# Lecture 18

## Linear Combination of Unitaries

### - Quantum Walk for Sparse Hamiltonian Simulation

## 1 Non-unitary $LCU$ with approximation

Theorem. Let $A$ be a Hermitian operator with eigenvalues in a domain $D \subseteq \mathbb{R}$ (Common choice: $D = [-1, 1]$). Suppose the function $f : D \to \mathbb{R}$ satisfies $|f(x)| \geqslant 1$ for all $x \in D$ and is $\varepsilon$-close to $\sum_i \alpha_i T_i$ on $D$ for some $\varepsilon \in (0, 1/2)$, coefficients $\alpha_i > 0$, and functions $T_i : D \to \mathbb{C}$. Let $\{U_i\}$ be a set of unitaries such that $U_i |0^t\rangle |\phi\rangle = |0^t\rangle T_i(A)|\phi\rangle + |\Phi_i^\perp\rangle$ for all states $|\phi\rangle$, where $t$ is a nonnegative integer and $(|0^t\rangle \langle 0^t| \otimes I) |\Phi_i^\perp\rangle = 0$.

Given an algorithm $U_B$ for preparing $|b\rangle$, there is a quantum algorithm that prepares a quantum state $4\varepsilon$ -close to $f(A)|b\rangle/\|f(A)|b\rangle\|$, succeeding with constant probability, that makes $O(\alpha/\|f(A)\,|b\rangle\,\|) = O(\alpha)$ uses of $U_B, U$, and $V$, where

$$U = \sum_i |i\rangle \langle i| \otimes U_i, \qquad V |0^n\rangle = \frac{1}{\sqrt{\alpha}} \sum_i \sqrt{\alpha_i}\, |i\rangle\,, \qquad \alpha = \sum_i \alpha_i.$$

and an output bit indicating whether it was successful.

For a Hermitian $A$: $A = \sum_i \lambda_i |\lambda_i\rangle \langle \lambda_i|$, $f(A) = \sum_i f(\lambda_i) |\lambda_i\rangle \langle \lambda_i|$.

| Input | Further combination |
|---|---|
| Unitary | $LCU$ |
| Block of unitary | Non-unitary $LCU$ |
| Block of unitary with approximation | Non-unitary $LCU$ with approximation |

To apply $LCU$ results, we need to implement $U$, in particular the $U_i$ 's.

In our class, we consider the case where all $U_i$ are correlated, and are actually powers of a simple unitary $Y$. In this case. we have:

Theorem. Let $U = \sum_{i=0}^{N-1} |i\rangle \langle i| \otimes Y^i$, where $Y$ is a unitary with gate complexity $G$. Assume $N = 2^n$. Then the gate complexity of implementing $U$ is $O(NG)$.

Note: A brute-force way of implementing each $|i\rangle \langle i| \otimes Y^i$ cost

$$G(1 + 2 + \cdots + N - 1) = O\left(N^2 G\right).$$

*Proof.* - The unitary $Y^{2j}$ for $j \in \{0.1, \ldots, n-1\}$ has gate complexity at most $2^j G$.

- We implement $U = \sum_{i=1}^{N-1} |i\rangle \langle i| \otimes Y^i$ by having the operator $c - Y^{2^j}$ on the second register controlled by $j^{\text{th}}$ qubit of the first register $|i\rangle$.

$$\text{Total gate complexity: } G(1+2+\cdots+2^{n-1}) = O(NG)$$

What's the $Y$ we use here? (Discrete-time) quantum walk for a Hamiltonian.

Let $A$ be an s-sparse $N \times N$ Hamiltonian. $\|A\|_{\max} = \max_{i,j\in[a]} |A_{ij}| \le 1$. $\square$

Denote $s = 2^{\mathfrak{s}}$, $H = \frac{1}{s}A$. From the part of quantum walks, we know that taking $Z_\Pi = 2\Pi - I, \Pi = |0^{\mathfrak{s}}\rangle\langle 0^{\mathfrak{s}}| \otimes I, O_H = U_A Z_\Pi$, we have

$$\langle 0^{\mathfrak{s}}| \, c_i | O_H^k \, |0^{\mathfrak{s}}\rangle \, |j\rangle = (T_k(H))_{ij} \quad \forall i \cdot j \in [N].$$

Recall: $T_k$ is the degree-$k$ Chebyshev polynomial.

This is basically what we want!

Query complexity: $2k$ for $O_c$ and $O_A \Rightarrow$ in total $O(k)$ quantum queries.

The core idea is:

1. Quantum walk for $A/s = H$ gives Chebyshev polynomials of $H$.
2. Combine them by non-unitary $LCU$.
3. Which to combine: polynomial approximation.

## 2 Quantum Walk for Sparse Hamiltonian Simulation

In our lecture, we have proved that sparse Hamiltonian can be efficiently simulated, ie., an $s$-sparse Hamiltonian with $n$ quits can be simulated with cost poly $(n, s, t, 1/\varepsilon)$.

However, poly can be large. and it's also not precise. Can we give a better bound?

We use quantum walk for Hamiltonian + non-unitary $LCU$.

How to do this? Approximate $e^{-iH/s\cdot st}$ by $T_k(H/s)$.

This is basically representing $e^{-itx}$ by polynomials $T_k(x)$ for different $k$.

$e^{-itx} = \cos(tx) - i\sin(tx) \Rightarrow$ suffices to approximate $\cos(tx)$ and $\sin(tx)$ by Chebyshev polynomials.

Jacobi-Anger expansion:

$$\cos(tx) = J_0(t) + 2\sum_{n=1}^{\infty}(-1)^n J_{2n}(t) T_{2n}(x)$$

$$\sin(tx) = 2\sum_{n=0}^{\infty}(-1)^n J_{2n+1}(t) T_{2n+1}(x)$$

Here, $J_n(z)$ denotes the Bessel functions of the first kind.

Specifically, for any $\nu, e^{z\left(\nu - \frac{1}{\nu}\right)/2} = \sum_{n=-\infty}^{+\infty} \nu^n J_n(z)$.

Or in a series: far any $n \in \mathbb{Z}$, $J_n(z) = \sum_{l=0}^{\infty} \frac{(-1)^l}{2^{2l+n} l!(n+l)!} z^{2l+n}$.

Properties of the Bessel function:

- For any real $z$ and integer $n$, $J_{-n}(z) = (-1)^n J_n(z)$.
- For any real $z$ and integer $n$, $|J_n(z)| \leqslant \frac{1}{|n|!}\left|\frac{z}{2}\right|^{|n|}$ Eq. (1).
- By Eq. (1), for any positive integer $k$ and real $z$ s.t. $|z| \le k, \sum_{n=k+1}^{\infty} |J_n(z)| \le 2\frac{|z/2|^{k+1}}{(k+1)!}$. Eq. (2).
- For real $z$, $\sum_{n=-\infty}^{+\infty} |J_n(z)|^2 = 1$. By Cauchy-Schwart, this gives $\sum_{n=0}^{k} |J_n(z)| < \sqrt{k+1}$ Eq. (3).

Note: Eq. (2) bounds the tail of Jacobi-Anger expansion, but the form looks simple only for small $z$. Eq. (3) bounds the cost needed for $LCU$ (the $\alpha$).

Simulate in piece: Each piece for a shout the $z=2$ (total number of pieces $=\frac{t}{2}$). and precision $\frac{\varepsilon}{t}$ for each piece (two terms in each piece: $\cos 2H$ and $\sin 2H$ ). Total error: $\leqslant \frac{t}{2}\cdot\frac{\varepsilon}{t}\cdot 2=\varepsilon$.

This requires that $\frac{2}{(k+1)!}\leq\frac{\varepsilon}{t}$. By Stirling's formula, $k!\sim\sqrt{2\pi k}\cdot\left(\frac{k}{e}\right)^k$

$$\Rightarrow k=O\left(\log\frac{t}{\varepsilon}/\log\log\frac{t}{\varepsilon}\right).$$

Final algorithm:

Input: An s-sparse Hamiltonian A such that $\|A\|_{\max}\leqslant 1$. We assume its quantum query oracle.

1. Implement the quantum walk for Hamiltonian $H=\frac{A}{s}$, as introduced above.
2. Approximate $\cos 2H$ and $\sin 2H$ with precision $\frac{\varepsilon}{st}$. respectively. Using the Jacobi-Anger expansion. $k=O\left(\log\frac{st}{\varepsilon}/\log\log\frac{st}{\varepsilon}\right)$ and the non-unitary $LCU$ framework.

$$\cos(tx)=J_0(t)+2\sum_{n=1}^{\infty}(-1)^n J_{2n}(t)T_{2n}(x)\Rightarrow\cos(tx)\approx J_0(t)+2\sum_{n=1}^{\lceil\frac{k}{2}\rceil}(-1)^n J_{2n}(t)T_{2n}(x)$$

$$\sin(tx)=2\sum_{n=0}^{\infty}(-1)^n J_{2n+1}(t)T_{2n+1}(x)\Rightarrow\sin(tx)\approx 2\sum_{n=0}^{\lceil\frac{k}{2}\rceil}(-1)^n J_{2n+1}(t)T_{2n+1}(x).$$

   This approximates the map $e^{-2iH}$ with precision $\frac{2\varepsilon}{st}$.

3. Apply this for $\frac{st}{s}$ times, which gives a quantum algorithm for implementing $\left(e^{-2iH}\right)^{\frac{st}{2}}=e^{-iAt}$ with precision $\left(\frac{2\varepsilon}{st}\right)\cdot\frac{st}{2}=\varepsilon$.

Correctness: Since $f(x)=e^{-ixt}$ satisfies $|f(x)|=1\quad\forall x\in\mathbb{R}$. This condition is met in non-unitary $LCU$.
$\alpha_i\geqslant 0:$ This is can be released by rotating a phase on the quantum walk
$\Rightarrow$ Need to compute $\alpha=\sum_i|\alpha_i|$ instead.
Cost: $O(st)$ times of non-unitary $LCU$, each with

$$\alpha=\sum_i|\alpha_i|=O\left(\sum_{n=0}^{k}J_n(2)\right)=O(\sqrt{k}).$$

Complexity of implementing each $LCU$: $O(k)$. $k$ is the degree of polynomial approximation.
In total: $O(st)\cdot O(\sqrt{k})\cdot O(k)=O\left(stk^{1.5}\right)=O\left(st\cdot\left(\frac{\log(st/\varepsilon)}{\log\log(st/\varepsilon)}\right)^{1.5}\right)$.
This is much better than using the Trotter formula!
We achieve: (almost) linear in s, (almost) linear in $t$, poly-logarithmic in $\varepsilon$.
On the other hand, this is not far from the optical band: $\Theta\left(st\|A\|_{\max}+\frac{\log(1/\varepsilon)}{\log\log(1/\varepsilon)}\right)$.

Reference. Low and Chang. Optimal Hamiltonian simulation by quantum signal processing. PRL 2017: arxiv: 1606.02685.

# 3 Solving Linear Systems

One of the most basic problems in linear algebra.

In quantum computing we consider the following problem:

Definition. (Quantum Linear system problem, QLSP) Let $A$ be an $N \times N$ Hermitian matrix with condition number $\kappa$, $\|A\| = 1$, and is $d$-sparse. Let $\vec{b}$ be an $N$-dimensional vector, and let $\vec{x} = A^{-1}\vec{b}$. We define the quartan states $|b\rangle$ and $|x\rangle$ :

$$|b\rangle = \frac{\sum_i b_i |i\rangle}{\|\sum_i b_i\, |i\rangle\|} \text{ and } |x\rangle = \frac{\sum_i x_i |i\rangle}{\|\sum_i x_i |i\rangle\|}.$$

Given a quantum query oracle $O_A$ and a unitary $U_B$ that prepares $(b)$, the goal is to output a state $|\bar{x}\rangle$ such that $\||\bar{x}\rangle - |x\rangle\| \leqslant \varepsilon$. succeeding with probability $\geqslant 2/3$.

$\|A\| = 1$, condition number $K \Rightarrow$ all eigenvalues of $A$ are in $D_k = [-1, -1/k] \cup [1/k, 1]$.

As a result, all eigenvalues of $H = A/d$ are in $[-1/d, -1/dk] \cup [1/dk, 1/d] \subseteq D_{dk}$.

Next Class: non-unitary $LCU$ + quantum walk for solving linear systems.