Background

Variational Quantum Eigen Value Solver (VQE)

- Physical System:
  - Hamiltonian
    - Describes energy of the physical system
    - From this one can compute the behavior of the system & which state the system is in
  - Eigen Vector:
    - Represent the "State" of the system
  - Eigen value
    - Represents the "Energy" of the system in that state
  - Lowest Eigen Value: Ground State
- Variational Principle
  - Let's say we have a Hamiltonian H with eigenstates $|\phi_1>, \ldots, |\phi_j>$ and associated eigenvalues $\lambda_1, \ldots, \lambda_n$ then

$$H\left|\phi_j\right> = \lambda_j\left|\phi_j\right>$$

- Energy of the Physical System at a given state $|\phi>$

$$E(|\phi>) = <\phi|H|\phi>$$

- Energy at Eigen states $|\phi_j>$

$$E_j = <\phi_j|H|\phi_j> = <\phi_j\left|\lambda_j\right|\phi_j> = \lambda_j \;<\phi_j|\phi_j>$$

Minimum Eigen Value:

The minimum Eigen value can be found using optimization algorithm by minimizing the energy of the physical system.

$$\lambda_{Min} = Min_j E_j = Min_j <\phi_j|H|\phi_j>$$

Solution

Steps

1. Decomposition into Pauli Matrices
2. VQE
    a. Ansatz
    b. Hamiltonian
    c. Measurement

Decomposition into Pauli Matrices

Every matrix H can be written as some linear combination of Pauli matrices I, Z, X, Y.

$$I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$H = aI + bX + cY + dZ$$

The coefficients can be found by the formulas:

$$a = \frac{1}{2} trace(H * I^*), b = \frac{1}{2} trace(H * X^*), c = \frac{1}{2} trace(H * Y^*), d = \frac{1}{2} trace(H * Z^*)$$

The given Hamiltonian matrix is 4×4

$$H = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

This can be written as

$$H = aII + bXX + cYY + dZZ$$

Where

$$II = I \otimes I, \qquad XX = X \otimes X, \qquad YY = Y \otimes Y, \qquad ZZ = Z \otimes Z$$

Each new matrix is Tensor product of 2×2 Pauli matrices.

The coefficients can be found by the formulas:

$$a = \frac{1}{4} trace(H * II^*), b = \frac{1}{4} trace(H * XX^*), c = \frac{1}{4} trace(H * YY^*), d = \frac{1}{4} trace(H * ZZ^*)$$

In particular

$$H = (0.5)II + (-0.5)XX + (-0.5)YY + (0.5)ZZ$$

VQE

Ansatz

- Gates used:

$$(RX\ I)\ (CX)\ (HI)\ |00>$$

- The angle in RX is variational parameter.

Hamiltonian

$$H = (0.5)II + (-0.5)XX + (-0.5)YY + (0.5)ZZ$$

Measurement

- For II
  - Expectation = 1
- For XX
  - Apply $H \otimes H$ then apply measurement
- For YY
  - Apply $Y_{Gate} \otimes Y_{Gate}$ then apply measurement
  - $Y_{Gate} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & -i \\ 1 & i \end{bmatrix}$
- For ZZ
  - No gates required. Directly apply measurement

Expectation:

$$\langle H \rangle = (0.5) * \langle II \rangle + (-0.5) * \langle XX \rangle + (-0.5) * \langle YY \rangle + (0.5) * \langle ZZ \rangle$$