Hamiltonian Simulation

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1 Simulating Hamiltonian dynamics

In quantum mechanics, time evolution of the state $|\psi(t)\rangle$ is governed by the Schrodinger equation,

$$i\frac{d}{dt}|\psi(t)\rangle = H(t)|\psi(t)\rangle,$$

where $H(t)$ is the Hamiltonian. Given an initial state $|\psi(0)\rangle$, we can solve this differential equation to determine $|\psi(t)\rangle$ at any time t.

For H independent of time, the solution of the Schrodinger equation is

$$|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle.$$

A Hamiltonian acting on n qubits is said to be *efficiently simulated* if for any $t > 0$, $\epsilon > 0$, there is a quantum circuit U consisting of $\mathrm{poly}(n, t, 1/\epsilon)$ gates such that

$$||U - e^{-iHt}|| < \epsilon.$$

$$\int dte^{-i\omega t}\langle\psi(0)|e^{-iHt}|\psi(0)\rangle$$

2 Trotter-Suzuki

3 Quantum walk

The quantum walk approach gives optimal complexity as a function of the simulation time t, while its performance as a function of the required error ϵ is worse than PF.

4 Linear combinations of unitaries

We can achieve complexity poly(log($1/\epsilon$)) by techniques for implementing linear combinations of unitary operators.

Basic idea of LCU is that given the ability to implement

$$\mathrm{SELECT}(W) = \sum_{j=0} |j\rangle\langle j| \otimes W_j$$

implement $V = \sum \alpha_i W_i$, where each W_i is an easy-to-implement unitary. For instance, let $V = W_0 + W_1$,

$$\begin{aligned}
\mathrm{SELECT}(W) \left|+\right\rangle \left|\psi\right\rangle &= \frac{1}{\sqrt{2}}(\left|0\right\rangle W_0 + \left|1\right\rangle W_1) \left|\psi\right\rangle \\
&= \frac{1}{2}(\left|+\right\rangle (W_0 + W_1) + \left|-\right\rangle (W_0 - W_1)) \left|\psi\right\rangle \\
&= \frac{1}{2} \left|+\right\rangle V \left|\psi\right\rangle + \frac{1}{2} \left|-\right\rangle (W_0 - W_1)) \left|\psi\right\rangle,
\end{aligned}$$

which is a probabilistic implementation of V.

More generally, suppose we can decompose the given Hamiltonian in the form

$$H = \sum_{\ell=1}^{L} \alpha_\ell H_\ell,$$

where α_ℓ are some real positive coefficients and H_ℓ are both unitary and Hermitian. This is straightforward if H is k-local, since in that case H can be expressed as linear combinations of Pauli operators.

We denote the Taylor series for e^{-iHt} up to time t, truncated at order K, by

$$\begin{aligned}
\tilde{U}(t) &= \sum_{k=0}^{K} \frac{(-iHt)^k}{k!} \\
&= I + (-it) \sum_{\ell=1}^{L} \alpha_\ell H_\ell + \cdots + \frac{(-it)^K}{K!} \left(\sum_{\ell=1}^{L} \alpha_\ell H_\ell \right)^K \\
&= \sum_{k=0}^{K} \sum_{\ell_1=1}^{L} \cdots \sum_{\ell_k=1}^{L} \frac{t^k}{k!} \alpha_{\ell_1} \cdots \alpha_{\ell_k} (-i)^k H_{\ell_1} \cdots H_{\ell_k} \\
&= \sum_{j=0}^{m-1} \beta_j V_j
\end{aligned}$$

Let B be an operator that prepares the state

$$B|0\rangle = |\beta\rangle = \frac{1}{s}\sum_{j=0}^{m-1}\sqrt{\beta_j}\,|j\rangle\,,$$

where

$$\begin{aligned}
s &= \sum_{j=0}^{m-1}\beta_j \\
&= \sum_{k=0}^{K}\sum_{\ell_1=1}^{L}\cdots\sum_{\ell_k=1}^{L}\frac{t^k}{k!}\alpha_{\ell_1}\cdots\alpha_{\ell_k} \\
&= \sum_{k=0}^{K}\frac{t^k}{k!}\left(\sum_{\ell=1}^{L}\alpha_\ell\right)^k.
\end{aligned}$$

Let

$$\mathrm{SELECT}(V) = \sum_{j=0}^{m-1}|j\rangle\langle j|\otimes V_j$$

and

$$W = (B^\dagger\otimes I)\mathrm{SELECT}(V)(B\otimes I)$$

Then we have

$$\begin{aligned}
(\langle 0|\otimes I)W(|0\rangle\otimes|\psi\rangle) &= (\langle 0|\otimes I)B^\dagger\mathrm{SELECT}(V)B(|0\rangle\otimes|\psi\rangle) \\
&= \frac{1}{s}\left(\sum_{i}^{m-1}\sqrt{\beta_i}\,\langle i|\otimes I\right)\mathrm{SELECT}(V)\left(\sum_{j}^{m-1}\sqrt{\beta_k}\,|k\rangle\otimes|\psi\rangle\right) \\
&= \frac{1}{s}\left(\sum_{i}^{m-1}\sqrt{\beta_i}\,\langle i|\otimes I\right)\left(\sum_{j=0}^{m-1}|j\rangle\langle j|\otimes V_j\right)\left(\sum_{j}^{m-1}\sqrt{\beta_k}\,|k\rangle\otimes|\psi\rangle\right) \\
&= \frac{1}{s}\sum_{j=0}^{m-1}\beta_j V_j\,|\psi\rangle \\
&= \frac{1}{s}\tilde{U}(t)\,|\psi\rangle
\end{aligned}$$

If we postselect the state $W(|0\rangle\otimes|\psi\rangle)$ on having its first register in the state $|\psi\rangle$, we obtain the desired result, with the success probability of approximately $1/s^2$. W is called *probabilistic implementation* of U with probability $1/s$, or W *block-encodes* the operator U/s.

The action of W on the full space is

$$W(|0\rangle \otimes |\psi\rangle) = \frac{1}{s} |0\rangle \otimes \tilde{U}(t) |\psi\rangle + \sqrt{1 - \frac{1}{s^2}} |\Phi\rangle$$

where subspace of $|\Phi\rangle$ is orthogonal to $|0\rangle$, or

$$(|0\rangle\langle 0| \otimes I) |\Phi\rangle = 0$$

To boost the chance of success, we would like to apply amplitude amplification to W. Note however that $|\psi\rangle$, about which we would like to reflect, is unknown. Alternatively we can apply the reflection about the subspace $|0\rangle$

$$R = (I - 2 |0\rangle\langle 0|) \otimes I$$

Let the projection $P = |0\rangle\langle 0|$, we have

$$\begin{aligned} WRW^\dagger RW &= W((I - 2P) \otimes I)W^\dagger((I - 2P) \otimes I)W \\ &= WW^\dagger W - 2WPW^\dagger W - 2WW^\dagger PW + 4WPW^\dagger PW, \end{aligned}$$

hence

$$(\langle 0| \otimes I)WRW^\dagger RW(|0\rangle \otimes I) = (\langle 0| \otimes I)(-3W + 4WPW^\dagger PW)(|0\rangle \otimes I)$$

TODO: check

1. Is $W^\dagger = W^{-1}$?
2. $\langle 0| B^\dagger B |0\rangle = 1$, then what is $B^\dagger |0\rangle$?

Therefore

$$(\langle 0| \otimes I)WRW^\dagger RW(|0\rangle \otimes |\psi\rangle) = -\frac{3}{s}\tilde{U}(t) |\psi\rangle + \frac{4}{s^3}\tilde{U}(t)\tilde{U}^\dagger(t)\tilde{U}(t) |\psi\rangle ,$$

which is close to $-(3/s - 4/s^3)\tilde{U}(t)$ since $\tilde{U}(t)$ is close to unitary. For the purpose of Hamiltonian simulation, we can choose the parameters such that a single segment of the evolution has the value of s, and we repeat the process, called *oblivious amplitude amplification*. More generally, the operation $WRW^\dagger RW$ is applied many times to boost the amplitude for success to a value close to unity. LCU can be implemented with complexity $O(1/s)$. It is important to note that U is (closed to) unitary for OAA to work.

5 Quantum signal processing

Suppose we can decompose the given Hamiltonian in the form

$$H = \sum_{\ell=1}^{L} \alpha_\ell H_\ell,$$

where α_ℓ are some real positive coefficients and H_ℓ are both unitary and Hermitian.

Let

$$\mathrm{SELECT}(H) = \sum_{\ell=1}^{L} |\ell\rangle\langle\ell| \otimes H_\ell$$

and

$$\mathrm{PREPARE}\,|0\rangle = \frac{1}{\sqrt{\alpha}} \sum_{\ell=1}^{L} \sqrt{\alpha_\ell}\,|\ell\rangle = |G\rangle\,,$$

where $\alpha = \sum_{\ell=1}^{L} \alpha_\ell$. Then we have

$$\begin{aligned}
(\langle G| \otimes I)\mathrm{SELECT}(H)(|G\rangle \otimes I) &= \left(\frac{1}{\sqrt{\alpha}} \sum_{j=1}^{L} \sqrt{\alpha_j}\,\langle j| \otimes I\right) \sum_{\ell=1}^{L} |\ell\rangle\langle\ell| \otimes H_\ell \left(\frac{1}{\sqrt{\alpha}} \sum_{k=1}^{L} \sqrt{\alpha_k}\,|k\rangle \otimes I\right) \\
&= \frac{1}{\alpha} \sum_{\ell=1}^{L} \alpha_\ell H_\ell \\
&= \frac{1}{\alpha} H
\end{aligned}$$

Let the spectral decompositions of H/α is

$$\frac{H}{\alpha} = \sum_{\lambda} \lambda\,|\lambda\rangle\langle\lambda|\,,$$

where the sum runs over all eigenvalues of H/α and $|\lambda| \leq 1$.

The concept of *qubitization* relates the spectral decompositions of H/α and

$$\mathcal{W} = ((2\,|G\rangle\langle G| - I) \otimes I)\,\mathrm{SELECT}(H).$$

$$\mathcal{R} = ((2\,|G\rangle\langle G| - I) \otimes I)$$

Theorem 2 of [Low and Chuang 2016] asserts that for each eigenvalue $\lambda \in (-1, 1)$, $\mathcal{W}$ has two corresponding eigenvalues (TODO: proof)

$$\lambda_\pm = \mp\sqrt{1 - \lambda^2} - i\lambda = \mp e^{\pm i \arcsin(\lambda)},$$

with eigenvectors $|\lambda_\pm\rangle = (|G_\lambda\rangle \pm i\,|G_\lambda^\perp\rangle)/\sqrt{2}$, where

$$\begin{aligned}
|G_\lambda\rangle &= |G\rangle \otimes |\lambda\rangle \\
|G_\lambda^\perp\rangle &= \frac{\lambda\,|G_\lambda\rangle - \mathrm{SELECT}(H)\,|G_\lambda\rangle}{\sqrt{1-\lambda^2}}
\end{aligned}$$

(TODO: proof)

$$\mathcal{W} = e^{i\arccos(\lambda)Y}$$

To perform Hamiltonian simulation by qubitization, we implement a function of θ that converts the eigenvalues $\lambda_\pm$ of $-iQ$ to the desired phase $e^{-i\lambda t}$, where

$$\theta(\lambda_\pm) = \mp\arccos(\lambda)$$

We approximate $e^{-i\lambda t}$ with the Jacobi-Anger expansion

$$e^{-i\cos(z)t} = \sum_{k=-\infty}^{\infty} i^k J_k(t) e^{ikz}$$

where $J_k(t)$ are Bessel function of the first kind. By identifying $\cos(z) = \lambda$, we obtain

$$\begin{aligned}
e^{-i\lambda t} &= \sum_{k=-\infty}^{\infty} i^k J_k(t) e^{ik\arccos(\lambda)} \\
&= J_0(t) + 2\sum_{k=1}^{\infty}(-1)^k J_{2k}(t)T_{2k}(\lambda) + 2i\sum_{k=1}^{\infty}(-1)^{k-1}J_{2k-1}(t)T_{2k-1}(\lambda) \\
&= \mathcal{A}(\lambda) + i\mathcal{C}(\lambda)
\end{aligned}$$

where $T_k(x) = \cos(k\arccos(x))$ is the Chebyshev polynomials.

$$T_k(\lambda) = \cos(k\arccos(\lambda)) = \cos\left(k\left(\frac{\pi}{2} + \theta(\lambda_\pm)\right)\right)$$

hence

$$e^{-i\lambda t} = \mathcal{A}\left(\frac{\pi}{2} + \theta(\lambda_\pm)\right) + i\mathcal{C}\left(\frac{\pi}{2} + \theta(\lambda_\pm)\right)$$

The QSP algorithm applies a sequence of *phased iterates*. We introduce an additional ancilla qubit and define the operator. Given any unitary V with eigenstates $V\,|\lambda\rangle = e^{i\theta_\lambda}\,|\lambda\rangle$ and

$$V_0 = |+\rangle\langle+| \otimes I + |-\rangle\langle-| \otimes V$$

controlled by the single-qubit ancilla register where $X\,|\pm\rangle = \pm\,|\pm\rangle$.

$$V_\varphi = (e^{-i\varphi Z/2} \otimes I)V_0(e^{i\varphi Z/2} \otimes I)$$

To simulate evolution of an initial state $|\psi\rangle$, the QSP algorithm applies V to the state $|+\rangle \otimes |G\rangle \otimes |\psi\rangle$

$$
\begin{aligned}
e^{-i\phi Z/2} |+\rangle &= e^{-i\phi/2}(|0\rangle + e^{-i\phi/2} |1\rangle) \\
&= e^{-i\phi/2}/2(1 + e^{-i\phi/2}) |+\rangle + (1 - e^{-i\phi/2}) |-\rangle \\
&= e^{-i\phi/2}(\cos(\phi/2) |+\rangle + i \sin(\phi/2) |-\rangle)
\end{aligned}
$$

$$
\begin{aligned}
V_\phi(|+\rangle \otimes |G\rangle \otimes |\lambda\rangle) &= (e^{-i\phi Z/2} \otimes I)(|+\rangle\langle+| \otimes I + |-\rangle\langle-| \otimes (-iQ))(e^{-i\phi Z/2} \otimes I)(|+\rangle \otimes |G\rangle \otimes |\lambda\rangle) \\
&= e^{i\phi}(e^{-i\phi Z/2} \otimes I)(|+\rangle\langle+| \otimes I + |-\rangle\langle-| \otimes (-iQ))(\cos(\phi/2) |+\rangle + i \sin(\phi/2) |-\rangle) \otimes |G\rangle \otimes |\lambda \\
&= (e^{-i\phi Z/2} \otimes I)(\cos(\phi/2) |+\rangle + ie^{-i\theta_\lambda} \sin(\phi/2) |-\rangle) \otimes |G\rangle \otimes |\lambda\rangle) \\
&= (\cos(\theta_\lambda) |+\rangle + \sin(\theta_\lambda) |-\rangle) \otimes |G\rangle \otimes |\lambda\rangle)
\end{aligned}
$$

and post-selects the ancilla register of the output on the $|+\rangle \otimes |G\rangle$.

Consider the sequence,

$$
V_{\bar{\varphi}} = V^\dagger_{\varphi_Q+\pi} V_{\varphi_{Q-1}} \cdots V^\dagger_{\varphi_2+\pi} V_{\varphi_1}
$$

(TODO: add cancellation of phase) For each eigenstate $|\lambda\rangle$, we obtain a product of single qubit operators $R_{\varphi_Q}(\theta_\lambda) \cdots R_{\varphi_1}(\theta_\lambda)$ acting only on the ancilla $|+\rangle$. The choice of $\{\varphi_1, \cdots, \varphi_Q\}$ determines the effective single-qubit ancilla operator

$$
V_{\bar{\varphi}} = \oplus_\lambda (\mathcal{A}(\theta_\lambda) I + i\mathcal{B}(\theta_\lambda) Z + i\mathcal{C}(\theta_\lambda) X + i\mathcal{D}(\theta_\lambda) Y) \otimes |\lambda\rangle\langle\lambda|
$$

$$
(\langle G| \otimes \langle+|) V_{\bar{\varphi}} (|+\rangle \otimes |G\rangle) = \oplus_{\lambda,\pm} \frac{1}{2} \left(\mathcal{A}\left(\frac{\pi}{2} + \theta_{\lambda_\pm}\right) I + i\mathcal{C}\left(\frac{\pi}{2} + \theta_{\lambda_\pm}\right) X \right) \otimes |\lambda\rangle\langle\lambda|
$$

$$
\begin{aligned}
V_\phi &= (e^{-i\phi Z/2} \otimes I)(|+\rangle\langle+| \otimes I + |-\rangle\langle-| \otimes (-iQ))(e^{-i\phi Z/2} \otimes I) \\
&= \sum_\nu e^{i\theta_\nu/2} R_\phi(\theta_\nu) \otimes |\nu\rangle\langle\nu|
\end{aligned}
$$

where

$$
R_\phi(\theta) = e^{-i\theta(\cos\phi X + \sin\phi Y)/2}
$$

6 Equations for slides

$$\begin{aligned} H\left|n\right\rangle &= E_n\left|n\right\rangle \\ e^{-iHt}\left|n\right\rangle &= e^{-iE_nt}\left|n\right\rangle = e^{-i\phi_n}\left|n\right\rangle \end{aligned}$$

$$\frac{\tilde{\phi}_n}{2\pi} = \frac{j_1}{2} + \frac{j_2}{2^2} + \cdots + \frac{j_t}{2^t} = 0.j_1 j_2 \ldots j_t$$

$$\left|\psi\right\rangle\left|0\right\rangle^{\otimes t} \xrightarrow{\text{QPE}} \left|\psi\right\rangle\left|\tilde{\phi}_n\right\rangle = \left|\psi\right\rangle\left|j_1 j_2 \ldots j_t\right\rangle$$

$$\begin{aligned} H\left|\psi\right\rangle &= \sum_n c_n H\left|n\right\rangle = \sum_n c_n E_n\left|n\right\rangle \\ e^{-iHt}\left|\psi\right\rangle &= \sum_n c_n e^{-iE_nt}\left|n\right\rangle = \sum_n c_n e^{-i\phi_n}\left|n\right\rangle \end{aligned}$$

$$\begin{aligned} \left|+\right\rangle\left|n\right\rangle &\to \frac{1}{\sqrt{2}}(\left|0\right\rangle + e^{-i\phi_n}\left|1\right\rangle)\left|n\right\rangle \\ &\to \frac{1}{2}\Big[(1+e^{-i\phi_n})\left|0\right\rangle + (1-e^{-i\phi_n})\left|1\right\rangle\Big]\left|n\right\rangle \end{aligned}$$

$$\begin{aligned} \text{Prob}(0) &= 1 + \cos(\phi_n) \\ \text{Prob}(1) &= 1 - \cos(\phi_n) \end{aligned}$$

$$\begin{aligned} \left|\psi\right\rangle &= \sum_n c_n\left|n\right\rangle \\ \left|+\right\rangle\left|\psi\right\rangle &\to \frac{1}{\sqrt{2}}\sum_n c_n(\left|0\right\rangle + e^{-i\phi_n}\left|1\right\rangle)\left|n\right\rangle \\ &\to \frac{1}{2}\sum_n c_n\Big[(1+e^{-i\phi_n})\left|0\right\rangle + (1-e^{-i\phi_n})\left|1\right\rangle\Big]\left|n\right\rangle \end{aligned}$$

$$\begin{aligned} U(t) &= e^{-iHt} \\ e^{-iHt} &= \left(\prod_{\ell=1}^{L} e^{-i\alpha_\ell H_\ell t/\rho}\right)^{\rho} \end{aligned}$$

$$e^A e^B = e^{A+B+\frac{1}{2}[A,B]+\frac{1}{2}[A,[A,B]]+\frac{1}{2}[B,[B,A]]+\cdots}$$

$$e^{-i(H_0+H_1)t} = e^{-iH_0t}e^{-iH_1t} + \mathcal{O}(t^2)$$
$$e^{-i(H_0+H_1)t} = e^{-iH_0t/2}e^{-iH_1t}e^{-iH_0t/2} + \mathcal{O}(t^3)$$

$$W = e^{i\theta_\lambda} |\lambda\rangle\langle\lambda|$$

$$f(W) = \sum_\lambda f(\lambda) |\lambda\rangle\langle\lambda| = \sum_\lambda e^{-i\lambda t} |\lambda\rangle\langle\lambda|$$

$$e^{-i\lambda t} = J_0(t) + 2\sum_{k=1}^{\infty}(-1)^k J_{2k}(t)T_{2k}(\cos\theta_\lambda) + 2i\sum_{k=1}^{\infty}(-1)^{k-1}J_{2k-1}(t)T_{2k-1}(\cos\theta_\lambda)$$

$$\mathcal{A}(\theta_\lambda)I + i\mathcal{B}(\theta_\lambda)Z + i\mathcal{C}(\theta_\lambda)X + i\mathcal{D}(\theta_\lambda)Y$$

$$\mathcal{A}(\lambda) \approx J_0(t) + 2\sum_{k=1}^{Q}(-1)^k J_{2k}(t)T_{2k}(\cos\theta_\lambda)$$

$$\mathcal{C}(\lambda) \approx 2\sum_{k=1}^{Q}(-1)^{k-1}J_{2k-1}(t)T_{2k-1}(\cos\theta_\lambda)$$

$$\mathcal{W} = e^{-i\arccos(H/\alpha)Y}$$

$$f(e^{-i\arccos(H/\alpha)}) = e^{-iHt}$$

$$\alpha = \sum_{\ell=1}^{L} |\alpha_\ell|$$