Lecture 4: Hamiltonian Simulation Algorithms (Pt. 2)

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Review: Trotter-Suzuki

Trotter-Suzuki decomposition:

- Pro: Very simple and intuitive. Works well in practice, too.
- Con: Scaling in inverse error is polynomial. This is not optimal.

Some history

In the early 2010s, an entirely new way of implementing Hamiltonian simulation was introduced. These approaches are not intuitive at all, and seem very unnatural from the physics perspective. However, they are often the best approaches when it comes down to the complexity.

Reviewing all of these things are beyond the scope of this lecture. What I will try to do is to explain the key ideas behind quantum signal processing [Low and Chuang (2016)], which is the state-of-the-art approach.

Guiding example

Let $|\psi\rangle$ be a single-qubit state. Let O be an arbitrary 2×2 matrix. How can we apply

$$|\psi\rangle \to O|\psi\rangle / \|O|\psi\rangle\|.$$

Is this possible at all?

Step 1: Linear Combination of Unitary

It turns out that O be can be decomposed into a linear combination of unitaries:

$$O = \alpha_I I + \alpha_X X + \alpha_Y Y + \alpha_Z Z,$$

where $\alpha_I, \alpha_X, \alpha_Y, \alpha_Z \in \mathbb{C}$.

$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ $X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ $Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ $Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$X^2 = Y^2 = Z^2 = I$

Let

$$|\alpha\rangle = (\alpha_I|I\rangle + \alpha_X|X\rangle + \alpha_Y|Y\rangle + \alpha_Z|Z\rangle)/\sqrt{\sum_k |\alpha_k|^2}.$$

Now we can apply a controlled unitary to create something that looks similar to what we want.

$$CU\ |I\rangle \otimes |\psi\rangle = |I\rangle \otimes I|\psi\rangle$$
$$CU\ |X\rangle \otimes |\psi\rangle = |X\rangle \otimes X|\psi\rangle$$
$$CU\ |Y\rangle \otimes |\psi\rangle = |Y\rangle \otimes Y|\psi\rangle$$
$$CU\ |Z\rangle \otimes |\psi\rangle = |Z\rangle \otimes Z|\psi\rangle$$
$$CU(|\alpha\rangle \otimes |\psi\rangle) = \alpha_I|I\rangle \otimes |\psi\rangle + \alpha_X|X\rangle \otimes X|\psi\rangle + \alpha_Y|Y\rangle \otimes Y|\psi\rangle + \alpha_Z|Z\rangle \otimes Z|\psi\rangle$$

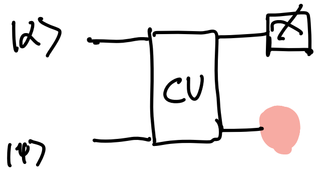
Step 3: Postselection

Now suppose we measure the ancillary register in a basis that includes $\frac{1}{2}(|I\rangle + |X\rangle + |Y\rangle + |Z\rangle)$. What happens?

$\hookrightarrow |\phi_1\rangle$

$|\phi_2\rangle, |\phi_3\rangle, |\phi_4\rangle$

$$(\langle\phi_2| \otimes I)\, CU\, (|\alpha\rangle \otimes |\psi\rangle) \neq c\, O\, |\psi\rangle$$



	Success?	Probability
$\lvert\phi_1\rangle$	Yes	$\lVert(\langle\phi_1\rvert \otimes I)\, CU\, (\lvert\alpha\rangle \otimes \lvert\psi\rangle)\rVert$
$\lvert\phi_2\rangle$	No	$\lVert(\langle\phi_2\rvert \otimes I)\, CU\, (\lvert\alpha\rangle \otimes \lvert\psi\rangle)\rVert$
$\lvert\phi_3\rangle$	No	
$\lvert\phi_4\rangle$	No	

$$CU\ |I\rangle \otimes |\psi\rangle = |I\rangle \otimes I|\psi\rangle$$
$$CU\ |X\rangle \otimes |\psi\rangle = |X\rangle \otimes X|\psi\rangle$$
$$CU\ |Y\rangle \otimes |\psi\rangle = |Y\rangle \otimes Y|\psi\rangle$$
$$CU\ |Z\rangle \otimes |\psi\rangle = |Z\rangle \otimes Z|\psi\rangle$$

$$CU\,(|\alpha\rangle \otimes |\psi\rangle) = \alpha_I |I\rangle \otimes |\psi\rangle + \alpha_X |X\rangle \otimes X|\psi\rangle + \alpha_Y |Y\rangle \otimes Y|\psi\rangle + \alpha_Z |Z\rangle \otimes Z|\psi\rangle$$

$$\left(\frac{1}{2}(\langle I| + \langle X| + \langle Y| + \langle Z|) \otimes I\right) CU\,(|\alpha\rangle \otimes |\psi\rangle)$$
$$= \frac{1}{2}(\alpha_I |\psi\rangle + \alpha_X X|\psi\rangle + \alpha_Y Y|\psi\rangle + \alpha_Z Z|\psi\rangle)$$
$$= \frac{1}{2}(\alpha_I I + \alpha_X X + \alpha_Y Y + \alpha_Z Z)|\psi\rangle$$
$$= \frac{1}{2} O|\psi\rangle$$

Lessons

- It is possible with to apply a non-unitary transformation to an unknown quantum state, as long as you are willing to accept a nonzero failure probability.
- However, when we succeed, we will know that we succeeded.
- Similarly, when we fail, we will know that we failed.

One approach

$$e^{-iHT} = \sum_n a_n H^n T^n$$

$$e^{-iHT}|\psi\rangle \simeq \sum_n a_n H^n T^n |\psi\rangle$$

1. Truncate the sum.
2. Find ways to implement $|\psi\rangle \rightarrow H|\psi\rangle$.
3. Conditionally apply 1 many times.
4. Postselect.

Problems

- Not clear how to implement $|\psi\rangle \rightarrow H|\psi\rangle$.
- This operation is not deterministic. The success probability will decay exponentially in n.

Part 1. $|\psi\rangle \to \dfrac{H|\psi\rangle}{\| H|\psi\rangle \|}$

Setup

$$H = \sum_i \alpha_i P_i,$$

where $\{P_i\}$ is a set of Paulis.

This is a reasonable choice for locally interacting many-body quantum spin systems or fermions.

$|\psi\rangle \to H|\psi\rangle$

$$H = \sum_i \alpha_i P_i,$$

where $\{P_i\}$ is a set of Paulis.

Select+Prepare

- Select: $|i\rangle \otimes |\psi\rangle \to |i\rangle \otimes \cancel{P_i|\psi\rangle}$ $P_i|\psi\rangle$
- Prepare: $|0\ldots0\rangle \to \sum_i \sqrt{|\alpha_i|}|i\rangle$.

* For convenience, let's suppose that $|\alpha\rangle = \sum_i \alpha_i|i\rangle$ is normalized.

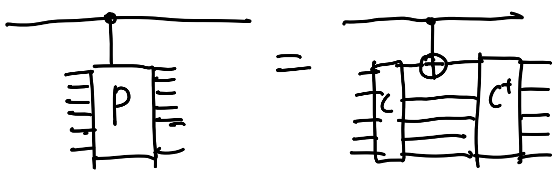
Select

Basic idea: For any Pauli P, $P = CXC^\dagger$ for some Clifford C.

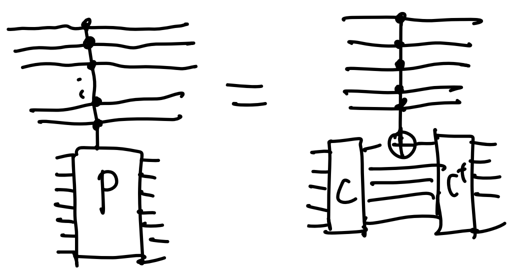
$$\text{SEL}\,|i\rangle \otimes |\psi\rangle = |i\rangle \otimes P_i|\psi\rangle$$

i	P_i
0	$X_1X_2Z_1Z_2$
1	Z_1
2	Y_3
3	X_4Y_{100}
⋮	
100	

i	P_i
0	I
1	P



i	P_i
$00\cdots0$	I
⋮	⋮
⋮	I
$11\cdots1$	P



Prepare

$$H = \sum_i \alpha_i P_i$$

$$|0 \ldots 0\rangle \to |\alpha\rangle. \qquad |\alpha\rangle = \sum_i \sqrt{|\alpha_i|}\, |i\rangle$$

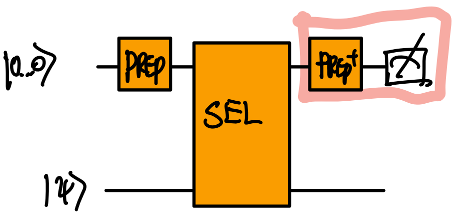
The gate complexity of this operation is $O(N \log(N/\epsilon))$, where N is the number of nonzero α_i and ϵ is the error.

Select+ Prepare

Using $O(1)$ number of Select and Prepare, we can realize

$$|\psi\rangle \to H|\psi\rangle$$

with a nonzero probability.



$$|0\ldots0\rangle \otimes |\psi\rangle \to |\alpha\rangle \otimes |\psi\rangle$$

$$\to \sum_i \sqrt{|\alpha_i|}\, |i\rangle \otimes P_i|\psi\rangle$$

$$\to \sum_{i,j} \sqrt{|\alpha_i||\alpha_j|}\, \langle j||i\rangle \otimes P_i|\psi\rangle$$

$$= \sum_i |\alpha_i| P_i|\psi\rangle \quad \text{if } \alpha_i \geq 0$$

$$= \sum_i \alpha_i P_i|\psi\rangle$$

$$= H|\psi\rangle$$

$$\mathrm{PREP}\,|0\ldots0\rangle = |\alpha\rangle$$

$$\to \boxed{\langle 0\ldots0|\mathrm{PREP}^\dagger} = \underline{\langle\alpha|}$$

$$H = \sum \alpha_i P_i$$

$$|\alpha\rangle = \sum_i \sqrt{|\alpha_i|}\, |i\rangle \qquad H = \sum_i \alpha_i P_i$$

\# terms $O(n)$

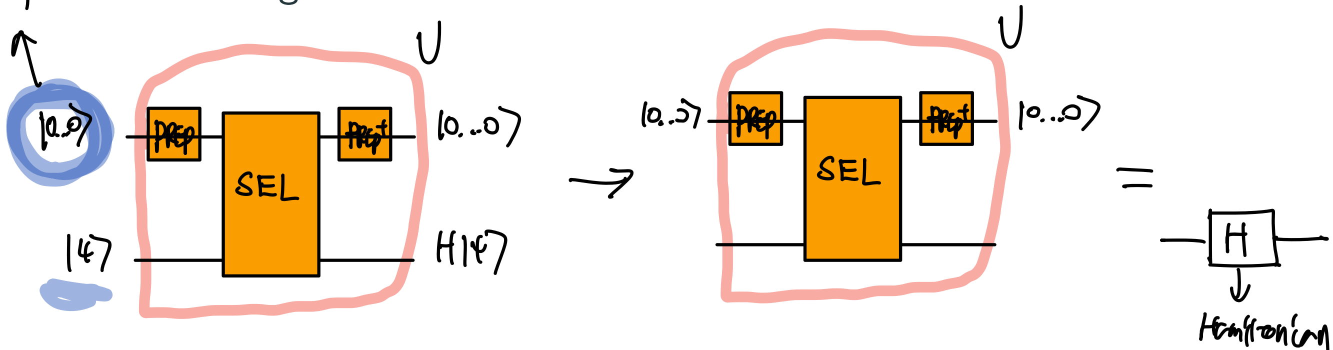
↳ system size

We say that a unitary U is a block-encoding of H if

$$(\langle 0 \ldots 0|_a \otimes I_s) U (|0 \ldots 0\rangle_a \otimes I_s) = H.$$

The Select+Prepare provides a natural framework to implement a block-encoding of H.

$O(\log n)$



Part 2. Quantum Signal Processing (=Qubitization)

One approach

$$e^{-iHT} = \sum_n a_n H^n T^n$$

1. Truncate the sum.
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- This operation is not deterministic. The success probability will decay exponentially in n.

Simplification

We will make a simplification that will make our analysis easier. Suppose we have a block encoding of H:

$U^2 \neq I$

$$(\langle 0\ldots 0|_a \otimes I_s)U(|0\ldots 0\rangle_a \otimes I_s) = H.$$

Moreover, suppose we can somehow guarantee that $U^2 = I$. This may seem like a very strong assumption but it is not. [Low and Chuang (2016)] discusses a method to convert a general block encoding into a block encoding that squares to identity. Let me emphasize that the extra cost is acceptable; one only needs $O(1)$ factor blowup in the cost (plus negligible amount of additional gates).

Another simplification

We will make a yet another(!) simplification that will make our analysis easier. We will assume that

$$(\langle 0|_a \otimes I_s)U(|0\rangle_a \otimes I_s) = H.$$

"ancilla"

Unlike the previous simplification, it is generally not possible to reduce the number of ancilla qubits to 1. However, what we are about to show can be generalized easily to the case in which we have more than one ancilla qubits. (You can ask me later if you are curious.)

Acting on an eigenstate

Let U be the aforementioned block encoding of H. Let $|n\rangle$ be an eigenstate of H (with an eigenvalue of E_n).

$$U(|0\rangle \otimes |n\rangle) = E_n|0\rangle|n\rangle + \sqrt{1-E_n^2}|1\rangle|\psi_n\rangle,$$

where $|\psi_n\rangle$ is some unknown normalized state.

Question:

$$U(|1\rangle \otimes |\overset{\psi_n}{\cancel{n}}\rangle) = ?$$

$$(\langle 0| \otimes I)\, U |0\rangle \otimes |n\rangle = H|n\rangle = E_n|n\rangle \qquad U|0\rangle \otimes |n\rangle = E_n|0\rangle|n\rangle + \sqrt{1-E_n^2}\,|1\rangle|\psi_n\rangle$$

$$U^2 = I$$

$$\underbrace{U^2(|0\rangle \otimes |n\rangle)}_{|0\rangle \otimes |n\rangle} = \underbrace{U\ E_n|0\rangle|n\rangle} + \sqrt{1-E_n^2}\,U|1\rangle|\psi_n\rangle$$

$$= E_n^2|0\rangle|n\rangle + E_n\sqrt{1-E_n^2}\,|1\rangle|\psi_n\rangle + \sqrt{1-E_n^2}\,U|1\rangle|\psi_n\rangle$$

$$\boxed{U|1\rangle \otimes |\psi_n\rangle = \sqrt{1-E_n^2}\,|0\rangle|n\rangle - E_n|1\rangle|\psi_n\rangle}$$

Two-dimensional subspace

From our assumptions, we showed that U preserves a two-dimensional subspace spanned by

$$\{|0\rangle \otimes |n\rangle, |1\rangle \otimes |\psi_n\rangle\}.$$

Moreover, on this subspace U acts in the following form:

$$\begin{pmatrix} E_n & \sqrt{1-E_n^2} \\ \sqrt{1-E_n^2} & -E_n \end{pmatrix},$$

a 2×2 unitary that squares to 1.

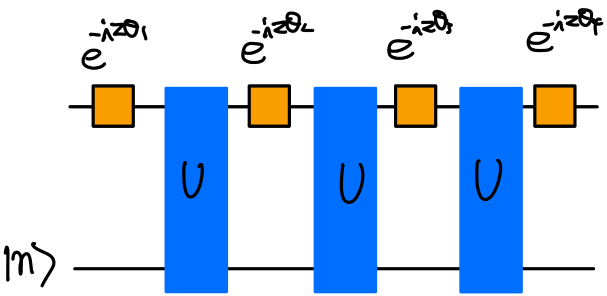
Two-dimensional subspace

From our assumptions, we showed that U preserves a two-dimensional subspace spanned by

$$\{|0\rangle \otimes |n\rangle, |1\rangle \otimes |\psi_n\rangle\}.$$

There is another unitary that we can easily apply in this subspace: $e^{-iZ\theta}$ acting on the ancilla qubit. On our subspace, this is again a 2×2 unitary:

$$\begin{pmatrix} e^{-i\theta} & 0 \\ 0 & e^{i\theta} \end{pmatrix}$$



U: Block encoding of H

Qubitization (=Quantum Signal Processing)

By interleaving the two unitaries d times, we can obtain a 2×2 unitary of some particular form.

polynomials

$$\boxed{\begin{pmatrix} P(E_n) & iQ(E_n)\sqrt{1-E_n^2} \\ iQ^*(E_n)\sqrt{1-E_n^2} & P^*(E_n), \end{pmatrix}}$$

where P and Q are polynomial of degrees of at most d and $d-1$ respectively. (Moreover, they have different parities.)

Question. Given this fact, suppose we apply the same sequence of unitaries to $|0\rangle|\psi\rangle$, where $|\psi\rangle$ is an arbitrary state, and then measure the ancilla qubit. If we measure $|0\rangle$, what is the post-measurement state?

$$|0\rangle\otimes|n\rangle \longrightarrow \begin{pmatrix} P(E_n) & iQ(E_n)\sqrt{1-E_n^2} \\ iQ^*(E_n)\sqrt{1-E_n^2} & P^*(E_n) \end{pmatrix} |0\rangle\otimes|n\rangle$$

$$\langle 0| \begin{pmatrix} P(E_n) & iQ(E_n)\sqrt{1-E_n^2} \\ iQ^*(E_n)\sqrt{1-E_n^2} & P^*(E_n) \end{pmatrix} |0\rangle\otimes|n\rangle = P(E_n)\,|n\rangle$$

$$|\psi\rangle = \sum_n a_n|n\rangle \rightarrow \sum_n a_n P(E_n)\,|n\rangle = \sum_n a_n P(H)\,|n\rangle = P(H)\sum_n a_n|n\rangle = P(H)\,|\psi\rangle$$

Qubitization (=Quantum Signal Processing)

By interleaving the two unitaries d times, we can obtain a 2×2 unitary of some particular form.

$$\begin{pmatrix} P(E_n) & iQ(E_n)\sqrt{1-E_n^2} \\ iQ^*(E_n)\sqrt{1-E_n^2} & P^*(E_n), \end{pmatrix}$$

where P and Q are polynomial of degrees of at most d and $d-1$ respectively. (Moreover, they have different parities.)

We found that we can implement

$$|\psi\rangle \to P(H)|\psi\rangle$$

for some polynomial $P(x)$. The success probability is exactly $\|P(H)|\psi\rangle\|$.

Qubitization (=Qiuantum Signal Processing)

We now have a very general framework to apply a polynomial transformation to the Hamiltonian H and apply it to an arbitrary state.

Important facts

1. For any real polynomial $P(x)$, as long as $|P(x)| < 1$, by choosing a different measurement basis we can apply $P(H)$.
   - No need to worry about the pesky $Q(x)$.
2. Given a real polynomial $P(x)$, there is an efficient classical algorithm that computes the set of angles (used in single-qubit rotations).

$\rightarrow$ If you have a good polynomial approximation of any function $f(x)$, you can apply $f(H)$ to an arbitrary quantum state using qubitization. The complexity scales linearly with the degree of the polynomial.

Example. e^{-ixt}

To apply e^{-iHt}, we need to use a function $f(x) = e^{-ixt}$. $f(H) = e^{-iHt}$

Jacobi-Anger expansion

$e^{-ixt} = \cos xt - i \sin xt$

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

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

$J_i(t)$: Bessel function of the first kind of order i

$T_k(x)$: Chebyshev polynomial

This expansion leads to complexity of

precision (error)

$$\boxed{O\left(t + \frac{\log 1/\epsilon}{\log\log(1/\epsilon)}\right),}$$

which is optimal in all the parameters. [Low and Chuang (2016)]

Recap

- The state-of-the-art method for Hamiltonian simulation uses highly non-intuitive facts.
  - Application of non-unitary transformation.
  - Polynomial approximation of a transcendental function.
- Quantum computers seem to be very good at applying low-order polynomial of the Hamiltonian to an arbitrary quantum state.

At this point, the standard approach to Hamiltonian simulation is the qubitization. And the main innovation lies in optimizing the block encoding of a Hamiltonian into a unitary.