5. Hamiltonian simulation (LCU): pt.1

Linear combination of Unitaries

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Recap

e^{-iHt}

- QPE is very useful for
  - ❖ energy estimation
  - ❖ ground state preparation
- QPE cost $\approx 1/\epsilon$ times Hamiltonian simulation cost for a unit time.
- Better Hamiltonian simulation → Better time-evolution simulation, energy estimation, ground state preparation, …
- Trotter-Suzuki: An efficient algorithm for Hamiltonian simulation on a quantum computer

Post-Trotter methods

- Hamiltonian simulation from Trotter-Suzuki decomposition was first proposed by Lloyd (1996).
- In the 2010s, many new ideas appeared. They are interesting, because they come with a better complexity bound than the Trotter-Suzuki method.
- Strangely, many of these algorithms attempt to approximate e^{-iHt} by a *non-unitary operation*.
- We will talk about one such method, known as the LCU(=linear combination of unitaries).

Basic intuition

- What we want: $|\psi\rangle \rightarrow |\psi'\rangle = e^{-iHt}|\psi\rangle$.
- What we do: $|\psi\rangle|0\rangle \rightarrow \sqrt{p}\,|\widetilde{\psi}'\rangle|Success\rangle + \sqrt{1-p}\,|Fail\rangle$, where $|\widetilde{\psi}'\rangle \approx |\psi'\rangle$, by applying a linear combination of unitaries (LCU). [Childs and Wiebe (2012)]
- Then we "boost" the success probability to 1.

Measure the 2nd register
- Prob p: $|\tilde{\psi}'\rangle$
- Prob $1-p$: "Fail"

Toy example 1

- Suppose we want to apply an arbitrary 2×2 matrix on a qubit, using a unitary quantum circuit. What can we do?

A : 2x2 matrix

$|\psi\rangle$: 1-qubit state

$|\psi\rangle \longrightarrow A|\psi\rangle / \| A|\psi\rangle \|$ $\quad \left(\| |\phi\rangle \| = \sqrt{\langle \phi | \phi \rangle} \right)$

Fact: $A = \alpha_I I + \alpha_X X + \alpha_Y Y + \alpha_Z Z$, $\quad (\alpha_I, \alpha_X, \alpha_Y, \alpha_Z \in \mathbb{C})$

Register with 2 qubits $|I\rangle, |X\rangle, |Y\rangle, |Z\rangle$
$|00\rangle \quad |01\rangle \quad |10\rangle \quad |11\rangle$

$$(\alpha_I|I\rangle + \alpha_X|X\rangle + \alpha_Y|Y\rangle + \alpha_Z|Z\rangle)|\psi\rangle \xrightarrow{U} \alpha_I|I\rangle|\psi\rangle + \alpha_X|X\rangle X|\psi\rangle + \alpha_Y|Y\rangle Y|\psi\rangle + \alpha_Z|Z\rangle Z|\psi\rangle$$

$\downarrow$

Measure in the basis of $\left\{ \frac{1}{2}(|I\rangle + |X\rangle + |Y\rangle + |Z\rangle), \ldots \right\}$

$U|I\rangle|\psi\rangle = |I\rangle|\psi\rangle$

$U|X\rangle|\psi\rangle = |X\rangle X|\psi\rangle$

$U|Y\rangle|\psi\rangle = |Y\rangle Y|\psi\rangle$ $\quad U^2 = I$

$U|Z\rangle|\psi\rangle = |Z\rangle Z|\psi\rangle$

$|\phi_1\rangle$

↓ If I measure $|\phi_1\rangle$

$\alpha_I|\psi\rangle + \alpha_X X|\psi\rangle + \alpha_Y Y|\psi\rangle + \alpha_Z Z|\psi\rangle$

$\frac{1}{2}\left(ZI|+\rangle|+\rangle + ZX|+\rangle|-\rangle + ZY|-\rangle|+\rangle + ZZ|-\rangle|-\rangle\right)\left(\alpha_I|I\rangle|\psi\rangle + \alpha_X|X\rangle X|\psi\rangle + \alpha_Y|Y\rangle Y|\psi\rangle + \alpha_Z|Z\rangle Z|\psi\rangle\right)$

Toy example 2

- Suppose we want to apply $e^{-iH\delta t} \approx I - iH\delta t$, where H is a local Hamiltonian. What can we do?

$$H = -t \sum_i (a_i^\dagger a_{i+1} + h.c.) + U \sum_i \hat{n}_i \hat{n}_{i+1} .$$

$$H = -\frac{t}{2} \sum_i (X_i X_{i+1} + Y_i Y_{i+1}) + U \sum_i \frac{(Z_i + 1)(Z_{i+1} + 1)}{4} .$$

X_i, Y_i, Z_i

$H = \sum_P \alpha_P P$

P ← Tensor product of Pauli operators

ex) $X_1 \otimes X_2 \otimes Y_3 \otimes I_4 \cdots$

$\left(|I\rangle - i\delta t \sum_P \alpha_P |P\rangle\right) |\psi\rangle \xrightarrow{U} |I\rangle|\psi\rangle - i\delta t \sum_P \alpha_P |P\rangle P|\psi\rangle$

$U|p\rangle|\psi\rangle = |p\rangle P|\psi\rangle$

Hamiltonian Simulation

- Suppose we want to apply $e^{-iH\delta t}$, where H is a local Hamiltonian and the norm of $H\delta t$ is ≈ 0. What can we do?
- A: Taylor expansion! [Berry, Childs, Cleve, Kohtari, and Somma (2014)]

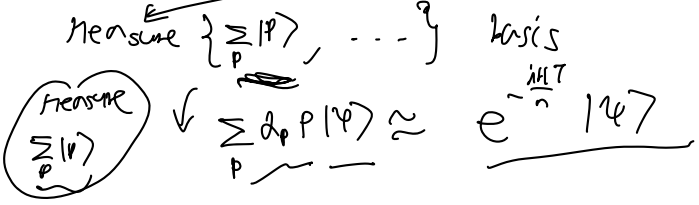
$$H = -\frac{t}{2}\sum_i (X_i X_{i+1} + Y_i Y_{i+1}) + U\sum_i \frac{(Z_i+1)(Z_{i+1}+1)}{4}.$$

$e^{-iHT} = \left(e^{-\frac{iHT}{n}}\right)^n$ → norm is $O(1)$

$e^{-\frac{iHT}{n}} = I - \frac{iHT}{n} - \frac{H^2T^2}{2n^2} + \cdots$

$= \sum_p \alpha_p P$

$\left(\sum_p \alpha_p |p\rangle\right)|\psi\rangle \xrightarrow{U} \sum_p \alpha_p |p\rangle P|\psi\rangle$



SELECT

- SELECT is an important subroutine used in modern quantum algorithms.
- Think of it as a “lookup table.”
- We will see this subroutine again, later in the course.

$\{P_1, P_2, \ldots P_n\}$

$|K\rangle|\psi\rangle \longrightarrow \text{SELECT}\,|K\rangle|\psi\rangle$

$= |K\rangle P_K|\psi\rangle$

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$\cup |p\rangle|\psi\rangle = |p\rangle P|\psi\rangle$

PREPARE

- PREPARE is another important subroutine.
- In the context of the Hamiltonian simulation, this prepares the state that encodes the coefficients of the Hamiltonian.
- We will see this subroutine again, later in the course.

$\sum_p \alpha_p |p\rangle$

$\text{PREPARE}|0\cdots0\rangle = \sum_{k=1}^{n} \alpha_k |k\rangle$

$\text{SELECT}|k\rangle|\psi\rangle = |k\rangle P_k|\psi\rangle$ $\quad \{P_1, \cdots P_n\}$

SELECT + PREPARE

- With these two, we can implement the desired operation.

$\log_2 n$-qubit state

$$\text{PREPARE}\,|0\cdots0\rangle = \sum_{k=1}^{n} \alpha_k |k\rangle$$

$$\text{SELECT}\,|k\rangle|\psi\rangle = |k\rangle P_k|\psi\rangle \qquad \{P_1, \cdots P_n\}$$

$$\text{PREPARE}^\dagger\,\text{SELECT}\,\text{PREPARE}\left(|0\cdots0\rangle|\psi\rangle\right)$$

$$= \text{PREPARE}^\dagger\,\text{SELECT}\left(\sum_{k=1}^{n} \alpha_k |k\rangle|\psi\rangle\right)$$

$$= \text{PREPARE}^\dagger \sum_{k=1}^{n} \alpha_k |k\rangle P_k|\psi\rangle$$

$$\langle 0\cdots0|\,\text{PREPARE}^\dagger \sum_{k=1}^{n} \alpha_k |k\rangle P_k|\psi\rangle = \sum_{k'=1}^{n}\sum_{k=1}^{n} \alpha_{k'}^{*}\alpha_k \langle k'|k\rangle P_k|\psi\rangle$$

$$= \sum_{k=1}^{n} |\alpha_k|^2 P_k|\psi\rangle$$

$k=1$

$$e^{-iHt} \simeq \sum_k |\alpha_k|^2 P_k$$

$$H_1 = \sum_{i=1}^{n} Z_i Z_{i+1} |\alpha_i|^2$$

↓

SELECT $|i\rangle|\psi\rangle$

$= |i\rangle Z_i Z_{i+1} |\psi\rangle$

PREPARE $= \sum_{i=1}^{n} \alpha_i |i\rangle$

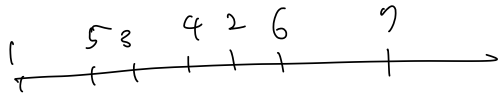
$$H_2 = \sum_{i=1}^{n} X_i X_{i+1}$$

↓

SELECT $|i\rangle|\psi\rangle$

$= |i\rangle X_i X_{i+1} |\psi\rangle$

PREPARE $= \sum_{i=1}^{n} \frac{1}{\sqrt{n}} |i\rangle$



$\geq$ $\rangle$

Why bother with this approach?

- In the Trotter-based Hamiltonian simulation, there is an inevitable $O(poly(\epsilon^{-1}))$ scaling in the precision ϵ .
- Using the LCU approach, one can get a sub-logarithmic scaling in $1/\epsilon$. [Berry, Childs, Cleve, Kohtari, and Somma (2013, 2014)]
- This is especially important for quantum chemistry applications, because they tend to require high-precision calculations.

Summary

- In the Trotter-based Hamiltonian simulation, there is an inevitable $O(poly(\epsilon^{-1}))$ scaling in the precision ϵ .
- Using the LCU approach, one can get a sub-logarithmic scaling in $1/\epsilon$. [Berry, Childs, Cleve, Kohtari, and Somma (2013, 2014)]
- Using SELECT + PREPARE, we can apply the desired unitary with a nonzero probability.
- However, we haven't discussed how to boost this probability. That will come in the next lecture.