

Lecture 4: Linear combination of unitaries (solutions)

*Lecturer: Simon Apers***Exercise 1 (1 point)**

- Verify that the Chebyshev polynomials form an orthogonal set w.r.t. the inner product

$$\langle f, g \rangle = \int_{-1}^{+1} f(x)g(x) \frac{dx}{\sqrt{1-x^2}}.$$

Hint: use that $T_t(\cos(\theta)) = \cos(t\theta)$.

Using the change of variables $x = \cos(\theta)$, we can rewrite

$$\langle f, g \rangle = \int_0^\pi f(\cos(\theta))g(\cos(\theta)) d\theta.$$

For $f(x) = T_k(x)$ and $g(x) = T_\ell(x)$, this is

$$\langle T_k, T_\ell \rangle = \int_0^\pi \cos(k\theta) \cos(\ell\theta) d\theta.$$

This equals zero when $k \neq \ell$.

- Moreover, they form a basis: any degree- d polynomial can be described as a linear combination of the first $d+1$ Chebyshev polynomials. Prove this by finding the coefficients of the expansion

$$x^\tau = \sum_{t=0}^{\tau} \alpha_t T_t(x). \quad (1)$$

Hint: use the fact that $\cos(\theta) = (e^{i\theta} + e^{-i\theta})/2$.

Again using the change of variables $x = \cos(\theta)$, we wish to find an expansion

$$\cos(\theta)^\tau = \sum_{t=0}^{\tau} \alpha_t \cos(t\theta).$$

By rewriting $\cos(\theta) = (e^{i\theta} + e^{-i\theta})/2$ and using binomial expansion, the left hand side is

$$\cos(\theta)^\tau = \frac{1}{2^\tau} \sum_{k=0}^{\tau} \binom{\tau}{k} e^{i(\tau-2k)\theta}.$$

Combining terms to form cosines, this gives the expansion $\cos(\theta)^\tau = \sum_{t=0}^{\tau} \alpha_t T_t(\cos(\theta))$ with

$$\alpha_t = \begin{cases} \frac{1}{2^\tau} \binom{\tau}{\tau/2} & \text{if } t = 0, \tau \text{ even} \\ \frac{1}{2^{\tau-1}} \binom{\tau}{(\tau-t)/2} & \text{if } t > 0 \text{ and } \tau = t \bmod 2. \end{cases}$$

Exercise 2 (1 point)

- Analyze what the (projected) output of the LCU algorithm corresponds to, given by

$$(I \otimes \Pi_0)(I \otimes U_{\text{cl}}^\dagger) cW (I \otimes U_{\text{cl}}) |\phi\rangle |0\rangle.$$

First note that

$$cW (I \otimes U_{\text{cl}}) |\phi\rangle |0\rangle = cW \sum_t \sqrt{\alpha_t} |\phi\rangle |t\rangle = \sum_t \sqrt{\alpha_t} W^t |\phi\rangle |t\rangle.$$

Then, use that

$$(I \otimes \Pi_0)(I \otimes U_{\text{cl}}^\dagger) = I \otimes (|0\rangle\langle 0| U_{\text{cl}}^\dagger) = I \otimes \left(\sum_t \sqrt{\alpha_t} |0\rangle\langle t| \right).$$

Combining these expressions we find that

$$(I \otimes \Pi_0)(I \otimes U_{\text{cl}}^\dagger) cW (I \otimes U_{\text{cl}}) |\phi\rangle |0\rangle = \left(\sum_t \alpha_t W^t |\phi\rangle \right) |0\rangle.$$

So, if we look at the projection into the Π_0 subspace, then we see that the algorithm effectively implements a linear combination of the unitaries I, W, W^2, \dots

- Analyze what the following state corresponds to:

$$(I \otimes \Pi_0 \otimes \Pi_0)(I \otimes U_{\text{cl}}^\dagger)(U_\psi^\dagger \otimes I) cW (U_\psi \otimes I)(I \otimes U_{\text{cl}}) |\chi\rangle |0\rangle |0\rangle.$$

We first simplify

$$\begin{aligned} (U_\psi^\dagger \otimes I) cW (U_\psi \otimes I)(I \otimes U_{\text{cl}}) |\chi\rangle |0\rangle |0\rangle &= (U_\psi^\dagger \otimes I) cW (U_\psi \otimes I) \sum_t \sqrt{\alpha_t} |\chi\rangle |0\rangle |t\rangle \\ &= \sum_t \sqrt{\alpha_t} (U_\psi^\dagger W^t U_\psi) |\chi\rangle |0\rangle |t\rangle. \end{aligned}$$

Now rewrite $I \otimes \Pi_0 \otimes \Pi_0 = (I \otimes \Pi_0 \otimes I)(I \otimes I \otimes \Pi_0)$. Using the previous exercise we can rewrite the full expression as

$$\begin{aligned} (I \otimes \Pi_0 \otimes I)(I \otimes I \otimes \Pi_0)(I \otimes U_{\text{cl}}^\dagger) \sum_t \sqrt{\alpha_t} (U_\psi^\dagger W^t U_\psi |\chi\rangle |0\rangle) |t\rangle \\ = (I \otimes \Pi_0 \otimes I) \sum_t \alpha_t (U_\psi^\dagger W^t U_\psi |\chi\rangle |0\rangle) |0\rangle \\ = \sum_t \alpha_t ((I \otimes \Pi_0) U_\psi^\dagger W^t U_\psi |\chi\rangle |0\rangle) |0\rangle \\ = \left(\sum_t \alpha_t T_t(H) |\chi\rangle \right) |0\rangle |0\rangle. \end{aligned}$$

Hence, by combining LCU with quantum walks, we can implement linear combinations of Chebyshev polynomials $T_t(H)$ to a quantum state.

Exercise 3 (2 points)

- Let W be the QW operator associated to H . Explicitly describe the LCU algorithm based on W for constructing the state $H^\tau |\psi\rangle / \|H^\tau |\psi\rangle\|_2$. What is the cost of this algorithm?

We can use the expansion $x^\tau = \sum_{t=0}^{\tau} \alpha_t T_t(x)$ from Exercise 1. Then the algorithm is described as follows:

1. Create controlled QW operator cW and unitary U_ψ based on H . Create unitary U_{cl} such that $U_{cl} |0\rangle = \sum_t \sqrt{\alpha_t} |t\rangle$.

2. Apply operators

$$(I \otimes U_{cl}^\dagger)(U_\psi^\dagger \otimes I) cW (U_\psi \otimes I)(I \otimes U_{cl})$$

to the initial state $|\chi\rangle |0\rangle |0\rangle$.

3. Measure the last 2 registers. If outcome “00”, then return the resulting state. If not, go back to step 2.

The cost of this algorithm is determined by (i) the cost of the main routine in step 2., and (ii) the number of times we have to repeat step 2. The cost of step 2. is dominated by applying the controlled QW operator cW , whose cost corresponds to applying τ steps of the QW. The expected number of repetitions is inversely proportional to the success probability in step 3., which is

$$\begin{aligned} & \left\| (I \otimes \Pi_0 \otimes \Pi_0)(I \otimes U_{cl}^\dagger)(U_\psi^\dagger \otimes I) cW (U_\psi \otimes I)(I \otimes U_{cl}) |\chi\rangle |0\rangle |0\rangle \right\|_2^2 \\ &= \left\| \sum_t \alpha_t T_t(H) |\chi\rangle \right\|_2^2 = \|H^\tau |\chi\rangle\|_2^2. \end{aligned}$$

Hence, the total cost corresponds to $O(\tau / \|H^\tau |\chi\rangle\|_2^2)$ steps of the quantum walk. Using amplitude amplification we could boost the success probability in step 3., so that the total cost becomes $O(\tau / \|H^\tau |\chi\rangle\|_2)$ QW steps.

- Consider independent and uniformly distributed random variables $X_1, \dots, X_\tau \in \{+1, -1\}$, and let $Y_\tau = \sum_{k=1}^{\tau} X_k$. Prove that the coefficients in Eq. (1) satisfy $\alpha_t = \Pr(|Y_\tau| = t)$.

If $t = 0$ and τ is even, then indeed $\Pr(|Y_\tau| = t) = \frac{1}{2^\tau} \binom{\tau}{\tau/2} = \alpha_0$, since this is simply the probability that exactly half of the X_i 's are +1. For $t > 0$, we use that $\Pr(|Y_\tau| = t) = \Pr(Y_\tau = t) + \Pr(Y_\tau = -t) = 2 \Pr(Y_\tau = t)$ by symmetry. Now notice that $\Pr(Y_\tau = t)$ is only nonzero when τ and t have the same parity ($\tau = t \bmod 2$). Moreover, $Y_\tau = t$ only if exactly $\tau - 2t$ of the X_i 's equals one, which has probability

$$\Pr(Y_\tau = t) = \frac{1}{2^\tau} \binom{\tau}{(\tau-t)/2},$$

and so $\Pr(|Y_\tau| = t) = \binom{\tau}{(\tau-t)/2} / 2^{\tau-1} = \alpha_t$.

- By Hoeffding's theorem we know that $\Pr(|Y_\tau| > r) \leq 2 \exp(-r^2/(2\tau))$ for any $r \geq 0$. Use this to prove that there exists $d \in O(\sqrt{\tau \log(1/\varepsilon)})$ such that the degree- d polynomial

$$h(x) = \sum_{t=0}^d \alpha_t T_t(x)$$

satisfies $|h(x) - x^\tau| \leq \varepsilon$ for all $x \in [-1, 1]$.

Using that $|T_t(x)| \leq 1$ and $\alpha_t \geq 0$, we can bound

$$|h(x) - x^\tau| = \left| \sum_{t=d+1}^{\tau} \alpha_t T_t(x) \right| \leq \left| \sum_{t=d+1}^{\tau} \alpha_t \right| = \sum_{t=d+1}^{\tau} \alpha_t.$$

By the former exercise, we know that $\alpha_t = \Pr(|Y_\tau| = t)$, and hence $\sum_{t=d+1}^{\tau} \alpha_t = \Pr(|Y_\tau| > d)$. By Hoeffding's theorem, this is upper bounded by ε if $d \geq \sqrt{2\tau \log(2/\varepsilon)}$.

- What is the cost of the LCU algorithm based on the polynomial h for implementing the function H^τ with error ε ?

The cost of step 2. improves from τ to $O(\sqrt{\tau \log(1/\varepsilon)})$. The total cost is hence

$$O(\sqrt{\tau \log(1/\varepsilon)} / \|H^\tau |\chi\rangle\|_2^2).$$

Exercise 4 (1 point)

- Find an expansion $e^{ix\tau} = \sum_{t \geq 0} \alpha_t T_t(x)$ using the Jacobi-Anger expansion

$$e^{i \cos(\theta)\tau} = J_0(\tau) + 2 \sum_{k=1}^{+\infty} i^k J_k(\tau) \cos(k\theta).$$

Here the function $J_k(y)$ corresponds to the k -th Bessel function of the first kind.

Simply replace $\cos(\theta)$ by x to get

$$e^{ix\tau} = J_0(\tau) + 2 \sum_{k=1}^{+\infty} i^k J_k(\tau) T_k(x),$$

and so $\alpha_0 = J_0(\tau)$ and $\alpha_t = 2i^t J_t(\tau)$ for $t > 0$.

- Use that $|J_k(\tau)| \leq \frac{1}{k!2^k}$ for $\tau \leq 1$ to show that $\sum_t |\alpha_t| \in \Theta(1)$.

We use that $|\alpha_t| \leq 2|J_t(\tau)|$ for all $t \geq 0$ to bound

$$\sum_t |\alpha_t| \leq 2 \sum_t |J_t(\tau)| \leq 2 \sum_t \frac{1}{t!2^t} = 2e^{1/2} \in O(1),$$

where we used the identity $e^y = \sum_t \frac{y^t}{t!}$. To prove that $\sum_t |\alpha_t| \in \Omega(1)$, note that for any $x \in [-1, 1]$ we have that

$$\sum_t |\alpha_t| \geq \sum_t |\alpha_t T_t(x)| \geq \left| \sum_t \alpha_t T_t(x) \right| = |e^{ix\tau}| = 1.$$

- Show that there exists $d \in O(\log(1/\varepsilon))$ such that $h(x) = \sum_{t=0}^d \alpha_t T_t(x)$ satisfies $|h(x) - e^{ix}| \leq \varepsilon$ for $|x| < 1$.¹

¹While harder to prove, you could even choose $d \in O(\log(1/\varepsilon)/\log \log(1/\varepsilon))$.

Here we can use a very rough (but near-optimal) bound:

$$|e^{ix\tau} - h(x)| = \left| \sum_{t=d+1}^{\infty} \alpha_t T_t(x) \right| \leq 2 \sum_{t=d+1}^{\infty} |J_t(\tau)| \leq 2 \sum_{t=d+1}^{\infty} \frac{1}{t!2^t} \leq 2 \sum_{t=d+1}^{\infty} \frac{1}{2^t} = \frac{1}{2^{d-1}}.$$

The right hand side is at most ε if $d \in \Omega(\log(1/\varepsilon))$.

- What is the cost of the LCU algorithm based on h for Hamiltonian simulation with $\|H\|_1 < 1$, $\tau \leq 1$ and error $\varepsilon > 0$?

Using the same algorithm as previous exercise, and the fact that $\|e^{iH\tau} |\chi\rangle\|_2^2 = \|\chi\rangle\|_2^2 = 1$, the cost scales with

$$O(d/\|e^{iH\tau} |\chi\rangle\|_2^2) = O(\log(1/\varepsilon)).$$