Quantum algorithms (CO 781, Winter 2008)
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LECTURE 14: Discrete-time quantum walk

So far, we have focused mainly on continuous-time quantum walk. We now turn our attention to discrete-time quantum walk, which provides a convenient framework for quantum search algorithms.

How to quantize a Markov chain Recall that a discrete-time classical random walk on an N-vertex graph can be represented by an $N \times N$ matrix P. The entry P_{jk} represents the probability of making a transition to j from k, so that an initial probability distribution $p \in \mathbb{R}^N$ becomes Pp after one step of the walk. To preserve normalization, we must have $\sum_{j=1}^N P_{jk} = 1$; we say that such a matrix is *stochastic*.

For any $N \times N$ stochastic matrix P (not necessarily symmetric), we can define a corresponding discrete-time quantum walk, a unitary operation on the Hilbert space $\mathbb{C}^N \otimes \mathbb{C}^N$. To define this walk, we introduce the states

$$|\psi_j\rangle := |j\rangle \otimes \sum_{k=1}^N \sqrt{P_{kj}}|k\rangle \tag{1}$$

$$= \sum_{k=1}^N \sqrt{P_{kj}}|j,k\rangle \tag{2}$$

for $j = 1, \ldots, N$. Each such state is normalized since P is stochastic. Now let

$$\Pi := \sum_{j=1}^N |\psi_j\rangle\langle\psi_j| \tag{3}$$

denote the projection onto $\operatorname{span}\{|\psi_j\rangle : j = 1, \ldots, N\}$, and let

$$S := \sum_{j,k=1}^N |j,k\rangle\langle k,j| \tag{4}$$

be the operator that swaps the two registers. Then a single step of the quantum walk is defined as the unitary operator $U := S(2\Pi - 1)$.

Notice that if $P_{jk} = A_{jk}/\deg(k)$ (i.e., if the walk simply chooses an outgoing edge of an underlying digraph uniformly at random), then this is exactly the coined quantum walk with the Grover diffusion operator as the coin flip.

If we take two steps of the walk, then the corresponding unitary operator is

$$[S(2\Pi - 1)][S(2\Pi - 1)] = [S(2\Pi - 1)S][2\Pi - 1] \tag{5}$$

$$= (2S\Pi S - 1)(2\Pi - 1), \tag{6}$$

which can be interpreted as the reflection about $\operatorname{span}\{|\psi_j\rangle\}$ followed by the reflection about $\operatorname{span}\{S|\psi_j\rangle\}$ (the states where we condition on the second register to do a coin operation on the first). To understand the behavior of the walk, we will now compute the spectrum of U; but note that it is also possible to compute the spectrum of a product of reflections more generally.

Spectrum of the quantum walk To understand the behavior of a discrete-time quantum walk, it will be helpful to compute its spectral decomposition. Let us show the following:

Theorem. *Fix an* $N \times N$ *stochastic matrix* P*, and let* $\{|\lambda\rangle\}$ *denote a complete set of orthonormal eigenvectors of the* $N \times N$ *matrix* D *with entries* $D_{jk} = \sqrt{P_{jk}P_{kj}}$ *with eigenvalues* $\{\lambda\}$*. Then the eigenvalues of the discrete-time quantum walk* $U = S(2\Pi - 1)$ *corresponding to* P *are* ± 1 *and* $\lambda \pm i\sqrt{1-\lambda^2} = e^{\pm i \arccos \lambda}$*.*

Proof. Define an isometry

$$T := \sum_{j=1}^{N} |\psi_j\rangle\langle j| \tag{7}$$

$$= \sum_{j,k=1}^{N} \sqrt{P_{kj}}|j,k\rangle\langle j| \tag{8}$$

mapping states in $\mathbb{C}^n$ to states in $\mathbb{C}^n \otimes \mathbb{C}^n$, and let $|\tilde{\lambda}\rangle := T|\lambda\rangle$. Notice that

$$TT^\dagger = \sum_{j,k=1}^{N} |\psi_j\rangle\langle j|k\rangle\langle\psi_k| \tag{9}$$

$$= \sum_{j=1}^{N} |\psi_j\rangle\langle\psi_j| \tag{10}$$

$$= \Pi, \tag{11}$$

whereas

$$T^\dagger T = \sum_{j,k=1}^{N} |j\rangle\langle\psi_j|\psi_k\rangle\langle k| \tag{12}$$

$$= \sum_{j,k,\ell,m=1}^{N} \sqrt{P_{\ell j}P_{mk}}|j\rangle\langle j,\ell|k,m\rangle\langle k| \tag{13}$$

$$= \sum_{j,\ell=1}^{N} P_{\ell j}|j\rangle\langle j| \tag{14}$$

$$= I \tag{15}$$

and

$$T^\dagger S T = \sum_{j,k=1}^{N} |j\rangle\langle\psi_j|S|\psi_k\rangle\langle k| \tag{16}$$

$$= \sum_{j,k,\ell,m=1}^{N} \sqrt{P_{\ell j}P_{mk}}|j\rangle\langle j,\ell|S|k,m\rangle\langle k| \tag{17}$$

$$= \sum_{j=1}^{N} \sqrt{P_{jk}P_{kj}}|j\rangle\langle k| \tag{18}$$

$$= D. \tag{19}$$

Applying the walk operator U to $|\tilde{\lambda}\rangle$ gives

$$U|\tilde{\lambda}\rangle = S(2\Pi - 1)|\tilde{\lambda}\rangle \tag{20}$$
$$= S(2TT^\dagger - 1)T|\lambda\rangle \tag{21}$$
$$= 2ST|\lambda\rangle - ST|\lambda\rangle \tag{22}$$
$$= S|\tilde{\lambda}\rangle, \tag{23}$$

and applying U to $S|\tilde{\lambda}\rangle$ gives

$$US|\tilde{\lambda}\rangle = S(2\Pi - 1)S|\tilde{\lambda}\rangle \tag{24}$$
$$= S(2TT^\dagger - 1)ST|\lambda\rangle \tag{25}$$
$$= (2STD - T)|\lambda\rangle \tag{26}$$
$$= 2\lambda S|\tilde{\lambda}\rangle - |\tilde{\lambda}\rangle. \tag{27}$$

We see that the subspace $\operatorname{span}\{|\tilde{\lambda}\rangle, S|\tilde{\lambda}\rangle\}$ is invariant under U, so we can find eigenvectors of U within this subspace.

Now let $|\mu\rangle := |\tilde{\lambda}\rangle - \mu S|\tilde{\lambda}\rangle$, and let us choose $\mu \in \mathbb{C}$ so that $|\mu\rangle$ is an eigenvector of U. We have

$$U|\mu\rangle = S|\tilde{\lambda}\rangle - \mu(2\lambda S|\tilde{\lambda}\rangle - |\tilde{\lambda}\rangle) \tag{28}$$
$$= \mu|\tilde{\lambda}\rangle + (1 - 2\lambda\mu)S|\tilde{\lambda}\rangle. \tag{29}$$

Thus μ will be an eigenvalue of U corresponding to the eigenvector $|\mu\rangle$ provided $(1-2\lambda\mu) = \mu(-\mu)$, i.e. $\mu^2 - 2\lambda\mu + 1 = 0$, so

$$\mu = \lambda \pm i\sqrt{1 - \lambda^2}. \tag{30}$$

Finally, note that for any vector in the orthogonal complement of $\operatorname{span}\{|\tilde{\lambda}\rangle\} = \operatorname{span}\{|\psi_j\rangle\}$ (these spaces are the same since $\sum_\lambda |\tilde{\lambda}\rangle\langle\tilde{\lambda}| = \sum_\lambda T|\lambda\rangle\langle\lambda|T^\dagger = TT^\dagger = \Pi$), U simply acts as $-S$, which has eigenvalues ± 1. □

Hitting times We can use random walks to formulate a generic search algorithm, and quantizing this algorithm gives a generic square root speedup. Consider a graph $G = (V, E)$, with some subset $M \subset V$ of the vertices designated as *marked*. We will compare classical and quantum walk algorithms for deciding whether any vertex in G is marked.

Classically, a straightforward approach to this problem is to take a random walk defined by some stochastic matrix P, stopping if we encounter a marked vertex. In other words, we modify the original walk P to give a walk P' defined as

$$P'_{jk} = \begin{cases} 1 & k \in M \text{ and } j = k \\ 0 & k \in M \text{ and } j \neq k \\ P_{jk} & k \notin M. \end{cases} \tag{31}$$

Let us assume from now on that the original walk P is symmetric, though the modified walk P' clearly is not provided M is non-empty. If we order the vertices so that the marked ones come last, the matrix P' has the block form

$$P' = \begin{pmatrix} P_M & 0 \\ Q & I \end{pmatrix} \tag{32}$$

where P_M is obtained by deleting the rows and columns of P corresponding to vertices in M.

Suppose we take t steps of the walk. A simple calculation shows

$$(P')^t = \begin{pmatrix} P_M^t & 0 \\ Q(I + P_M + \cdots + P_M^{t-1}) & I \end{pmatrix} \tag{33}$$

$$= \begin{pmatrix} P_M^t & 0 \\ Q\frac{P_M^t - I}{P_M - I} & I \end{pmatrix}. \tag{34}$$

Now if we start from the uniform distribution over unmarked items (if we start from a marked item we are done, so we might as well condition on this not happening), then the probability of not reaching a marked item after t steps is $\frac{1}{N-|M|}\sum_{j,k\notin M}[P_M^t]_{jk} \leq \|P_M^t\| = \|P_M\|^t$, where the inequality follows because the left hand side is the expectation of P_M in the normalized state $|V \setminus M\rangle = \frac{1}{\sqrt{N-|M|}}\sum_{j\notin M}|j\rangle$. Now if $\|P_M\| = 1-\Delta$, then the probability of reaching a marked item after t steps is at least $1 - \|P_M\|^t = 1-(1-\Delta)^t$, which is $\Omega(1)$ provided $t = O(1/\Delta) = O(\frac{1}{1-\|P_M\|})$.

It turns out that we can bound $\|P_M\|$ away from 1 knowing only the fraction of marked vertices and the spectrum of the original walk. Thus we can upper bound the *hitting time*, the time required to reach some marked vertex with constant probability.

Lemma. *If the second largest eigenvalue of P (in absolute value) is at most $1-\delta$ and $|M| \leq \epsilon N$, then $\|P_M\| \leq 1 - \delta\epsilon/2$.*

Proof. Let $|v\rangle \in \mathbb{R}^{N-|M|}$ be the principal eigenvector of P_M, and let $|w\rangle \in \mathbb{R}^N$ be the vector obtained by padding $|v\rangle$ with 0's for all the marked vertices.

We will decompose $|w\rangle$ in the eigenbasis of P. Since P is symmetric, it is actually doubly stochastic, and the uniform vector $|V\rangle = \frac{1}{\sqrt{N}}\sum_j |j\rangle$ corresponds to the eigenvalue 1. All other eigenvectors $|\lambda\rangle$ have eigenvalues at most $1-\delta$ by assumption. Now

$$\|P_M\|^2 = \|P|w\rangle\|^2 \tag{35}$$

$$= |\langle V|w\rangle|^2 + \sum_{\lambda\neq 1} \lambda^2 |\langle\lambda|w\rangle|^2 \tag{36}$$

$$\leq |\langle V|w\rangle|^2 + (1-\delta)^2 \sum_{\lambda\neq 1} |\langle\lambda|w\rangle|^2 \tag{37}$$

$$\leq |\langle V|w\rangle|^2 + (1-\delta) \sum_{\lambda\neq 1} |\langle\lambda|w\rangle|^2 \tag{38}$$

$$= 1 - \delta \sum_{\lambda\neq 1} |\langle\lambda|w\rangle|^2 \tag{39}$$

$$= 1 - \delta(1 - |\langle V|w\rangle|^2). \tag{40}$$

But by the Cauchy-Schwarz inequality,

$$|\langle V|w\rangle|^2 = |\langle V|\Pi_{V\setminus M}|w\rangle|^2 \tag{41}$$

$$\leq \|\Pi_{V\setminus M}|V\rangle\|^2 \cdot \||w\rangle\|^2 \tag{42}$$

$$= \frac{N-|M|}{N} \tag{43}$$

$$= 1-\epsilon \tag{44}$$

where $\Pi_{V\setminus M} = \sum_{j\notin M}|j\rangle\langle j|$. Thus $\|P_M\| \leq \sqrt{1-\delta\epsilon} \leq 1-\delta\epsilon/2$ as claimed. $\square$

Thus we see that the classical hitting time is $O(1/\delta\epsilon)$.

Now we turn to the quantum case. Our strategy will be to perform phase estimation with sufficiently high precision on the operator U, the quantum walk corresponding to P', with the state

$$|\psi\rangle := \frac{1}{\sqrt{N}} \sum_{j \notin M} |\psi_j\rangle. \tag{45}$$

This state can easily be prepared by starting from the state

$$\frac{1}{\sqrt{N}} \sum_{j} |\psi_j\rangle \tag{46}$$

and measuring whether the first register corresponds to a marked vertex; if it does then we are done, and if not then we have prepared $|\psi\rangle$.

The matrix D for the walk P' is

$$\begin{pmatrix} P_M & 0 \\ 0 & I \end{pmatrix}, \tag{47}$$

so according to the spectral theorem, the eigenvalues of the resulting walk operator U are ± 1 and $e^{\pm i \arccos \lambda}$, where λ runs over the eigenvalues of P_M. If the marked set M is empty, then $P' = P$, and $|\psi\rangle$ is an eigenvector of U with eigenvalue 1, so phase estimation on U is guaranteed to return a phase of 0. But if M is non-empty, then the state $|\psi\rangle$ lives entirely within the subspace with eigenvalues $e^{\pm i \arccos \lambda}$. Thus if we perform phase estimation on U with precision $O(\min_\lambda \arccos \lambda)$, we will see a phase different from 0. Since $\arccos \lambda \geq \sqrt{1-\lambda}$, we see that precision $O(\sqrt{1 - \|P_M\|})$ suffices. So the quantum algorithm can decide whether there is a marked vertex in time $O(1/\sqrt{1 - \|P_M\|}) = O(1/\sqrt{\delta\epsilon})$.