Phase estimation implementation

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I. SCALING THE HAMILTONIAN FOR QUANTUM PHASE ESTIMATION

Consider an eigensystem

$$H|u_j\rangle = u_j|u_j\rangle \tag{1}$$

We choose $\tau > 0$ so that upon rescaling $H' = -\tau H$, the unitary describing evolution is

$$U = e^{-iH'} = e^{i\tau H}. \tag{2}$$

Then the phase imparted is determined by

$$U|u_j\rangle = e^{i2\pi\phi_j}|u_j\rangle, \quad \text{with } \phi_j = \tau\frac{u_j}{2\pi}. \tag{3}$$

Recall that $e^{i2\pi(\phi_j+m)}$ has the same value for all integers m. The phase approximation algorithm provides an estimate $\tilde{\phi}$ of $\phi_j \mod 1$. We would like to choose τ such that the phase satisfies $0 \le \phi_j < 1$, which then guarantees a one-to-one correspondence between u_j and ϕ_j.

A. A single eigenstate and positive spectrum

Suppose the spectrum is positive

$$u_j \ge 0, \quad \text{for all } j. \tag{4}$$

The algorithm ideally measures the phase as $\tilde{\phi} = \phi_j \mod 1$. So, we choose a bound $u_b > u_{\max}$ where $u_{\max} = \max_j u_j$ so that $\tau = 2\pi/u_b$, and $\phi_j = u_j/u_b$ satisfies $0 \le \phi_j < 1$. Then there is a one-to-one correspondence between values of ϕ and u_j.

In summary, we supply to the algorithm an eigenstate $|u_j\rangle$ and a unitary constructed[1] from

$$-\tau H = -\frac{2\pi}{u_b}H. \tag{5}$$

We read the output $\tilde{\phi}$ and obtain our estimate of $\tilde{u_j}$ of u_j as

$$\tilde{u_j} = u_b\tilde{\phi}. \tag{6}$$

In fact, the phase is read from a register with a finite number n of bits and so takes discrete values

$$\tilde{\phi} \in \{0, \epsilon, 2\epsilon, 3\epsilon, \ldots, 1-\epsilon\}, \quad \text{where } \epsilon = 2^{-n}. \tag{7}$$

The estimate $\tilde{u_j}$ takes values

$$\tilde{u_j} \in \{0, \epsilon_u, 2\epsilon_u, 3\epsilon_u, \ldots, u_b - \epsilon_u\}, \quad \text{where } \epsilon_u = u_b 2^{-n}. \tag{8}$$

In particular, if we choose $u_b = u_{\max}$, then $u_{\max}$ is mapped to zero. This is why we required $u_b > u_{\max}$ rather than $u_b \ge u_{\max}$.

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[1] On quantum hardware, we might construct $-H$ and evolve for time $\tau = 2\pi/u_b$.

1. Example: Exact representation of minimum eigenvalue

When testing implementations, one may encounter problems such as the following. Still assuming $u_j > 0$ for all j, we look for a scaling that allows at the same time

1. an exact representation of $u_{\min}$ in the n bits of the phase register.
2. $u_b > u_{\max}$.

The second condition is required if we expect that a component $|u_{\max}\rangle$ will be present in the input state. Referring to (8) we see that for the first condition we must have $u_{\min} = m\epsilon_u$ or

$$u_b = \frac{2^n}{m} u_{\min}, \quad \text{for some } m \in 1, 2, \ldots, n-1. \tag{9}$$

Note that we do not include $m = 0$ as a possibility. We only scale the phase interval, but do not shift it. In particular, the phase $\phi = 0$ corresponds only to $u = 0$ (unless $u_{\max} >= u_b$, which we want to avoid.) The second condition, $u_b > u_{\max}$ may be written

$$u_{\max} < \frac{2^n}{m} u_{\min} \tag{10}$$

Clearly if (10) is satisfied for any $m > 1$, then it is satisfied for $m = 1$. That is $m = 1$ gives the largest u_b. Thus, setting $m = 1$, we find the condition for the number of qubits in the phase register n.

$$n > \log_2 \left(\frac{u_{\max}}{u_{\min}} \right) \tag{11}$$

This is the number of qubits necessary to satisfy both conditions 1 and 2 above. On the other hand, to get the best resolution, we want to choose m as large as possible. From (10) we find that for fixed n, we can choose the largest m satisfying

$$m < 2^n \frac{u_{\max}}{u_{\min}}, \tag{12}$$

Explicitly,

$$m = \left\lfloor 2^n \frac{u_{\max}}{u_{\min}} \right\rfloor, \tag{13}$$

B. Single eigenstate and positive and negative eigenvalues

Here we present a straigtforward scaling that makes good use of the resolution in case the spectrum has both positive and negative values of the same magnitude. We map the positive eigenvalues to $(0, \pi)$ and the negative eigenvalues to $(-\pi, 0)$. We choose u_b satisfying

$$u_b > \max \{|u_{\min}|, |u_{\max}|\}. \tag{14}$$

For a positive spectrum we chose $\tau = 2\pi/u_b$. Here, we choose $\tau = \pi/u_b$, so that $\phi_j = u_j/(2u_b)$ satisfies

$$-\frac{1}{2} \le \phi_j < \frac{1}{2}. \tag{15}$$

We obtain the unwrapped observed phase $\tilde{\phi}'$ satisfying $-(1/2) \le \tilde{\phi}' < (1/2)$ via

$$\tilde{\phi}' = \begin{cases} \tilde{\phi} & \text{if } \tilde{\phi} < \frac{1}{2} \\ 1 - \tilde{\phi} & \text{if } \tilde{\phi} \ge \frac{1}{2} \end{cases}. \tag{16}$$

The sorted possible values of $\tilde{\phi}'$ are given by

$$\tilde{\phi}' \in \left\{ -\frac{1}{2}, -\frac{1}{2} + \epsilon, -\frac{1}{2} + 2\epsilon, \ldots, \frac{1}{2} - \epsilon \right\}, \quad \text{where } \epsilon = 2^{-n}. \tag{17}$$

The estimated eigenvalue, obtained via $\tilde{u} = 2u_b\tilde{\phi}'$, has value given by

$$\tilde{u} \in \{-u_b, -u_b + \epsilon_u, \ldots, u_b - \epsilon_u\}, \quad \text{where } \epsilon_u = u_b 2^{-n+1}. \tag{18}$$

II. FAST SIMULATION OF THE PHASE REGISTER PROBABILITIES

Here, we present a method to compute numerically the probabilities of the states of phase-estimation register in parallel QPE. The method is very straightforward. We simply compute intermediate steps classically rather than with quantum circuits. Recall that QPE works with a composite system with Hilbert space $V_p \otimes V_U$ where V_p corresponds to an n-qubit phase-estimation register and V_U is the space of the eigenphase problem. Suppose for the moment that the input state $|u\rangle \in V_U$ is an eigenvector of U, that is $U|u\rangle = e^{2\pi i \phi_u}|u\rangle$. For our purposes, we break QPE into three steps.

1. Preparation of a state

$$\frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} e^{2\pi i j \phi_u} |j\rangle |u\rangle, \tag{19}$$

where $N = 2^n$ and the states $|j\rangle$ are the computational basis vectors of the phase register.

2. Application of the inverse (quantum) Fourier transform of the prepared state, with the result

$$|\tilde{\phi}_u\rangle |u\rangle. \tag{20}$$

If ϕ_u can be representated exactly in n-qubits, then $\phi_u = k/N$ for some integer k. In this case we are performing the inverse Fourier transform of a Fourier transform with a single frequency component, given by k. In this case, the phase estimation register will be in the computational basis state $|k\rangle$.

3. Measurement of the state $|\tilde{\phi}_u\rangle$ in the computational basis to obtain an estimate of ϕ_u

Our procedure for computing the amplitudes of $|\tilde{\phi}_u\rangle$ takes as input the phase ϕ_u, and the number of qubits n. In particular, we make no use of $|u\rangle$ and U. We first prepare complex floating point vector $x_0, \ldots, x_{N-1}$ with values

$$x_j = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} e^{2\pi i j \phi_u}. \tag{21}$$

We then compute the inverse Fourier transform, via the FFT, of the vector $x_0, \ldots, x_{N-1}$. The result is a numerical approximation of amplitudes of $|\tilde{\phi}_u\rangle$ in the computational basis, that is $\langle j|\tilde{\phi}_u\rangle$ for $j = 0, \ldots, N-1$. These are amplitudes of the phases in (7)

Suppose that instead of an eigenstate $|u\rangle$ we have as input a generic pure state $\sum_u c_u |u\rangle$, where the sum runs over eigenvectors of U. In this case, the QPE algorithm leaves the phase register in the state

$$\sum_u c_u |\tilde{\phi}_u\rangle |u\rangle. \tag{22}$$

The state of the phase register alone is described by the reduced density matrix

$$\rho_{\text{phase}} = \sum_u |c_u|^2 |\tilde{\phi}_u\rangle\langle\tilde{\phi}_u|. \tag{23}$$

The probability of reading the computational basis state $|j\rangle$ is then

$$p(j) = \operatorname{tr}\left(|j\rangle\langle j|\rho_{\text{phase}}\right) = \sum_u |c_u|^2 |\langle j|\tilde{\phi}_u\rangle|^2. \tag{24}$$

Consider taking as input the number of qubits in the phase register n and pairs (ϕ_u, c_u) representing the input state. We can compute $p(j)$ numerically as follows. Initialize $p(j)$ to zero for all j. Loop over u. For each iteration with fixed u, compute the vector of $\langle j|\tilde{\phi}_u\rangle$ for $j = 0, \ldots, N-1$ as described above. For each j accumulate $|c_u|^2 |\langle j|\tilde{\phi}_u\rangle|^2$ into $p(j)$. Continue to the next u until finished.