APPLIED QUANTUM ALGORITHMS LECTURE: QUANTUM PHASE ESTIMATION

THOMAS O'BRIEN

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Notation 1. *Throughtout this course (and when clear), I will use $|E_j\rangle$ to represent the eigenstates of a Hamiltonian H — $H|E_j\rangle = E_j|E_j\rangle$.*

0.1. **Phase kickback**

Quantum phase estimation relies fundamentally on the idea of phase kickback

- Recall that in quantum computing we transform the state of a quantum register by unitary operations, which correspond to gates in a quantum circuit.
- Recall that every unitary operator U is generated by some Hermitian operator H as $U = e^{iHt}$.
- This implies that U shares the same eigenstates $|E_j\rangle$ as H

$$U|E_j\rangle = e^{iE_jt}|E_j\rangle. \tag{0.1}$$

- When we apply a unitary U to a state $|\Psi\rangle$, we can work in the basis of eigenstates $|E_j\rangle$ of U just as well as we can work in the computational basis:

$$|\Psi\rangle = \sum_j a_j|E_j\rangle \quad \rightarrow \quad U|\Psi\rangle = \sum_j a_j e^{iE_jt}|E_j\rangle. \tag{0.2}$$

- If U is a unitary operator, so is the operator $I \oplus U$, defined as

$$I \oplus U = \begin{pmatrix} I & 0 \\ 0 & U \end{pmatrix}. \tag{0.3}$$

- This is the quantum action of applying U conditional on or controlled by an ancilla qubit (i.e. we do nothing if the ancilla qubit is in 0, and apply U if the ancilla qubit is in 1, and we do this coherently).
- In operator form, the combined states of the ancilla and system take the form $|0\rangle|\Psi\rangle$ and $|1\rangle|\Psi\rangle$, and $(I \oplus U)|0\rangle|\Psi\rangle = |0\rangle|\Psi\rangle$, but $(I \oplus U)|1\rangle|\Psi\rangle = |1\rangle U|\Psi\rangle$.
- Then, if the ancilla qubit is prepared in the $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ state, and the system register in $|\Psi\rangle = \sum_j a_j|E_j\rangle$, applying $(I \oplus U)$ produces the state

$$\sum_j a_j|E_j\rangle \frac{1}{\sqrt{2}}(|0\rangle + e^{iE_jt}|1\rangle). \tag{0.4}$$

- We see that the phases are 'kicked back' onto the ancilla qubit. This is the basis for quantum phase estimation; our goal is now to extract the E_j from the ancilla.

It is simple to extend the circuits from last week to allow control by an ancilla

- One may perform a controlled unitary operation by controlling each of the individual gates.
- This may be compressed further; in the decomposition of $e^{i\theta\hat{P}}$ from last week, only the final $R_z(\theta)$ rotation need to be controlled, as without this the remaining gates evaluate to the identity.

- A controlled R_z gate may be constructed by a controlled-phase gate and single qubit rotation on the ancilla.
- A controlled CNOT gate is a Toffoli gate, which is much harder to decompose (preferable to avoid).

0.2. **Single-ancilla QPE for eigenstates**

If the initial state is an eigenstate, one may estimate the eigenvalue with an error scaling as $M^{-1/2}t^{-1}$.

- Let us consider the case when $|\Psi\rangle = |E_j\rangle$. Then, the state post-controlled-U is separable

$$(I \oplus U)\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)|E_j\rangle = \frac{1}{\sqrt{2}}(|0\rangle + e^{iE_jt}|1\rangle)|E_j\rangle. \tag{0.5}$$

- Consider a measurement of the ancilla qubit in the X basis (achievable by performing a Hadamard and measuring in the computational basis):

$$P(M_{\mathrm{a},X} = 0) = \frac{1}{2}(1 + \cos(E_jt)). \tag{0.6}$$

- Similarly, consider a measurement of the ancilla qubit in the Y basis (achievable by performing a S gate before the Hadamard)

$$P(M_{\mathrm{a},Y} = 0) = \frac{1}{2}(1 - \sin(E_jt)) \tag{0.7}$$

- Now, suppose E_j (and thus $P(M_{\mathrm{a},X} = 0)$) are unknown. We can estimate $P(M_{\mathrm{a},X} = 0)$ by repeating the circuit M times and counting the number M_0 of 0's recorded; the estimator $\hat{P}(M_{\mathrm{a},X} = 0) \sim \frac{M_0}{M}$ converges to the true result with variance

$$\frac{P(M_{\mathrm{a},X} = 0)(1 - P(M_{\mathrm{a},X} = 0))}{M}. \tag{0.8}$$

- Let us now introduce the convenient term

$$\hat{Q} = \frac{1 - 2\hat{P}(M_{\mathrm{a},Y} = 0)}{2\hat{P}(M_{\mathrm{a},X} = 0) - 1} \sim \tan(E_j t). \tag{0.9}$$

- We can propagate variances through to $\hat{Q}$

$$\begin{aligned}\mathrm{Var}[\hat{Q}] = &\frac{P(M_{\mathrm{a},X} = 0)(1 - P(M_{\mathrm{a},X} = 0))}{M} \left| \frac{1 - 2\hat{P}(M_{\mathrm{a},Y} = 0)}{(2\hat{P}(M_{\mathrm{a},X}) = 0) - 1)^2} 2\hat{P}(M_{a,X} = 0) \right|^2 \\ &+ \frac{P(M_{\mathrm{a},Y} = 0)(1 - P(M_{\mathrm{a},Y} = 0))}{M} \left| \frac{2}{2\hat{P}(M_{\mathrm{a},X} = 0) - 1} \right|^2 . \end{aligned} \tag{0.10}$$

- Then, the estimator

$$\hat{E}_j = \frac{1}{t} \tan^{-1} \left[\hat{Q} \right], \tag{0.11}$$

  converges with variance

$$\frac{1}{t^2(1 + \hat{Q}^2)^2} \mathrm{Var}[\hat{Q}] \sim O(t^{-2} M^{-1}). \tag{0.12}$$

As the phase is only known modulo 2π, one cannot simply make t arbitrarily large to achieve Heisenberg scaling.

- The cost of implementing e^{iHt} M times scales as $O(Mt)$, so in theory we would want to make t as large as possible and M as small as possible.
- This is known as Heisenberg scaling — a scheme that achieves $\mathrm{Var}[E_j] \sim T^{-2}$ after total time spent T (here, $T = Mt$), or error scaling as T^{-1}.
- However, the above analysis ignored the fact that $\tan[\hat{Q}]$ only obtains an estimate of $\hat{E}_j t$ modulo 2π.
- We can avoid this by the following
  1. Estimate $2^l \hat{E}_j t \mod 2\pi$ for $l = 1, 2, 3, \ldots, L$ from M_l measurements using the above scheme, with t chosen to ensure $E_j t < 2\pi$.
  2. Estimate $\hat{E_j}^{(1)} = \frac{1}{t} \hat{E_j t}$.

(3) Choose $\hat{E}_j^{(2)}$ as the number in $[\hat{E}_j^{(1)} - \frac{\pi}{2}, \hat{E}_j^{(1)} + \frac{\pi}{2})$ so that $2t\hat{E}_j^{(2)} = 2\hat{E}_j t$.

(4) Repeat for higher l — choose $\hat{E}_j^{(l)} \in [\hat{E}_j^{(l-1)} - \frac{\pi}{2^l}, \hat{E}_j^{(l-1)} + \frac{\pi}{2^l})$ such that $2^l t\hat{E}_j^{(l)} = 2^l\hat{E}_j t$.

- One may check that by choosing $M_l = \alpha(L-l)+\beta$ measurements, we retain Heisenberg scaling; $\mathrm{Var}[\hat{E}_j] \sim T^{-1}$.

0.3. **Multi-ancilla QPE for mixed states**

By using phase kickback on multiple ancilla qubits, one may extract phases via the quantum Fourier transform, which has the advantage of directly projecting a system on an eigenstate.

- Instead of processing the data for QPE on a classical computer, we can perform this via the quantum fourier transform.
- Let us take L ancilla qubits, and perform controlled-e^{i2^lHt} on the lth qubit.
- If we write the ancilla state as $|n\rangle$ for $n = 0, \ldots, 2^L - 1$, then we send the state

$$|n\rangle|E_j\rangle \rightarrow e^{inE_jt}|n\rangle|E_j\rangle. \tag{0.13}$$

- Then, if we start from

$$\frac{1}{2^{L/2}}\sum_n |n\rangle \sum_j a_j e^{iE_jt}|E_j\rangle, \tag{0.14}$$

applying controlled-U^{2^l}, and following with a quantum Fourier transform on the ancilla register sends the state to

$$\frac{1}{2^L}\sum_j\sum_m\sum_n a_j e^{-i\frac{2\pi nm}{2^L}} e^{iE_jnt}|m\rangle|E_j\rangle \sim \sum_j a_j|\tilde{E}_j\rangle|E_j\rangle, \tag{0.15}$$

where here, $\tilde{E}_j$ is a L-bit representation of the true energy E_j.

- Importantly here, measuring the ancilla register projects the state register from a mixed state into an eigenstate.

- However, the error in the above approximation scales as $2^{-L/2}$, and not the optimal 2^{-L}.

- It turns out that this is caused by the construction of the ancilla state $\frac{1}{2^{L/2}}\sum_n |n\rangle$. To achieve Heisenberg scaling we need to optimize the coefficients of $|n\rangle$ in this preparation; unfortunately we don't have time to cover this here.

0.4. **Single-ancilla QPE for mixed states**

Separating phases with single ancilla qubits may be achieved in a similar method to extracting single notes from a chord.

- Let us recall the state of our system following a controlled-e^{iHt} (on a mixed-starting state $\sum_j a_j|E_j\rangle$)

$$|\Psi(t)\rangle = \frac{1}{\sqrt{2}}\sum_j a_j|E_j\rangle(|0\rangle + e^{iE_jt}|1\rangle). \tag{0.16}$$

- Now, let us re-calculate the probability of measuring $M = 0, 1$ on the ancilla qubit after rotating into the X and Y bases as before

$$P(M_{a,\mathrm{X}} = 0|t) = \frac{1}{2}(1 + \sum_j |a_j|^2\cos(E_jt)), P(M_{a,\mathrm{Y}} = 0|t) = \frac{1}{2}(1 - \sum_j |a_j|^2\sin(E_jt)) \tag{0.17}$$

- We may now define a useful function

$$g(t) := P(M_{a,\mathrm{X}} = 0|t) - P(M_{a,\mathrm{X}} = 1|t) + iP(M_{a,\mathrm{Y}} = 1|t) - iP(M_{a,\mathrm{Y}} = 0|t) \tag{0.18}$$

$$:= \langle\Psi(t)|X + iY|\Psi(t)\rangle \tag{0.19}$$

$$= \sum_j |a_j|^2 e^{iE_jt}. \tag{0.20}$$

- The eigenvalues E_j may be estimated from $g(j)$ via standard signal processing techniques.

- One such method is known as Prony's method, or the matrix pencil technique: if we define the $K/2 \times K/2$ Hankel matrices $G^{(0)}$ and $G^{(1)}$ by

$$G^{(a)}_{i,j} = g(i+j+a), \tag{0.21}$$

then eigenvalues of $G^{(1)}[G^{(0)}]^{-1}$ are the eigenvalues E_j for sufficiently large K.

- (One can improve convergence by noting additionally that $g(k)^* = g(-k)$.)

- This method achieves a variance in the estimate of an eigenvalue E_j of size $O(|a_j|^{-4}K^{-3}M^{-1})$ if M copies of the state are used to estimate each $g(k)$ value (and making some assumptions on the gap between eigenvalues). This is optimal in M and $|a_j|$, but as we require estimation of each $g(k)$, the cost to estimate scales as K^2 — this is not Heisenberg scaling.

The expectation values of operators in eigenstates may be additionally obtained during single-ancilla QPE

- We can extend the above protocol by inserting additional unitaries in between rounds of QPE.

- For example: consider controlled time evolution by H (for time t_1), followed by controlled application of a unitary V, followed by controlled time evolution by H for time t_2. The combined system plus ancilla state evolves to

$$\sum_{j,k} a_j \left(|0\rangle|E_j\rangle + \langle E_k|V|E_j\rangle e^{iE_jt_1+iE_kt_2}|1\rangle|E_k\rangle\right). \tag{0.22}$$

- We may then calculate

$$g(t_1,t_2) = \sum_{j,k} a_j a_k^* \langle E_j|V|E_k\rangle e^{-iE_jt_1-iE_kt_2}. \tag{0.23}$$

- This is a two-dimensional wave with coefficients $a_j a_k^* \langle E_j|V|E_k\rangle$, which may be extracted by a similar analysis to the above.

Instituut Lorentz, Leiden University

Email address: `obrien@lorentz.leidenuniv.nl`