COE 466 Quantum Architecture and Algorithms

Lecture 24

Variational Quantum Algorithms

References:

Introduction to Variational Quantum Algorithms
“https://arxiv.org/pdf/2402.15879

https://qiskit.org/textbook/ch-applications/vqe-molecules.html

https://qiskit.org/textbook/ch-applications/qaoa.html

Disclaimer

- “I started writing them in 2019, when most of the community had big hopes for VQAs (and Noisy IntermediateScale Quantum (NISQ) devices in general) and there were still plenty of unknown unknowns. But by now (February 2024), there is an increasing consensus in the community that using VQAs on NISQ devices for any practical purposes faces **fundamental issues** and that fault-tolerant algorithms (like QPE) seem to be a still distant, but much safer bet. “

Variational Quantum Eigansolver (VQE)

- VQE is considered as a hybrid, machine learning algorithm
  - **Variational:** Because the VQE varies parameters in order to find the true value
  - **Quantum:** Because it is a quantum algorithm
  - **Eigensolver:** Because we are solving for the lowest eigenvalue
- Useful terminology
  - Hamiltonian
  - Qubit mapping (encoding): the process of encoding information on a qubit
  - Ansatz: an educated guess of something (e.g. wave function of a molecule)
  - Eiganvalues
- VQE can help us to estimate* the energy of the ground state of a given quantum mechanical system.**

  With the following caveats:

  *estimate by providing us an upper bound

  **if we know the Hamiltonian of this system 1

Background

Ass. $H = H^\dagger$

Recall that an eigenvector $|\varphi_i\rangle$ of H

$$H|\varphi_i\rangle = \lambda_i |\varphi_i\rangle \qquad \lambda_1, \lambda_2, \dots, \lambda_n$$

$$\lambda_{min} = \min(\lambda_1, \dots, \lambda_n)$$

Ex

$$H = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$\lambda_1 = +1 \quad |\varphi_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$

$\lambda_2 = -1 \quad |\varphi_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$

- Given a Hamiltonian H, the expectation of H on $|\psi\rangle$

$$\langle\psi|H|\psi\rangle = \langle\psi|\left(\sum_i \lambda_i |\varphi_i\rangle\langle\varphi_i|\right)|\psi\rangle$$

$$= \sum_i \lambda_i \langle\psi|\varphi_i\rangle\langle\varphi_i|\psi\rangle$$

$$= \sum_i \lambda_i |\langle\varphi_i|\psi\rangle|^2 \longrightarrow \lambda_{min} \le \sum_i \lambda_i |\langle\varphi_i|\psi\rangle|^2$$

ex

$$Z \quad \begin{matrix} +1 \\ -1 \end{matrix}$$

$$(1\ 0)\, Z \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 1$$

$$(0.3\ 0.7)\, Z \begin{pmatrix} 0.3 \\ 0.7 \end{pmatrix}$$

$$(0.3\ 0.7)\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 0.3 \\ 0.7 \end{pmatrix} = 0.3\ 0.7 \begin{pmatrix} 0.3 \\ -0.7 \end{pmatrix}$$

$$= 0.09 - 0.49$$

$$= -0.4$$

$$0.3(1) + 0.7(-1) = -0.4$$

Background

Objective of VQE

- In many applications, finding the minimum eigenvalue of a matrix is important
  - *For example, in chemistry the minimum eigenvalue of a Hermitian matrix characterizing the molecule is the ground state energy of that system*
  - Why not using phase estimation algorithm?
- *Problem:* Given a Hermitian matrix H with an unknown minimum eigenvalue $\lambda_{\min}$ associated with the eigenstate $|\psi_{\min}\rangle$, VQE provides an estimate λ_{θ} bounding $\lambda_{\min}$:

$$\lambda_{\min} \leq \lambda_{\theta} \equiv \langle \psi(\theta)|H|\psi(\theta)\rangle$$

Where $\psi(\theta)$ is the eigenstate associated with λ_{θ}

Objective of VQE

- Alternatively, the above problem can be posed as an optimization problem

$$\min_{\theta} \langle \psi(\theta) | H | \psi(\theta) \rangle$$

By the variational principle of quantum mechanics, the quantity

$$\langle \psi(\theta) | H | \psi(\theta) \rangle$$

can never be smaller than the ground state energy.

- Therefore, minimizing this quantity can give an approximation of the ground state energy
- The process of minimization is done using the **variational method** (or **variational principle**)

Variational Forms

- Variational method is implemented using a parametrized quantum circuit (gate)

$$U(\theta)$$

Which is applied on an ansatz state $|\psi\rangle$ such that

$$U(\theta)|\psi\rangle \equiv |\psi(\theta)\rangle$$

- Doing this process iteratively over $|\psi(\theta)\rangle$ yields an expectation value $\langle\psi(\theta)|H|\psi(\theta)\rangle \approx E_{gs} \equiv \lambda_{min}$
- Example of a variational form is

Process of VQE

- Once a variation form is selected, its parameters must be optimized to minimize the expectation value of the target Hamiltonian
- Quantum part
  - Mapping molecular Hamiltonian into a qubit Hamiltonian
  - Creating and ansatz
  - Calculating the energy of the trial state
- Classical part
  - Measure and optimize the parameters
  - Iterate through the loop