Lecture 14

Hamiltonian simulation

- Product formulas

- Sparse Hamiltonian

1 Product formulas

Many natural Hamiltonians have the form of a sum of terms, each of which can be efficiently simulated.

Ex. Hamiltonian of a n-qubit spin system:

$$H = \sum_i h_i X_i + \sum_{i,j} J_{i,j} Z_i Z_j,$$

where $h_i, J_{i,j} \in \mathbb{C}, X_i$ is Pauli-X acting on the i^{th} qubit (and I on other qubits), and z_i is Pauli-Z acting on the i^{th} qubit.

Definition. A Hamiltonian H is k-local if H is sum of Hamiltonians that each acts on at most k qubits.

Product formula: In general, if H_1 and H_2 can be efficiently simulated, then $H_1 + H_2$ can be efficiently simulated.

If H_1 and H_2 commute ($[H_1, H_2] = H_1H_2 - H_2H_1 = 0$), then this is trivial:

$$e^{-i(H_1+H_2)t} = e^{-iH_1t}e^{-iH_2t}$$

In general, for matrices, H_1 and H_2 don't commute, i.e., $[H_1, H_2] \neq 0$. In this case, $e^{-i(H_1+H_2)t} \neq e^{-iH_1t}e^{-iH_2t}$ in general. What can we do?

Lie product formula: $e^{-i(H_1+H_2)t} = \lim_{m\to\infty} \left(e^{-iH_1t/m}e^{-iH_2t/m}\right)^m$

For more quantitative versions, we truncate this expression to a finite number of times:

$$\left\| \left(e^{-iH_1t/m}e^{-iH_2t/m}\right)^m - \left(e^{-i(H_1+H_2)t/m}\right)^m \right\| \leq \varepsilon. \tag{*}$$

For convenience, $A = -iH_1t,\ B = -iH_2t$. Intuition: $a^m - b^m = (a-b)\left(a^{m-1} + a^{m-2}b + \cdots + b^{m-1}\right)$

Since for matrices a, b,

$$\begin{aligned}
&\|a^m - b^m\| \\
=&\left\|a^m - a^{m-1}b + a^{m-1}b - a^{m-2}b^2 + a^{m-2}b^2 + \cdots + ab^{m-1} - b^m\right\| \\
\leqslant&\left\|a^m - a^{m-1}b\right\| + \|a^{m-1}b - a^{m-2}b^2\| + \cdots + \|ab^{m-1} - b^m\| \qquad \|XY\| \leqslant \|X\| \cdot \|Y\| \\
=&\|a^{m-1}(a-b)\| + \|a^{m-2}(a-b)b\| + \cdots + \|(a-b)b^{m-1}\| \\
\leqslant&m\|a-b\| \cdot (\max\{\|a\|, \|b\|\})^{m-1}
\end{aligned}$$

$$\|e^a\| \leqslant e^{\|a\|} : \|e^a\| = \left\| I + a + \frac{a^2}{2!} + \cdots \right\| \leqslant 1 + \|a\| + \frac{\|a\|^2}{2!} + \cdots = e^{\|a\|}.$$

Taking $a = e^{A/m}e^{B/m}$ and $b = e^{(A+B)/m}$, we have:

$$\left\| \left(e^{A/m}e^{B/m}\right)^m - \left(e^{(A+B)/m}\right)^m \right\| \leqslant m \cdot \left\| e^{A/m}e^{B/m} - e^{(A+B)/m} \right\| \cdot \max\left\{ \left\| e^{A/m}e^{B/m} \right\|, \left\| e^{(A+B)/m} \right\| \right\}^{m-1}.$$

In our case, $e^{A/m}e^{B/m} = e^{-iH_1t/m}e^{-iH_2t/m}$ is a multiplication of two unitaries, $\left\|e^{A/m}e^{B/m}\right\| = 1$. Similarly, $e^{(A+B)/m} = e^{-i(H_1+H_2)t/m}$ is a unitary, so $\left\|e^{(A+B)/m}\right\| = 1$.

$$\begin{aligned}
e^{A/m}e^{B/m} - e^{A+B/m} &= \left(I + \frac{A}{m} + O\left(\frac{\|A\|^2}{m^2}\right)\right)\left(I + \frac{B}{m} + O\left(\frac{\|B\|^2}{m^2}\right)\right) - \left(I + \frac{A+B}{m} + O\left(\frac{\|A+B\|^2}{m^2}\right)\right) \\
&= \left(I + \frac{A}{m} + \frac{B}{m} + \frac{AB}{m^2} + O\left(\frac{\max\{\|H\|, \|B\|]^2}{m^2}\right)\right) - \left(I + \frac{A+B}{m} + O\left(\frac{\|A+B\|^2}{m^2}\right)\right). \\
&= O\left(\frac{\max\{\|A\|, \|B\|\}^2}{m^2}\right). \qquad \|A+B\| \le \|A\| + \|B\| \le 2\max\{\|A\|, \|B\|\}
\end{aligned}$$

In all, we have

$$\left\| \left(e^{A/m}e^{B/m}\right)^m - \left(e^{A+B/m}\right)^m \right\| = O\left(\frac{1}{m} \cdot \max\{\|A\|, \|B\|\}^2\right) \overset{?}{\le} \varepsilon. \tag{**}$$

Suppose H_1, H_2 satisfies $\|H_1\|, \|H_2\| = O(1)$. Then $\|A\|, \|B\| = O(t)$.

To make $(**) \le \varepsilon$, $\quad m = O\left(\frac{\max\{\|A\|,\|B\|\}^2}{\varepsilon}\right) = O\left(\frac{t^2}{\varepsilon}\right)$

Cost of simulation: Apply $\left(e^{-iH_1t/m}e^{-iH_2t/m}\right)^m$, in other words, $e^{-iH_1t/m}$ and $e^{-iH_2t/m}$ alternatively, for $m = O\left(t^2/\varepsilon\right)$ times.

Can we improve further the bound for m, i.e., can we make the error to 3rd power?

Consider $e^{A/2m}e^{B/m}e^{A/2m} \quad \left(e^{A/2m}e^{B/m}e^{A/2m}\right)^m$

WLOG $\|A\|, \|B\| \le 1$ for better presentation

$$\begin{aligned}
&e^{A/2m}e^{B/m}e^{A/2m} - e^{(A+B)/m} \\
&= \left(I + \frac{A}{2m} + \frac{A^2}{8m^2} + O\left(\frac{1}{m^3}\right)\right)\left(I + \frac{B}{m} + \frac{B^2}{2m^2} + O\left(\frac{1}{m^3}\right)\right)\left(I + \frac{A}{2m} + \frac{A^2}{8m^2} + O\left(\frac{1}{m^3}\right)\right) \\
&\quad - \left(I + \frac{A+B}{m} + \frac{(A+B)^2}{2m^2} + O\left(\frac{1}{m^3}\right)\right) \\
&= \left(I + \frac{A}{m} + \frac{B}{m} + \frac{A^2}{8m^2} + \frac{A^2}{8m^2} + \frac{A}{2m} \cdot \frac{A}{2m} + \frac{B^2}{2m^2} + \frac{AB}{2m^2} + \frac{BA}{2m} + O\left(\frac{1}{m^3}\right)\right) \\
&\quad - \left(I + \frac{A+B}{m} + \frac{A^2 + AB + BA + B^2}{2m^2} + O\left(\frac{1}{m^3}\right)\right) \\
&\qquad (A+B)^2 = (A+B)(A+B) = A^2 + AB + BA + B^2 \\
&\quad = O\left(\frac{1}{m^3}\right).
\end{aligned}$$

Overall: $\left\| \left(e^{-iH_1t/2m}e^{-iH_2t/m}e^{-iH_1t/2m}\right)^m - e^{-i(H_1+H_2)t} \right\| = O\left(\frac{t^3}{m^2}\right) \leqslant \varepsilon$

$\Rightarrow$ Cost: $m = O\left(\frac{t^{1.5}}{\varepsilon^{0.5}}\right)$. $\qquad$ Previous: $O\left(\frac{t^2}{\varepsilon}\right)$

$\left(e^{A/m}e^{B/m}\right)^m$: Trotter formula

High-order Trotter formula $\quad m = O\left(\frac{t^{1+\frac{1}{k}}}{\varepsilon^{\frac{1}{k}}}\right) \forall k \in \mathbb{N} \quad$ Trotter-Suzuki formula

Research paper. Berry, Ahokas, Cleve, Sanders. Efficient quantum algorithms for simulating sparse Hamittonians. CMP 2007. arXiv: quant-ph/0508139.

Similarly, for more terms we have $e^{-i(H_1+\cdots+H_l)t} = \lim_{m\to\infty}\left(e^{-iH_1 t/m}\cdots e^{-iH_l t/m}\right)^m$, and the product formulas still apply and give algorithms with cost $O\left(\frac{t^{1+\frac{1}{k}}}{\varepsilon^{\frac{1}{k}}}\right), \forall k \in \mathbb{N}$.

Corollary 1.1. *$O(1)$-local Hamiltonians can be efficiently simulated.*

- *For k-local Hamiltonians, at most $l = \left(\begin{array}{c} n \\ k \end{array}\right) = poly(n)$ terms when $k = O(1)$.*

Next class: Sparse Hamiltonian.