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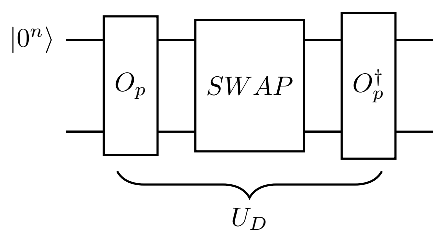
Lecture 11

Discrete-time Quantum Walk

- Qubitization
- Hitting time

1 Recap

Last lecture, we introduced quantum walks: Op $|0^n\rangle\,|j\rangle = \sum_k \sqrt{P_{jk}}|k\rangle|j\rangle$. We consider



UD: 1 step quantum walk.

Proposition 1.1. $\forall i, j \in [N]$, $\langle 0^n\,|\langle i\,|U_D|\,0^n\rangle|\,j\rangle = D_{ij}$. *Intuitively,* $U_D = \begin{pmatrix} D & \cdot \\ \cdot & \cdot \end{pmatrix} = |0^n\rangle\langle 0^n| \otimes D + \cdots$. *Such a form is called a block encoding of* D. .

2 Qubitization

Next: What can we obtain by using the block encoding?

Denote the eigendecomposition of D as $D = \sum_i \lambda_i\,|v_i\rangle\langle v_i|$. For each $|v_i\rangle$,

$$U_D\,|0^n\rangle\,|v_i\rangle = |0^n\rangle\,D\,|v_i\rangle + \left|\tilde{\perp}_i\right\rangle = \lambda_i\,|0^n\rangle\,|v_i\rangle + \left|\tilde{\perp}_i\right\rangle \qquad (*)$$

Here $\left|\tilde{\perp}_i\right\rangle$ is an unnormalized state satisfying $\Pi\left|\tilde{\perp}_i\right\rangle = 0$, where

$$\Pi = |0^n\rangle\langle 0^n| \otimes I$$

(*) should give a normalized state, so we may write $\left|\tilde{\perp}_i\right\rangle = \sqrt{1-\lambda_i^2}\,|\perp_i\rangle$, where $|\perp_i\rangle$ is a normalized state.

Suppose $\lambda_i \neq \pm 1$. First, notice that $U_D^\dagger = U_D$ $\qquad (ABC)^\dagger = C^\dagger (AB)^\dagger = C^\dagger B^\dagger A^\dagger$

$$U_D^\dagger = \left(\mathrm{Op}\,\mathrm{SWAP}\,\mathrm{Op}^\dagger\right)^\dagger = \left(\mathrm{Op}^\dagger\right)^\dagger \mathrm{SWAP}^\dagger\,\mathrm{Op}^\dagger = \mathrm{Op}\,\mathrm{SWAP}\,\mathrm{Op}^\dagger = U_D$$

Apply U_D to both sides of $(*)$, we have $\left(U_D^2 = U_D^\dagger U_D = I\right)$

$$\begin{aligned}
|0^n\rangle |v_i\rangle &= \lambda_i U_D |0^n\rangle |v_i\rangle + \sqrt{1-\lambda_i^2} U_D |\perp_i\rangle \\
&= \lambda_i \left(\lambda_i |0^n\rangle |v_i\rangle + \sqrt{1-\lambda_i^2} |\perp_i\rangle\right) + \sqrt{1-\lambda_i^2} U_D |\perp_i\rangle .\\
\Rightarrow \left(1-\lambda_i^2\right) |0^n\rangle |v_i\rangle &= \sqrt{1-\lambda_i^2}\lambda_i |\perp_i\rangle + \sqrt{1-\lambda_i^2} U_D |\perp_i\rangle \\
\Rightarrow \quad U_D |\perp_i\rangle &= \sqrt{1-\lambda_i^2} |0^n\rangle |v_i\rangle - \lambda_i |\perp_i\rangle . \qquad (**)
\end{aligned}$$

Conclusion: Denoting $\beta_i = \{|0^n\rangle |v_i\rangle, |\perp_i\rangle\}$, $\mathcal{H}_i = \mathrm{span}\{\beta_i\}$ is an invariant subspace of U_D.

When $\lambda_i = \pm 1$, $\mathrm{span}\{|0^n\rangle |v_i\rangle\}$ is already an invariant subspace.

The matrix representation of U_D w.r.t. β_i is

$$[U_D]_{\beta_i} = \begin{array}{cc} \begin{pmatrix} \lambda_i & \sqrt{1-\lambda_i^2} \\ \sqrt{1-\lambda_i^2} & -\lambda_i \end{pmatrix} & \begin{array}{c} |0^n\rangle |v_i\rangle \\ |\perp_i\rangle \end{array} \\ \begin{array}{cc} |0^n\rangle |v_i\rangle & \quad |\perp_i\rangle \end{array} & \end{array}$$

In literature, this phenomenon is known as qubitization - each eigenvector $|v_i\rangle$ is "qubitized" into two -dimensional space $\mathcal{H}_i$.

This also looks like Grover. But we need to make a rotation here.
Note that $\mathcal{H}_i$ is also an invariant subspace for Π :

$$[\pi]_{\beta_i} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

Define $Z_\pi = 2\pi - I$, then $[Z_\pi]_{\beta_i} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

Z_π acts as a reflection operator restricted to each subspace $\mathcal{H}_i$.

Now: $\mathcal{H}_i$ is an invariant subspace for the iterate $O_D = U_D Z_\pi$, where

$$[O_D]_{\beta_i} = \begin{pmatrix} \lambda_i & \sqrt{1-\lambda_i^2} \\ \sqrt{1-\lambda_i^2} & -\lambda_i \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} \lambda_i & -\sqrt{1-\lambda_i^2} \\ \sqrt{1-\lambda_i^2} & \lambda_i \end{pmatrix} \qquad \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$$

This is a desired rotation matrix! Applying it k times,

$$[0_D^k]_{\beta_i} = \left[(U_D Z_\pi)^k\right]_{\beta_i} = \begin{pmatrix} T_k(\lambda_i) & -\sqrt{1-\lambda_i^2} U_{k-1}(\lambda_i) \\ \sqrt{1-\lambda_i^2} U_{k-1}(\lambda_i) & T_k(\lambda_i) \end{pmatrix}.$$

Here T_k and U_k are Chebyshev polynomials of first and second kinds, respectively.

$$T_k(\cos\theta) = \cos k\theta \qquad U_{k-1}(\cos\theta) = \sin k\theta / \sin\theta$$

$$T_1(x) = x, \quad T_2(x) = 2x^2 - 1, \quad T_3(x) = 4x^3 - 3x, \ldots$$

$$U_1(x) = 2x, \quad U_2(x) = 4x^2 - 1, \quad U_3(x) = 8x^3 - 4x, \ldots$$

Since $\{|0^n\rangle |v_i\rangle\}_{i=1}^N$ spans the range of $\prod(\{|v_i\rangle\}$ is a complete, orthonormal basis), we have: $O_D^k = \begin{pmatrix} T_k(A) & * \\ * & * \end{pmatrix}$. $A = \sum_i \lambda_i |v_i\rangle \langle U_i|$, $T_k(A) = \sum_i T_k(\lambda_i) |v_i\rangle \langle v_i|$. i.e., $O_D^k = (U_D Z_\pi)^k$ is a block encoding of the Chebyshev polynomial $T_k(A)$:

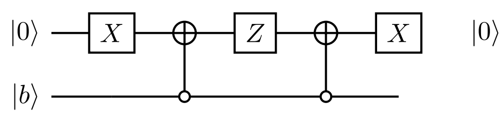
$$\langle 0^n| \langle i| O_D^k \mid 0^n\rangle|j\rangle = (T_k(A))_{ij}.$$

Now to implement O_D^k ? We know U_D; need to implement Z_π.

When $n = 1$ $\quad Z_\pi = Z$ (This reduces to amplitude amplification.)

For general $n, Z_\pi = 2\pi - I = 2|0^n\rangle \langle 0^n| - I$ $\qquad z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

Consider the following circuit with an ancilla qubit:

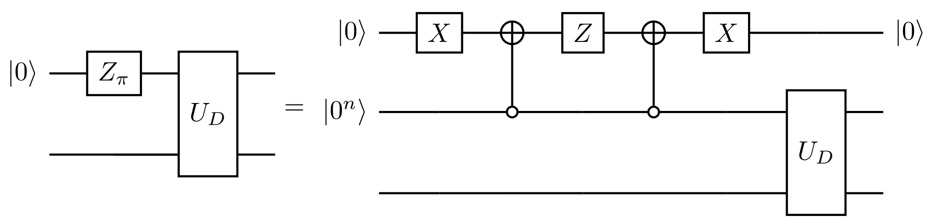


If $b = 0^n$: $\quad |0\rangle|b\rangle \xmapsto{X} |1\rangle|b\rangle \xmapsto{\text{CNOT}} |0\rangle|b\rangle \xmapsto{Z} |0\rangle|b\rangle \xmapsto{\text{CNOT}} |1\rangle|b\rangle \xmapsto{X} |0\rangle|b\rangle$

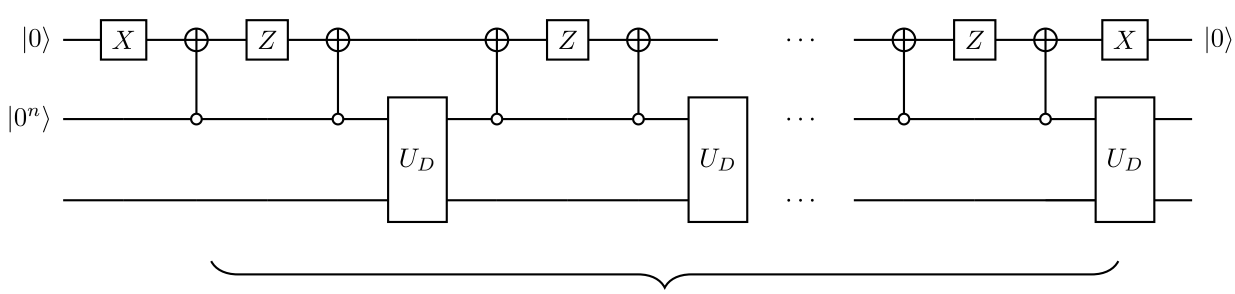
If $b \neq 0^n$: $\quad |0\rangle|b\rangle \xmapsto{X} |1\rangle|b\rangle \xmapsto{\text{CNOT}} |1\rangle|b\rangle \xmapsto{Z} -|1\rangle|b\rangle \xmapsto{\text{CNOT}} -|1\rangle|b\rangle \xmapsto{X} -|0\rangle|b\rangle$

In other words, it returns $|0\rangle|b\rangle$ if $b = 0^n$, and $-|0\rangle|b\rangle$ if $b \neq 0^n$. This is exactly Z_π. In all:

$O_D =$



$(O_D)^k$: $X^2 = I$.



repeat k times

3 Hitting time

In the above, we have shown that $\mathcal{H}_i = \text{span}\{|0^n\rangle|v_i\rangle, |\perp_i\rangle\}$ is an invariant subspace for the iterate $O_D = U_D Z_\pi$, where $[O_D]_{\beta_i} = \begin{pmatrix} \lambda_i & -\sqrt{1-\lambda_i^2} \\ \sqrt{1-\lambda_i^2} & \lambda_i \end{pmatrix}$.

Proposition 3.1. *The eigenvalues of* $[\mathrm{O}_D]_{\beta_i}$ *in the* 2×2 *matrix block are* $e^{\pm i \arccos(\lambda_i)}$.

Proof. Denote $\lambda_i = \cos\theta_i$. Then we need to find the eigenvalue of

$$[O_D]_{\beta_i} = \begin{pmatrix} \cos\theta_i & -\sin\theta_i \\ \sin\theta_i & \cos\theta_i \end{pmatrix} \qquad f(x) = \begin{vmatrix} x-\cos\theta_i & -\sin\theta_i \\ \sin\theta_i & x-\cos\theta_i \end{vmatrix}$$

Its characteristic function is $f(x) = (x-\cos\theta_i)^2 + \sin^2\theta_i = x^2 - 2\cos\theta_i x + 1$

$$x = \frac{2\cos\theta_i \pm \sqrt{4\cos^2\theta_i - 4}}{2} = \cos\theta_i \pm i\sin\theta_i = e^{\pm i\theta_i} = e^{\pm i \arccos(\lambda_i)}$$

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We have proved that if a random walk is ergodic and reversible, then eigenvalues of D and P are the same.

- The largest eigenvalue of D is unique is equal to 1 (with eigenvector π).
- The second largest eigenvalue of D is $1-\delta$, where $\delta > 0$ is called the spectral gap.

Since $\arccos 1 = 0$ and $\arccos(1-\delta) \approx \sqrt{2\delta}$, the spectral gap of O_D on the unit circle is in fact $O(\sqrt{\delta})$ instead of δ.

This is known as spectral gap amplification.

Ex. (Determining marked vertices in the complete graph)

Let $G = (V, E)$ be a complete graph of $N = 2^n$ vertices. We want to distinguish the following two scenarios:

(1) All vertices are the same, and the random walk is given by the transition matrix:

$$P = \frac{1}{N} e_N e_N^\top \quad e_N = (1, 1, \cdots, 1)^\top.$$

(2) There are M marked item (vertices). WLOG, we may assume that they are the 1st, 2nd,... M-th vertices for better notations (of course we do not have access to this information). In this case, the transition matrix is

$$\widetilde{P} = \begin{cases} \delta_{ij} & i \in [M] \\ P_{ij} & i \in \{M+1, \cdots, N\} \end{cases}$$