Lecture 3: Hamiltonian simulation & HHL

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last lecture:

RW P $\longrightarrow$ $\begin{cases} \text{star states } |\psi_x\rangle \\ \text{QW operator } W \\ \text{Szegedy's lemma:} \\ \quad \text{spectrum } \sigma(W) \Leftrightarrow \sigma(P) \end{cases}$

this lecture:

general Hermitian matrix H

$\downarrow$

$\langle y|\perp\rangle = 0, \forall y$

* star states: assume $\|H\|_1 \leq 1$!

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

* QW operator:

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$$W = S \cdot \left(2 \sum |\psi_x\rangle\langle\psi_x| - \mathbb{1}\right)$$

$$= S \cdot U_\psi \left(2\Pi_0 - \mathbb{1}\right) U_\psi^\dagger$$

$S|x,y\rangle = |y,x\rangle$, $S|x,\perp\rangle = |x,\perp\rangle$

<u>Exercise</u>: Verify that $\langle\psi_y|S|\psi_x\rangle = H_{x,y}$.

* <u>Szegedy's lemma</u>:

$\forall$ eigenpair $\left(\lambda_j = \cos(\theta_j) \neq \pm 1 \,,\, |v_j\rangle\right)$,

the QW operator has eigenpairs

$$\left(e^{\pm i\theta_j} \,,\, |\phi_j^\pm\rangle\right)$$

such that

$$\ldots = |\phi_j^+\rangle + |\phi_j^-\rangle$$

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

Hence, consider $|x\rangle = \sum \beta_j |v_j\rangle$:

$$W^t U_\psi |x\rangle|0\rangle$$

$$= \sum \beta_j \frac{e^{i\theta_j t}|\phi_j^+\rangle + e^{-i\theta_j t}|\phi_j^-\rangle}{\sqrt{2}}$$

$$= \sum \beta_j \left[\cos(\theta_j t)\frac{|\phi_j^+\rangle + |\phi_j^-\rangle}{\sqrt{2}} + i\sin(\theta_j t)\frac{|\phi_j^+\rangle - |\phi_j^-\rangle}{\sqrt{2}}\right]$$

such that

$$U_\psi^\dagger W^t U_\psi |x\rangle|0\rangle$$

$$= \sum \beta_j \Big[\cos(\theta_j t)|v_j\rangle|0\rangle$$

$$+ \; |\phi_j^+\rangle - |\phi_j^-\rangle \Big]$$

$$= \sum \beta_j \Big[\cos(\theta_j t) |v_j\rangle|0\rangle$$

$$+ i \sin(\theta_j t) \underbrace{U_\psi^\dagger \frac{|\phi_j^+\rangle - |\phi_j^-\rangle}{\sqrt{2}}}_{! \perp \operatorname{span}\{|x\rangle|0\rangle\}} \Big]$$

and $\Pi_0 U_\psi^\dagger W^t U_\psi |x\rangle|0\rangle$

$$= \sum \beta_j \cos(\theta_j t) |v_j\rangle|0\rangle$$

$$= \sum \beta_j \underbrace{T_t(\cos(\theta_j))}_{t\text{-th Cheb. pol. of } 1^{st} \text{ kind}} |v_j\rangle|0\rangle$$

$$= \left(\sum \beta_j T_t(\lambda_j) |v_j\rangle\right)|0\rangle$$

$$= T_t(H)|x\rangle|0\rangle.$$

↳ QW applies "function" of H on $|x\rangle$:

1. apply $U_\psi^\dagger W^t U_\psi$

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2. measure 2^{nd} register
$\rightarrow$ if outcome "0" (prob. $\| T_t(H)|x\rangle\|_2^2$),
then state $\dfrac{T_t(H)|x\rangle}{\|T_t(H)|x\rangle\|_2}$.

HAMILTONIAN SIMULATION.

"quantum system" described by ==Hamiltonian H==:

initial state $|\psi(0)\rangle$,

Schrödinger's equation

$$\boxed{i \frac{\partial}{\partial t}|x(t)\rangle = H|x(t)\rangle}$$

$$\boxed{i \frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle}$$

→ <u>solution:</u> $|\psi(t)\rangle = e^{-iHt}|\psi(t)\rangle$,

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

= unitary operator!

"other" fct. of H

"Hamiltonian simulation":

given "access" to H, implement e^{iHt}.

→ nontrivial, relevant & actual problem!

<u>ALGORITHM:</u> using QWs + phase estimation

! similar to QW reflection,

! similar to [illegible]

$$\text{function } f(x) = \operatorname{sgn}(x-1): \quad f(H) = \sum f(\lambda_j) |v_j\rangle\langle v_j|$$
$$= -|\pi\rangle\langle\pi| + (\mathbb{1} - |\pi\rangle\langle\pi|)$$

1. map to star subspace:

$$|\psi\rangle|0\rangle|0\rangle \xmapsto{U_\psi} \sum_j \beta_j \frac{|\phi_j^+\rangle + |\phi_j^-\rangle}{\sqrt{2}} |0\rangle$$

2. run phase estimation (precision $\hat{\varepsilon}$):

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

3. add phase $e^{i\cos(\theta)t}$ conditioned on phase reg. $|\theta\rangle$:

$$\xmapsto{R} \sum_j \beta_j e^{i\cos(\tilde{\theta}_j)t} \frac{|\phi_j^+\rangle|\tilde{\theta}_j\rangle + |\phi_j^-\rangle|-\tilde{\theta}_j\rangle}{\sqrt{2}}$$

4. uncompute phase estimate:

$$\xrightarrow{U_E^\dagger} \sum_j \beta_j e^{i\cos(\tilde{\theta}_j)t} \frac{|\phi_j^+\rangle + |\phi_j^-\rangle}{\sqrt{2}} |0\rangle$$

5. map back to original state space:

$$\xrightarrow{U_\psi^\dagger} \sum_j \beta_j e^{i\cos(\tilde{\theta}_j)t} |v_j\rangle |0\rangle |0\rangle.$$

TOTAL COST $= \tilde{O}(1/\hat{\varepsilon})$ $\in \tilde{O}(t/\varepsilon)$

CORRECTNESS:

Show that if $\hat{\varepsilon} \leq \varepsilon/t$, then

$$\left\| \sum \beta_j e^{i\cos(\tilde{\theta}_j)t} |v_j\rangle - e^{iHt} |\psi\rangle \right\|_2 \leq \varepsilon.$$

$$\hookrightarrow \; '' = \sum |\beta_j|^2 \cdot \underbrace{\left| e^{i\cos(\tilde{\theta}_j)t} - e^{i\cos(\theta_j)t} \right|}$$

$$= \left| 1 - e^{i(\cos(\theta_j) - \cos(\tilde{\theta}_j))t} \right|$$

if $\hat{\varepsilon} t \ll 1$

$$\leq \left| 1 - e^{i(\cos(\theta_j + \hat{\varepsilon}) - \cos(\theta_j))t} \right|$$

$$\leq \left| 1 - e^{i\hat{\varepsilon}t} \right|$$

$$= \left| 1 - 1 + i\hat{\varepsilon}t + O(\hat{\varepsilon}^2 t^2) \right|$$

$$\in O(\hat{\varepsilon}t) \in O(\varepsilon).$$