QUANTUM ALGORITHMS

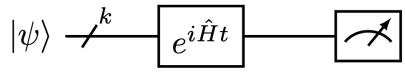
What can we use quantum computing for? At present, nothing that we cannot do classically, but plenty of things if we aren't trying to compete with classical methods.

Open quantum systems

- If we wanted to do simple Hamiltonian evolution,

$$|\psi(t)\rangle = e^{i\hat{H}t} |\psi(0)\rangle \,, \tag{1}$$

  in a unitary gate-based quantum algorithm, the challenge would be in circuit optimization (transpilation) since $\hat{H}$ is Hermitian and therefore $e^{i\hat{H}t}$ is unitary:



- What if instead we wanted to look at an open system whose dynamics are governed by Kraus operators in an operator-sum form:

$$\rho(t) = \sum_k M_k \rho(0) M_k^\dagger \tag{2}$$

  Starting with a pure state for simplicity,

$$|\psi(t)\rangle \langle\psi(t)| = \sum_k M_k |\psi(0)\rangle \langle\psi(0)| M_k^\dagger \tag{3}$$

- Let's look at the term,

$$M_k |\psi(0)\rangle \tag{4}$$

- ***Exercise 4***
- There are many different ways to either map non-unitary methods into quantum algorithm form but here we will focus on an operator decomposition approach that will let us learn a fun trick
- For any square operator M we can write,

$$M = S + A, \tag{5}$$

  where S is a symmetric (Hermitian) operator,

$$S = \frac{M + M^\dagger}{2} \tag{6}$$

and A is an antisymmetric (anti-Hermitian) operator,

$$A = \frac{M - M^\dagger}{2} \tag{7}$$

- ***Exercise 5***
- We can then rewrite both S and A in terms of their truncated Taylor expansions,

$$S = \lim_{\epsilon \to 0} \frac{i}{2\epsilon} \left(e^{-i\epsilon S} - e^{i\epsilon S} \right) \tag{8}$$

and

$$A = \lim_{\epsilon \to 0} \frac{1}{2\epsilon} \left(e^{\epsilon A} - e^{-\epsilon A} \right) \tag{9}$$

- ***Exercise 6***
- This allows us to rewrite a non-unitary operator as the linear combination of unitary operators,

$$M = \lim_{\epsilon \to 0} \frac{1}{2\epsilon} \left(ie^{-i\epsilon S} - ie^{i\epsilon S} + e^{\epsilon A} - e^{-\epsilon A} \right) \tag{10}$$

- ***Exercise 7***
- We can construct a unitary operator from M by taking the direct sum of the four unitaries above,

$$U_M = ie^{-i\epsilon S} \oplus -ie^{i\epsilon S} \oplus e^{\epsilon A} \oplus e^{-\epsilon A} \tag{11}$$

$$= \begin{pmatrix} ie^{-i\epsilon S} & 0 & 0 & 0 \\ 0 & -ie^{i\epsilon S} & 0 & 0 \\ 0 & 0 & e^{\epsilon A} & 0 \\ 0 & 0 & 0 & -e^{-\epsilon A} \end{pmatrix} \tag{12}$$

- In order to act this operator, we need the original system wavefunction to have the same dimensionality, which we can do by making copies in another direct sum,

$$|\psi_U\rangle = |\psi\rangle \oplus |\psi\rangle \oplus |\psi\rangle \oplus |\psi\rangle \tag{13}$$

$$= \begin{pmatrix} |\psi\rangle \\ |\psi\rangle \\ |\psi\rangle \\ |\psi\rangle \end{pmatrix} \tag{14}$$

- Now consider the product,

$$U_M |\psi_U\rangle = \begin{pmatrix} ie^{-i\epsilon S} |\psi\rangle \\ -ie^{i\epsilon S} |\psi\rangle \\ e^{\epsilon A} |\psi\rangle \\ -e^{-\epsilon A} |\psi\rangle \end{pmatrix} \tag{15}$$

- We have all the information we need but what would happen if we measure this state as is?
- ***Exercise 8***
- We need to invoke what is referred to as the **linear combination of unitaries** [1] technique which consists of a rotation gate to prepare the superpositions of interest,

$$R \cdot U_M \left|\psi_U\right\rangle, \tag{16}$$

with

$$R = \frac{1}{2}\begin{pmatrix} r & -r \\ r & r \end{pmatrix} \tag{17}$$

and

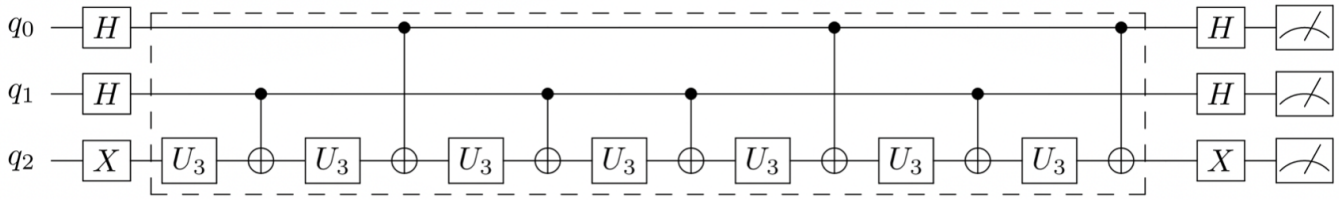
$$r = \frac{1}{2}\begin{pmatrix} \mathbb{1} & -\mathbb{1} \\ \mathbb{1} & \mathbb{1} \end{pmatrix} \tag{18}$$

which yields a vector containing every linear combination of elements

- As an example, we can consider the amplitude damping channel that we discussed on Monday,

$$\rho(t) = \sum_{k=0}^{1} M_k \rho(0) M_k^\dagger, \tag{19}$$

with $M_0 = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{e^{-\gamma t}} \end{pmatrix}$ and $M_1 = \begin{pmatrix} 0 & \sqrt{1-e^{-\gamma t}} \\ 0 & 0 \end{pmatrix}$. If we do this, we obtain the circuit,



Key Take-Away

- This is a probabilistic algorithm where we only get the answer we want when the ancilla are in specific states
- The alternative is a deterministic algorithm where everything generated is useful
- This has been applied to open dynamics (originally in Ref. [2]), but is generally a nice method of implementing non-unitary operators. A recent example is in excited state electronic structure theory by Ayush Asthana at the University of North Dakota. [3]

ENERGY ESTIMATION ALGORITHMS

Variational Quantum Eigensolvers (VQE)

- Relies on the variational principle,

$$\langle\psi|\hat{H}|\psi\rangle \leq E_0 \tag{20}$$

- Hybrid algorithm which relies on both classical and quantum computing:
  - ▷ Quantum computer: Prepares a state *ansatz*, $|\psi(\theta_i)\rangle$, and measures the expectation value of $\hat{H}$
  - ▷ Classical computer: Suggests a new ansatz via classical optimization
- Usually relies on the **Jordan-Wigner transformation** to map fermionic operators,

$$\hat{a}^\dagger|0\rangle = |1\rangle \qquad \hat{a}|1\rangle = |0\rangle \tag{21}$$

into Pauli strings. The simplest mapping would be to use the Pauli operators,

$$\hat{Q}^\dagger = \frac{1}{2}(X - iY) \qquad \hat{Q} = \frac{1}{2}(X + iY), \tag{22}$$

however these do not preserve the fermionic anticommutation relations,

$$\{a_j^\dagger, a_k^\dagger\} = 0 \qquad \{a_j, a_k\} = 0 \qquad \{a_j, a_k^\dagger\} = \delta_{jk}\mathbb{1}. \tag{23}$$

This is where the Jordan-Wigner transformation comes in, and a simple version is to take these relations and tensor product them with a series of Z gates,

$$\hat{a}_j^\dagger = \frac{1}{2}(X - iY)\bigotimes_{k<j} Z_k \qquad \hat{a}_j = \frac{1}{2}(X + iY)\bigotimes_{k<j} Z_k. \tag{24}$$

- The above is adapted from a nice tutorial in Pennylane, where more information is also available: https://pennylane.ai/qml/demos/tutorial_mapping
- The major challenge with VQEs is referred to as the challenge of **barren plateaus** where the energy landscapes are very flat and therefore the classical optimization step fails.

Quantum Phase Estimation (QPE)

- The general gist relies on estimating the phase in the expression,

$$U|\psi\rangle = e^{i\phi}|\psi\rangle, \tag{25}$$

which provides the eigenvalue of the operator, which will be the molecular ground-state energy if everything is mapped correctly

- There is a really nice tutorial through Pennylane here: https://pennylane.ai/qml/demos/tutorial_qpe
- This method is currently considered a gold standard for energy estimation, since it bypasses some of the major challenges of VQEs

MISCELLANEOUS OTHER INFORMATION

- This is a field with a million pedagogical resources that are all very nicely developed
- IBM Qiskit has years worth of great tutorials (videos, notebooks, blog posts, pretty much anything)
- Pennylane is another fantastic resource that has clean working examples embedded into lessons

SOME REFERENCES

[1] Quantum Information and Computation **12**, 10.26421/qic12.11-12 (2012).

[2] A. W. Schlimgen, K. Head-Marsden, L. M. Sager, P. Narang, and D. A. Mazziotti, Quantum simulation of open quantum systems using a unitary decomposition of operators, Phys. Rev. Lett. **127**, 270503 (2021).

[3] A. Asthana, Quantum krylov algorithm using unitary decomposition for exact eigenstates of fermionic systems using quantum computers (2025), arXiv:2512.11788 [quant-ph].