Lecture 3: Hamiltonian simulation and solving linear systems

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A key insight from previous lectures was that we can define a quantum walk so that (by Szegedy's lemma) its spectrum is characterized by that of an underlying random walk. This is the first example of a so-called *block encoding* [CGJ19], which more generally refers to a way of encoding an arbitrary matrix into a unitary operator. Such block encodings are the building blocks of the recent and exciting "grand unification of quantum algorithms " [GSLW19, MRTC21]. In the following we discuss how the quantum walk results extend to more general Hermitian matrices, and how this leads to quantum algorithms for Hamiltonian simulation and solving linear systems.

1 A quantum walk for any (Hermitian) matrix

We consider a Hermitian matrix H and we will assume that $\|H\|_1 \leq 1$, i.e., $\max_y \sum_x |H_{x,y}| \leq 1$. This trivially holds (and is tight) when H is a random walk transition matrix. In analogy to previous lectures, we wish to define star states associated to H. Since the rows of H will typically not sum to one, we define the star states slightly differently:

$$|\psi_x\rangle = \sum_y \sqrt{H_{x,y}}\,|x,y\rangle + \sqrt{1 - \sum_y |H_{x,y}|}\,|x,\perp\rangle\,,$$

where $|\perp\rangle$ is some state perpendicular to all other states (i.e., $\langle y|\perp\rangle = 0$ for all y). This ensures that $|\psi_x\rangle$ remains a normalized quantum state. In analogy to previous lectures, we can now define the preparation unitary U_ψ by $U_\psi\,|x,0\rangle = |\psi_x\rangle$ and the quantum walk operator W by

$$W = S \cdot \left(2\sum_x |\psi_x\rangle\langle\psi_x| - I\right). \tag{1}$$

Here we defined the swap operator S by $S\,|x,y\rangle = |y,x\rangle$ and $S\,|x,\perp\rangle = |\perp,x\rangle$.

Exercise 1. *Verify that* $\langle\psi_y|S|\psi_x\rangle = H_{x,y}$.

This generalizes a property of the quantum walks from last lectures, and in particular it allows us to again invoke Szegedy's lemma. It states that for any eigenvalue $\lambda_j = \cos(\theta_j) \neq \pm 1$ of H with eigenvector $|v_j\rangle$, the operator $W(H)$ has a pair of eigenvalues $e^{\pm i\theta_j}$ and eigenvectors $|\phi_j^{\pm}\rangle$ such that

$$U_\psi\,|v_j\rangle\,|0\rangle = \frac{|\phi_j^+\rangle + |\phi_j^-\rangle}{\sqrt{2}}.$$

Now consider a general state $|\chi\rangle$ with eigendecomposition $|\chi\rangle = \sum_j \beta_j\,|v_j\rangle$.[1] If we map this state to the star subspace and apply the QW operator, we get

$$\begin{aligned}W^t U_\psi\,|\chi\rangle\,|0\rangle &= \sum_j \beta_j \frac{e^{i\theta_j t}\,|\phi_i^+\rangle + e^{-i\theta_j t}\,|\phi_i^-\rangle}{\sqrt{2}}\\ &= \sum_j \beta_j \left[\cos(\theta_j t)\frac{|\phi_j^+\rangle + |\phi_j^-\rangle}{\sqrt{2}} + i\sin(\theta_j t)\frac{|\phi_j^+\rangle - |\phi_j^-\rangle}{\sqrt{2}}\right].\end{aligned}$$

[1] For clarify of exposition we assume that H has no eigenvalues ± 1 (and so $\|H\|_2 < 1$).

Mapping this state back to the original state space, and looking at the correct subspace, we see that this effectively implements a function of H on the $|\chi\rangle$. Specifically, it implements the t-th Chebyshev polynomial $T_t(\cdot)$ of the first kind, which is defined on the $[-1,1]$ interval by the equation $T_t(\cos(x)) = \cos(tx)$.

Exercise 2. *With* $\Pi_0 = I \otimes |0\rangle\langle 0|$, *show that*

$$\Pi_0 U_\psi^\dagger W^t U_\psi |\chi\rangle |0\rangle = \sum_j \beta_j \cos(\theta_j t) |v_j\rangle |0\rangle = T_t(H) |\chi\rangle |0\rangle .$$

In words, this means that if we measure the second register of the quantum state $U_\psi^\dagger W^t U_\psi |\chi\rangle |0\rangle$ and we receive outcome "0" (which happens with probability $\|T_t(H)|\chi\rangle\|_2 \leq 1$), then the new state of the system is

$$\frac{T_t(H)|\chi\rangle|0\rangle}{\|T_t(H)|\chi\rangle\|_2}.$$

2 Hamiltonian simulation

We can use phase estimation to apply a different function of H on an input state $|\chi\rangle$. A particular function of interest is the matrix exponential e^{iHt}, defined by its Taylor series

$$e^{iHt} = \sum_{k\geq 0} \frac{(iHt)^k}{k!}.$$

Equivalently, using the eigendecomposition $H = \sum_j \lambda_j |v_j\rangle\langle v_j|$, this is $e^{iHt} = \sum_j e^{i\lambda_j t} |v_j\rangle\langle v_j|$. If H is a Hermitian matrix then e^{iHt} is a unitary matrix. Moreover, it describes the evolution of a quantum state $|\chi(t)\rangle$ under Schrödinger's equation with Hamiltonian H, given by

$$i\frac{\partial}{\partial t}|\chi(t)\rangle = H|\chi(t)\rangle .$$

This has solution $|\chi(t)\rangle = e^{-iHt}|\chi(0)\rangle$ (we will ignore the "$-$"-factor in the exponential). Optimally simulating Hamiltonian dynamics is a central question in quantum algorithms research, and research in this direction has been a source of many new techniques.

We describe an algorithm for implementing the matrix exponential by combining the QW operator in Eq. (1) with quantum phase estimation.[2] We start from the initial state $|\chi\rangle|0\rangle|0\rangle = \sum_j \beta_j |v_j\rangle|0\rangle|0\rangle$, and recall our assumption that $\|H\|_1 \leq 1$.

1. Map the initial state $|\chi\rangle|0\rangle|0\rangle$ to the star subspace: $\overset{U_\psi}{\mapsto} \sum_j \beta_j \frac{|\phi_j^+\rangle + |\phi_j^-\rangle}{\sqrt{2}} |0\rangle$
2. Run phase estimation U_P to precision $\hat{\varepsilon}$: $\overset{U_P}{\mapsto} \sum_j \beta_j \frac{|\phi_j^+\rangle|\tilde{\theta}_j\rangle + |\phi_j^-\rangle|-\tilde{\theta}_j\rangle}{\sqrt{2}}$
3. Add phase $e^{i\cos(\theta)t}$ conditioned on phase register $|\theta\rangle$: $\mapsto \sum_j \beta_j e^{i\cos(\tilde{\theta}_j)t} \frac{|\phi_j^+\rangle|\tilde{\theta}_j\rangle + |\phi_j^-\rangle|-\tilde{\theta}_j\rangle}{\sqrt{2}}$
4. Uncompute the phase estimate: $\overset{U_P^\dagger}{\mapsto} \sum_j \beta_j e^{i\cos(\tilde{\theta}_j)t} \frac{|\phi_j^+\rangle + |\phi_j^-\rangle}{\sqrt{2}} |0\rangle$

[2] This scheme is a variation on the phase estimation algorithm for reflecting around the QW stationary state $|\pi\rangle$. There we implement the function $\mathrm{sgn}(x-1)$, with $\mathrm{sgn}(\cdot)$ the sign function.

5. Map back to the original state space: $\overset{U_\psi^\dagger}{\mapsto} \sum_j \beta_j e^{i\cos(\tilde{\theta}_j)t} |v_j\rangle |0\rangle |0\rangle$.

This algorithm has cost $\widetilde{O}(1/\hat{\varepsilon})$. The following exercise shows that if we set $\hat{\varepsilon} = \varepsilon/t$, then the resulting state is an ε-approximation of the target state.

Exercise 3. *Show that if $\hat{\varepsilon} \leq \varepsilon/t$, then $\left\| \sum_j \beta_j e^{i\cos(\tilde{\theta}_j)t} |v_j\rangle - e^{iHt} |\psi\rangle \right\|_2 \leq \varepsilon$. Hint:* [3]

3 Quantum linear system solving

As a different application, we can use this technique to construct a quantum state that describes the solution of a linear system, as in the famous quantum algorithm by Harrow, Hassidim and Lloyd [HHL09]. We consider an invertible, Hermitian matrix A and a vector b. We are interested in finding the solution x to the linear system

$$Ax = b,$$

given by $x = A^{-1}b$. This again corresponds to applying a function ($x \mapsto 1/x$) of a matrix (A) to a target state (b). We will use a similar approach as before to do this.

Exercise 4. *Assuming that A is Hermitian is without loss of generality. Show that for a general invertible A, we can always find a solution of the linear system $Ax = b$ by solving the alternative Hermitian linear system*

$$\begin{bmatrix} 0 & A \\ A^\dagger & 0 \end{bmatrix} y = \begin{bmatrix} b \\ 0 \end{bmatrix}.$$

We again assume that $\|A\|_1 \leq 1$ and moreover that A has eigenvalues λ_j such that $1/\kappa \leq |\lambda_j| < 1$ (so the *condition number* of A is less than κ). As in Section 1, we define star states and a QW operator W associated to A. As an initial state, we assume that we are given a quantum encoding of the vector b,

$$|b\rangle = \sum_i b(i) |i\rangle / \|b\|_2,$$

with decomposition $|b\rangle = \sum_j \beta_j |v_j\rangle$. We again map this state to the star subspace and apply phase estimation, yielding the state

$$\sum_j \beta_j \frac{|\phi_j^+\rangle |\tilde{\theta}_j\rangle + |\phi_j^-\rangle |-\tilde{\theta}_j\rangle}{\sqrt{2}}.$$

To obtain x, we would now like to implement the map $|\theta\rangle \mapsto \frac{1}{\cos(\theta)} |\theta\rangle$. However, unlike the map for Hamiltonian simulation ($|\theta\rangle \mapsto e^{i\cos(\theta)t} |\theta\rangle$), this is not a unitary operation. We resolve this by introducing an additional register and implementing the map R defined by

$$|\theta\rangle |0\rangle \overset{R}{\mapsto} |\theta\rangle \left(\frac{1}{\kappa\cos(\theta)} |0\rangle + \sqrt{1 - \frac{1}{\kappa^2\cos(\theta)^2}} |1\rangle \right).$$

Using the fact that $\lambda_j = \cos(\theta_j) \geq 1/\kappa$, we see that indeed this is a valid unitary transformation. This operation describes a *conditioned rotation* of the second qubit. Up to proportionality factor $1/\kappa$, the first component in the right hand side now describes the correct mapping. Based on this mapping, we propose the following algorithm, starting from the initial state $|b\rangle |0\rangle^{\otimes 3}$:

[3] Use the fact that $|\cos(\theta + \epsilon) - \cos(\theta)| \leq |\epsilon|$.

1. Map the initial state to the star subspace and run phase estimation to precision $\hat{\varepsilon}$:

$$|b\rangle\,|0\rangle^{\otimes 3} \overset{U_P U_\psi}{\mapsto} \sum_j \beta_j \frac{|\phi_j^+\rangle\,|\tilde{\theta}_j\rangle + |\phi_j^-\rangle\,|-\tilde{\theta}_j\rangle}{\sqrt{2}}\,|0\rangle$$

2. Apply rotation R, conditioned on phase register $|\theta\rangle$:

$$\overset{R}{\mapsto} \sum_j \beta_j \frac{|\phi_j^+\rangle\,|\tilde{\theta}_j\rangle + |\phi_j^-\rangle\,|-\tilde{\theta}_j\rangle}{\sqrt{2}} \left(\frac{1}{\kappa\cos(\tilde{\theta}_j)}\,|0\rangle + \sqrt{1-\frac{1}{\kappa^2\cos(\tilde{\theta}_j)^2}}\,|1\rangle\right)$$

3. Uncompute the phase estimate and map back to the original state space:

$$\overset{U_\psi^\dagger U_P^\dagger}{\mapsto} \sum_j \beta_j\,|v_j\rangle\,|0\rangle\,|0\rangle \left(\frac{1}{\kappa\cos(\tilde{\theta}_j)}\,|0\rangle + \sqrt{1-\frac{1}{\kappa^2\cos(\tilde{\theta}_j)^2}}\,|1\rangle\right) = |\psi\rangle\,.$$

This algorithm has cost $\widetilde{O}(1/\hat{\varepsilon})$. If we measure the three auxiliary registers of the outcome $|\psi\rangle$ and receive outcome "000", then the new state of the system is $\Pi_0\,|\psi\rangle\,/\|\Pi_0\,|\psi\rangle\,\|$, where $\Pi_0 = I\otimes|0\rangle\,\langle 0|^{\otimes 3}$. Similarly to the case of Hamiltonian simulation, one can prove that if $\hat{\varepsilon} \leq \varepsilon/\kappa$ then the outcome satisfies

$$\left\|\Pi_0\,|\psi\rangle\,/\|\Pi_0\,|\psi\rangle\,\| - |x\rangle\,|0\rangle^{\otimes 3}\right\|_2 \in O(\varepsilon),$$

where $|x\rangle = \sum_j x_j\,|j\rangle\,/\|x\|_2$ is the quantum state corresponding to the solution x.

In the final complexity we do have to take into account the probability of getting the correct outcome "000", which is $\|\Pi_0\,|\psi\rangle\,\|^2 \in \Omega(1/\kappa^2)$. So in order to get the correct outcome, we should repeat the algorithm some $\Omega(\kappa^2)$ times. Alternatively, we can use Grover search or amplitude amplification to boost the success probability with only $O(\kappa)$ repetitions. This yields a total complexity $\widetilde{O}(\kappa/\hat{\varepsilon}) \in \widetilde{O}(\kappa^2/\varepsilon)$. In the next lecture, we will see how a technique called "linear combination of unitaries" [CW12] allows us to exponentially improve the error dependency to $\log(1/\varepsilon)$. Using a different technique called "variable time amplitude amplification", Ambainis [Amb12] has also shown how to get a linear dependency on κ, which is optimal.

References

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