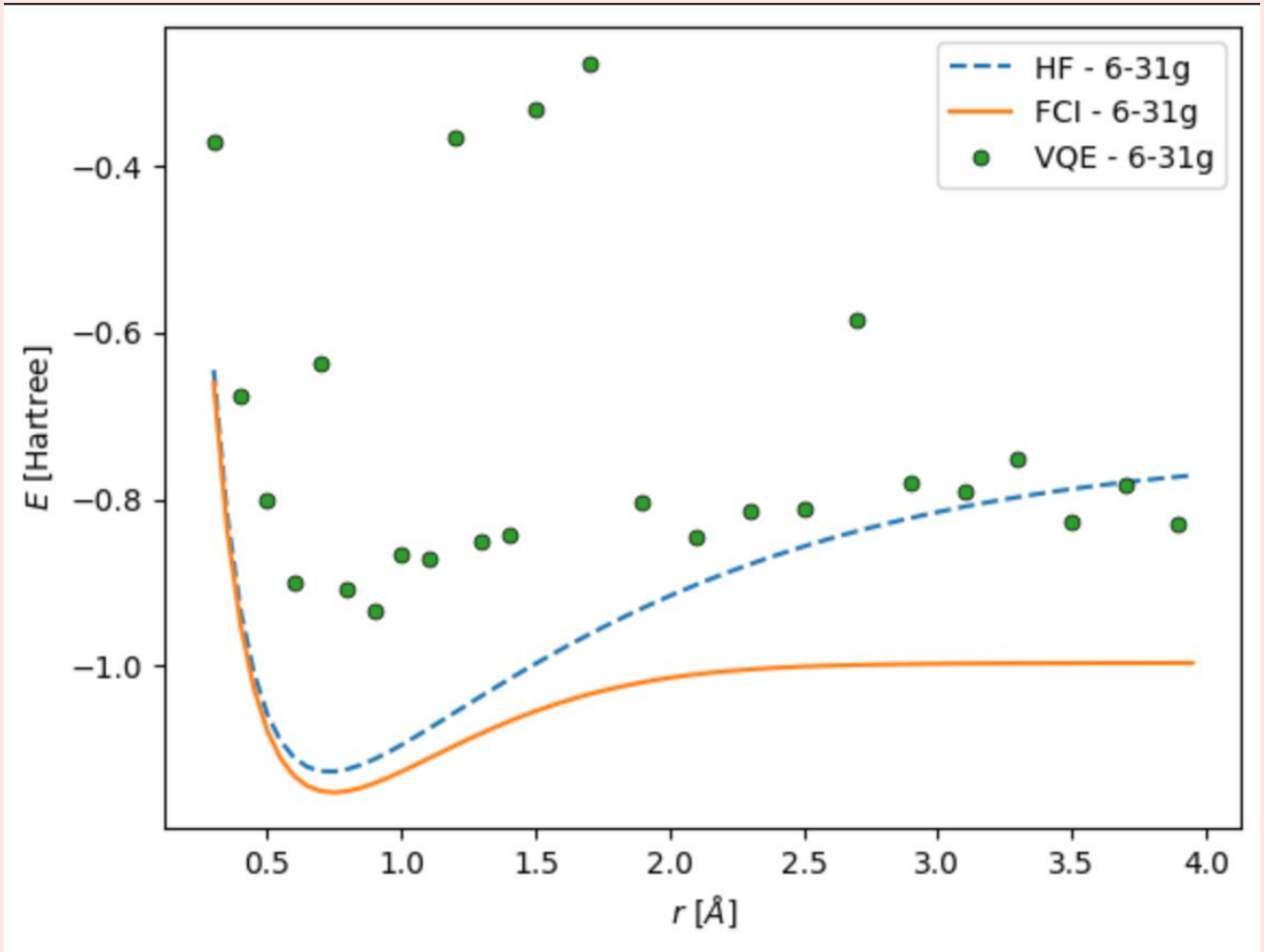
Measurement with Noise Models

Using the noise model *ibm brisbane* the following optimization graph was observed



Variational Quantum Eigensolver (VQE)

Measurement with Noise Models



Quantum Approximate Optimization Algorithms (QAOA)

Motivation

QAOA is a VQA that is used to solve *combinatorial optimization problems (COPs)*. A general class of COP is the *boolean satisfiability problem (SAT)*. This is helpful as most optimization problems can be **reduced to SAT** because it is *NP-complete*.

Quantum Approximate Optimization Algorithms (QAOA)

The Hamiltonian

NP complete problems can be mapped to a **classical** Hamiltonian called **Ising spin glass (ISG)** Hamiltonian.

$$H(s_1, s_2, \cdots, s_N) = -\sum_{i<j} J_{ij} s_i s_j - \sum_{i=1}^{N} h_i s_i$$

$s_j = \pm 1$, the task of finding the ground state is known to be *NP-hard*

Quantum Approximate Optimization Algorithms (QAOA)

The Hamiltonian

We now use *Quantum Adiabatic Optimization (QAO)*. Consider H as a quantum hamiltonian.

$$H_p = -\sum_{i<j} J_{ij} Z_i Z_j - \sum_{i=1}^{N} h_i Z_i$$

Introduce another hamiltonian,

$$H_0 = -h_0 \sum_{i=1}^{N} X_i$$

Each X_j has *eigenstates* $|+\rangle, |-\rangle$, hence the lowest energy state is $|+\rangle^{\otimes N}$

Quantum Approximate Optimization Algorithms (QAOA)

The Hamiltonian

Define the *time dependent hamiltonian*

$$H(t) = \left(1 - \frac{t}{T}\right) H_0 + \frac{t}{T} H_p$$

- The idea is to prepare a system in the state $|+\rangle^{\otimes N}$ at $t = 0$
- set T to be large enough so that dynamics is slow enough and the system stays *adiabatically* in the ground state
- system finally ends up in the ground state of H_p

Quantum Approximate Optimization Algorithms (QAOA)

Adiabatic Evolution

The issue with adiabatic evolution is that

$$\| \, |\psi(T)\rangle - |\psi_0\rangle \, \| \lesssim \frac{\langle H \rangle}{T\Delta^2}$$

- Δ is the minimal gap $= E_1 - E_0$ and it can decrease exponentially to 0 for systems of increasing size so we need T extremely long.
- another issue is that any time-dependent term in the Hamiltonian implies a loss of energy which violates the adiabatic criterion

Quantum Approximate Optimization Algorithms (QAOA)

Diabatic Evolution

A better solution is *diabatic* non-uniform time evolution

$$H(t) = (1 - f(t))H_0 + f(t)H_C$$

where $f(0) = 0, f(T) = 1$

Quantum Approximate Optimization Algorithms (QAOA)

Diabatic Evolution

We can parameterize the function $f(t)$ using many parameters(ξ) and run the time evolution several times adjusting the parameters each time, so as to minimize the expectation value of the energy.

$$\mathcal{E} = \langle \psi(T) | H_c | \psi(T) \rangle$$

This results in dramatic improvements in the value of T needed to achieve convergence.

Quantum Approximate Optimization Algorithms (QAOA)

Gradient Descent

$$\vec{\xi}_{n+1} = \vec{\xi}_n - \eta \nabla \mathcal{E}(\vec{\xi})|_{\vec{\xi}=\vec{\xi}_n}$$

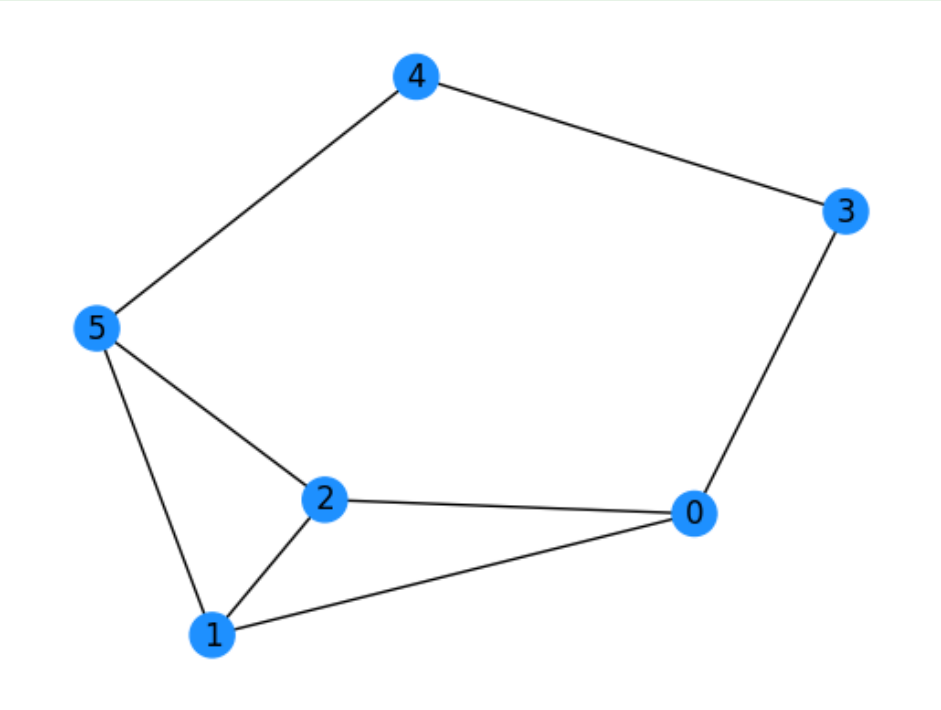
This approach is really accurate, but this requires estimating the gradient which is not possible analytically. Therefore we use gradient-less methods like

- Nelder-Mead method
- Simplex method
- COBYLA Optimizer
- Grid Search (Shallow Circuits)

Quantum Approximate Optimization Algorithms (QAOA)

Max-Cut Problem

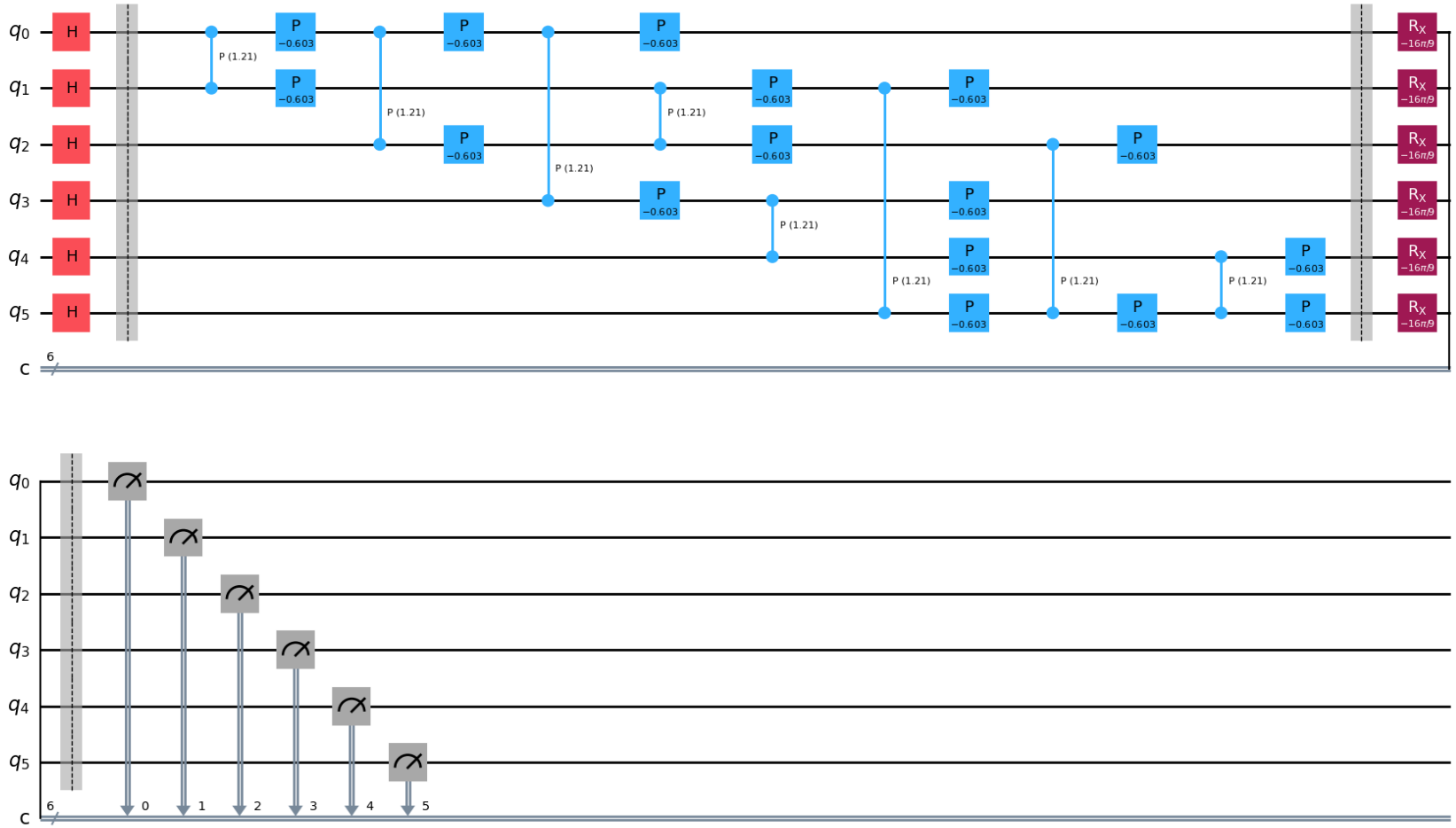
The following instance of the **Max-Cut Problem** has been evaluated.



Quantum Approximate Optimization Algorithms (QAOA)

Max-Cut Problem

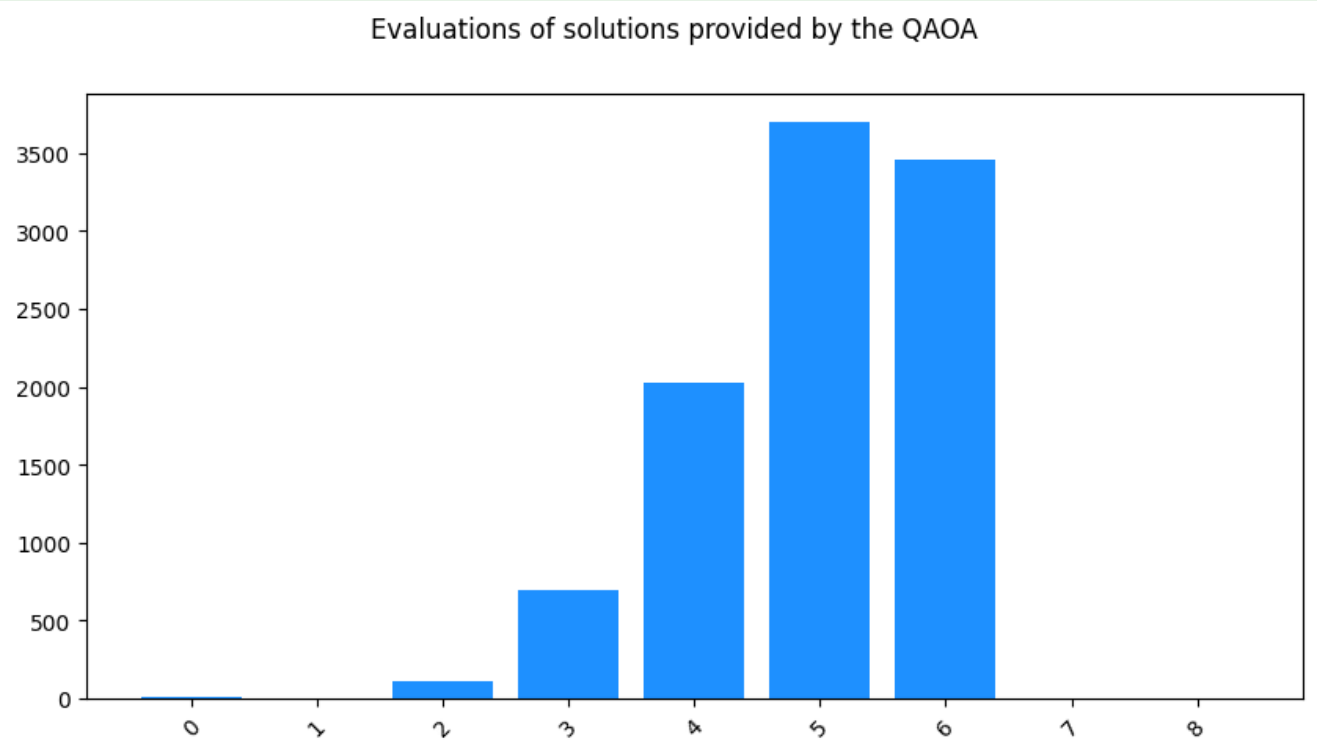
I use a **depth 1** circuit. This is parameterised by $\gamma = 0.603$ and $\beta = 2.793$. Which are optimized using **Grid Search**



Quantum Approximate Optimization Algorithms (QAOA)

Max-Cut Problem

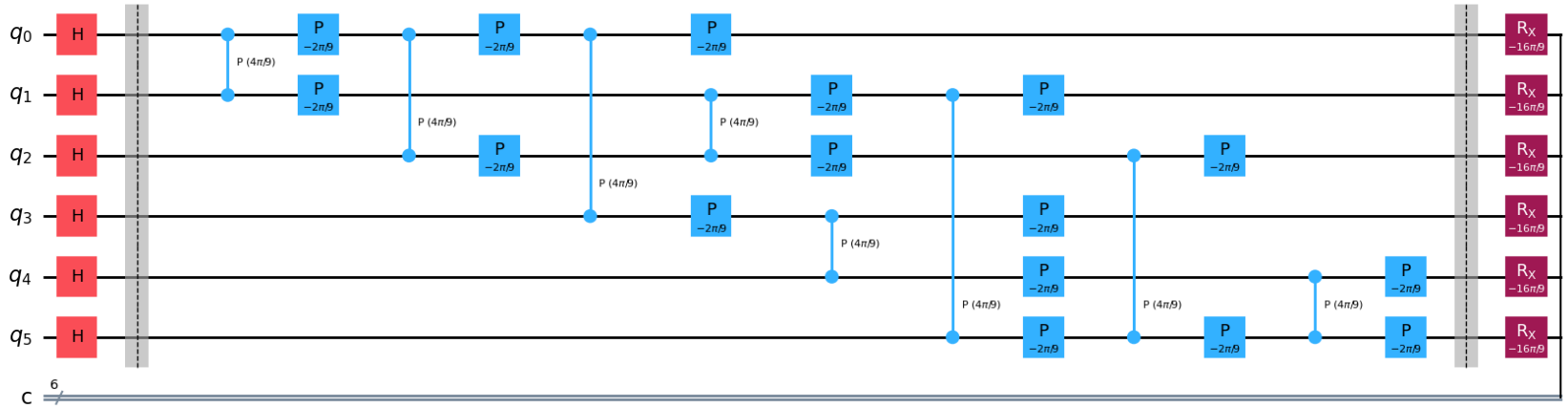
The following distribution of solutions with respect to cost is obtained. The approximate solution is $x^* = \{2, 3, 5\}, \{0, 1, 4\}(001101)$ with $C(x^*) = 6$

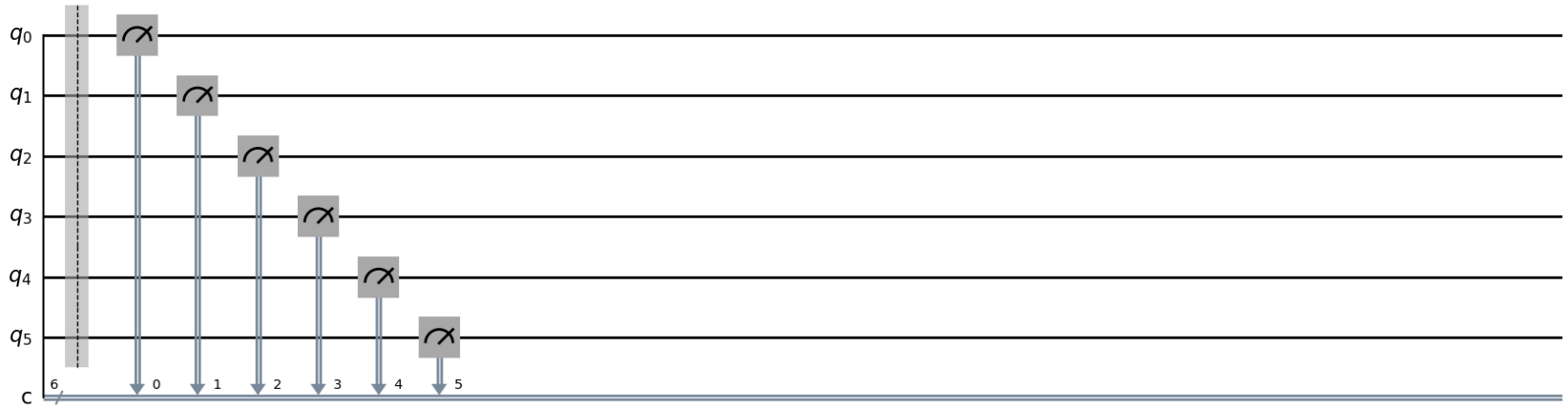


Quantum Approximate Optimization Algorithms (QAOA)

Measurement with Noise Models

Using the noise model *ibm brisbane* the parameters obtained from grid search were $\gamma = 0.698$ and $\beta = 2.793$

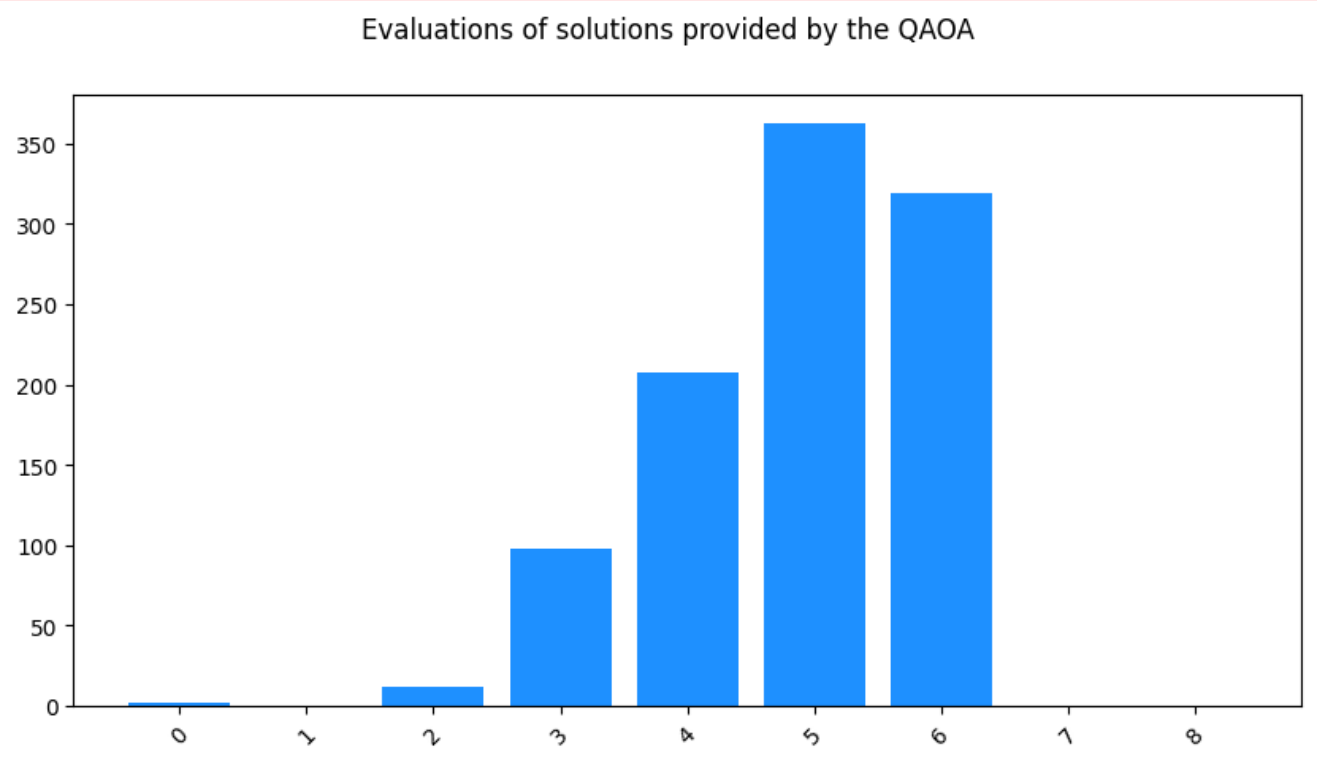




Quantum Approximate Optimization Algorithms (QAOA)

Measurement with Noise Models

The following evaluation was obtained



Conclusion

Solutions by VQA's

- The solutions obtained are extremely close to the actual solutions
- The amount of quantum gates used are low and shallow depth

Conclusion

Dealing with Noise

- VQE instance was not good at handling noise and the outputs diverge a lot
  - This may be due to gradient descent algorithm not executing enough steps
- QAOA instance implemented was really good at handling noise
  - We already found the best parameters for the problem by grid search