1 Quantum Phase Estimation - Why

First created in September 2018

Ref:

- Quantum phase estimation algorithm
- Quantum Phase Estimation but we are not following its illustration, as it is confusing.

1.1 Motivation

Quantum phase is useful in many algorithms due to its relative and modular nature. It is not distinguishable among $\phi_\kappa = \phi_0 + 2\kappa\pi \ (\kappa \in \mathbb{Z})$ so one can do modular arithmetic in calculation, e.g. Quantum Fourier Transform (QFT) and Shor's Algorithm.

However, phase is relative and cannot be directly measured with measurement gates. For example, $|+\rangle$ and $|-\rangle$ both measure 50-50 chance of a 0 and 1, but their phases differ by π.

Quantum Phase Estimation (QPE) is a process to measure how much phase change an operator U effects on its eigenstate $|\psi\rangle$. In other words, QPE is to measure the eigenvalue of U given an eigenstate.

1.2 Phase Saving

1.2.1 Modular Arithmetic

In this context, Θ is the count of 2π cycles, a "digitised cycle phase". $\Theta = 1$ is a phase of 2π. Fractional phase is represented in decimal or binary. e.g. $\pi/4 = 2\pi/8$ is presented as 0.125 in decimal or $[0.001]$ in binary.

For an angular phase ϕ, the cycle phase $\Theta = \phi/2\pi$. We further define $\phi_m \equiv 2\pi/m$, which is a unit of $1/m$ cycle.

$j\phi_m$ and $k\phi_m$ is in phase if and only if $j \equiv k \pmod m$.

Proof: $j \equiv k \pmod m \ \Leftrightarrow \ j = k + \kappa m \ \Leftrightarrow \ j\phi_m = k\phi_m + \kappa m \phi_m = k\phi_m + \kappa m \cdot 2\pi/m = k\phi_m + 2\kappa\pi$.

1.2.2 Eigenvalue as Phase

Given a unitary U and one of its eigenstates $|\psi\rangle$, the eigenvalue would be a unit-length complex number, or a phase. We have $U|\psi\rangle = e^{2\pi i\Theta}|\psi\rangle$, where $\Theta \in [0, 1)$.

The QPE algorithm estimates the value of Θ. In other words, it is to find the eigenvalue of a unitary operator, given an eigenstate.

The strategy is to have a "measuring" register $|x\rangle$ and an eigenstate register $|\psi\rangle$. By applying an x-controlled U to $|\psi\rangle$ one would "modulate" the phase $2\pi i\Theta$ into $|x\rangle$. Measuring $|x\rangle$ would give a bit pattern approximating Θ. The more qubits in $|x\rangle$, the more accurate the approximation is.

To illustrate, let cU^j be the q-controlled U^j operation. $U^j|\psi\rangle = e^{2\pi i\cdot j\Theta}|\psi\rangle$.

When $|q\rangle$ is initialised to $|+\rangle$, $cU^j(|q\rangle \otimes |\psi\rangle) = \frac{1}{\sqrt{2}}\left(|0\rangle|\psi\rangle + |1\rangle e^{2\pi i\cdot j\Theta}|\psi\rangle\right) = \frac{1}{\sqrt{2}}\left(|0\rangle + e^{2\pi i\cdot j\Theta}|1\rangle\right)|\psi\rangle$.

You can see the "kick back" of the phase change $e^{2\pi i\cdot j\Theta}$ from $|\psi\rangle$ to $|x\rangle$. This is not surprising given that phase is only relative. The trick is that we use $|\psi\rangle$ as a common reference that all qubits in $|x\rangle$ is relative to, such that there are phases differences built up among the qubits q_r.

When we apply the q_r-controlled U^{2^r} to $|\psi\rangle$, as $|\psi\rangle$ is an eigenstate of U, it will shift a phase of $2^r\Theta$, which will reflect on q_r given the common reference.

The measuring register $|x\rangle$ will build up a pattern of $\sum_{r=0}^{n} 2^r\Theta$. Such "phase modulation" can be read out by the inverse Quantum Fourier Transform QFT^{-1}.

1.2.3 Formulation

To measure $|\psi\rangle$ with n qubits, we apply a successive $|+\rangle$ controlled U^{2r} to $|\psi\rangle$, where $r \in [0, n-1]$.

Let the measuring register be $|x\rangle = |q_{n-1}q_{n-2}\ldots q_1q_0\rangle$, and $|k\rangle$ is standard basis vector with k being the numerical value of $q_{n-1}\cdots q_0$.

i.e. $|x\rangle = [x_0, x_1, \ldots, x_{N-1}]^T = \sum_{k=0}^{N-1} x_k |k\rangle$, where $N = 2^n$.

Note: While there are only n qubits of q_r, there are $N = 2^n$ states $x_k|k\rangle$, each x_k is represented as a unique pattern of $q_{n-1}\ldots q_0$.

Now let $c_r U^{2^r}|\psi\rangle$ be a controlled U^{2^r} operation on $|\psi\rangle$ with q_r being the control qubit. $|x\rangle$ was initialised to $\frac{1}{\sqrt{N}}(|0\rangle + |1\rangle)^{\otimes n}$. ($|\psi\rangle$ is omitted in the following to emphasise the phase change on $|x\rangle$.)

After the operation, x will become $\left(\prod_{r=1}^{n}{}^{\otimes}\, c_{n-r}U^{2^{(n-r)}}\right)\frac{1}{\sqrt{N}}(|0\rangle + |1\rangle)^{\otimes n}$

$$= \frac{1}{\sqrt{N}}\left(|0\rangle + e^{2\pi i\cdot 2^{n-1}\Theta}|1\rangle\right)\otimes\left(|0\rangle + e^{2\pi i\cdot 2^{n-2}\Theta}|1\rangle\right)\otimes\ldots\otimes\left(|0\rangle + e^{2\pi i\cdot 2\Theta}|1\rangle\right)\otimes\left(|0\rangle + e^{2\pi i\cdot\Theta}|1\rangle\right) = \frac{1}{\sqrt{N}}\sum_{k=0}^{N-1} e^{2\pi i\cdot k\Theta}|k\rangle .$$

This is very similar to QFT (Quantum Fourier Transform). If we apply F_N to a basis state $|q\rangle$,

$$F_N|q\rangle = \frac{1}{\sqrt{N}}\prod_{r=1}^{n}{}^{\otimes}\left(|0\rangle + e^{2\pi i\, q\cdot 2^{-r}}|1\rangle\right)$$

$$= \frac{1}{\sqrt{N}}\left(|0\rangle + e^{2\pi i\, q\cdot 2^{-1}}|1\rangle\right)\otimes\left(|0\rangle + e^{2\pi i\, q\cdot 2^{-2}}|1\rangle\right)\otimes\ldots\otimes\left(|0\rangle + e^{2\pi i\, q\cdot 2^{-n+1}}|1\rangle\right)\otimes\left(|0\rangle + e^{2\pi i\, q\cdot 2^{-n}}|1\rangle\right)$$

$$= \frac{1}{\sqrt{N}}\left(|0\rangle + e^{2\pi i\cdot 2^{n-1}(q/N)}|1\rangle\right)\otimes\left(|0\rangle + e^{2\pi i\cdot 2^{n-2}(q/N)}|1\rangle\right)\otimes\ldots\otimes\left(|0\rangle + e^{2\pi i\cdot 2(q/N)}|1\rangle\right)\otimes\left(|0\rangle + e^{2\pi i\cdot(q/N)}|1\rangle\right)$$

$$= \frac{1}{\sqrt{N}}\sum_{k=0}^{N-1} e^{2\pi i\cdot k(q/N)}|k\rangle .$$

By observation of $|x\rangle$ vs $F_N|q\rangle$, we can see that $\Theta \sim (q/N)$. In other words, $|x\rangle$ is "modulated" with the phase from $|\psi\rangle$.

So we can use QFT^{-1} to reverse the process to find the Θ pattern. The larger N is, the higher the precision of approximating Θ with q/N.

1.2.4 Visualisation

If we initialise the measuring register $|x\rangle$ to $|+\rangle^{\otimes} n$, it will be an unbiased superposition of $\frac{1}{\sqrt{N}}\sum_{k=0}^{N-1}|k\rangle$.

All standard basis states $|k\rangle$ are of the same "baseline" phase of zero. $|x\rangle = \frac{1}{\sqrt{N}}\sum_{k=0}^{N-1} e^{2\pi i\cdot 0}|k\rangle$.

After the q_r-controlled U^{2^r} operation, a phase is built up: $|x\rangle = \frac{1}{\sqrt{N}}\sum_{k=0}^{N-1} e^{2\pi i\cdot k\Theta}|k\rangle$.

So the originally zero rotation from $|0\rangle$ to $|N-1\rangle$, now it is spiraling through the states, adding a Θ phase per state in the numerical rank.

When F_N^{-1} is operating on $|x\rangle$, all rows would add up to zero, except for the row with q/N equal (or close) to Θ. Such row will add up to unity (or close). It is like the resonance in the continuous Fourier Transform, in which the phase in $|x\rangle$ "resonances" with $|\xi\rangle_q$, the q^{th} column of F_N, resulting in state $|q\rangle$.

Recall $|x\rangle = \left(\frac{1}{\sqrt{N}}\sum_{k=0}^{N-1} e^{2\pi i\cdot k\Theta}|k\rangle\right)$. Because $F_N|q\rangle \approx |x\rangle$, We have $F_N^{-1}|x\rangle \approx |q\rangle$.

1.3 Examples

Useful things:

$$R_x(\pi\Theta) = \begin{bmatrix} \cos\pi\Theta/2 & -i\sin\pi\Theta/2 \\ -i\sin\pi\Theta/2 & \cos\pi\Theta/2 \end{bmatrix}.$$

$$R_x(\pi/2) = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & -i \\ -i & 1 \end{bmatrix} = -i\sqrt{X}, \;\; R_x(\pi) = \begin{bmatrix} 0 & -i \\ -i & 0 \end{bmatrix} = -iX, \;\; R_x(2\pi) = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} = -I, \;\; R_x(4\pi) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = I.$$

$$F_2 = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & \omega_1 \end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} = H. \;\; F_2^{-1} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & \overline{\omega_1} \end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} = H.$$

$$F_4 = \frac{1}{\sqrt{4}}\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & \omega_2 & \omega_2^2 & \omega_2^3 \\ 1 & \omega_2^2 & \omega_2^4 & \omega_2^6 \\ 1 & \omega_2^3 & \omega_2^6 & \omega_2^9 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & i & -1 & -i \\ 1 & -1 & 1 & -1 \\ 1 & -i & -1 & i \end{bmatrix}.$$

$$F_4^{-1} = \frac{1}{\sqrt{4}}\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & \overline{\omega_2} & \overline{\omega_2^2} & \overline{\omega_2^3} \\ 1 & \overline{\omega_2^2} & \overline{\omega_2^4} & \overline{\omega_2^6} \\ 1 & \overline{\omega_2^3} & \overline{\omega_2^6} & \overline{\omega_2^9} \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -i & -1 & i \\ 1 & -1 & 1 & -1 \\ 1 & i & -1 & -i \end{bmatrix}.$$

1.3.1 1-Qubit Register

Case $n = 1, \;\; U = R_x(\pi), \;\; N = 2^n = 2$.

When $|\psi\rangle = |+\rangle, \;\; R_x(\pi)|\psi\rangle = -i|+\rangle, \;\; \Theta_+ = 0.75 = [0.11]$.

When $|\psi\rangle = |-\rangle, \;\; R_x(\pi)|\psi\rangle = i|-\rangle, \;\; \Theta_- = 0.25 = [0.01]$.

$|x\rangle$ was initialised to $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$, which is irrespective of $|\psi\rangle$. After the operation, $|x\rangle$ is changed.

When $|\psi\rangle = |+\rangle$:

$$(c_0R_x(\pi))|x\rangle|\psi\rangle = (c_0R_x(\pi))\frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle|+\rangle + |1\rangle R_x(\pi)|+\rangle) = \frac{1}{\sqrt{2}}(|0\rangle|+\rangle - i|1\rangle|+\rangle) = \frac{1}{\sqrt{2}}(|0\rangle - i|1\rangle)|+\rangle$$

$$= \frac{1}{\sqrt{2}}(|0\rangle + e^{2\pi i\cdot 1\times 0.75}|1\rangle)|+\rangle = \frac{1}{\sqrt{2}}\sum_{k=0}^{1} e^{2\pi i\cdot k\times 0.75}|k\rangle|+\rangle = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ -i\frac{1}{\sqrt{2}} \end{bmatrix} \otimes |+\rangle.$$

$F_2^{-1}|x\rangle = H\begin{bmatrix} \frac{1}{\sqrt{2}} \\ -i\frac{1}{\sqrt{2}} \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 1-i \\ 1+i \end{bmatrix}$. Measuring this will give you half a chance of 0 and 1.

When $|\psi\rangle = |-\rangle$:

$$|x\rangle|\psi\rangle = (c_0R_x(\pi))\frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)|-\rangle = \frac{1}{\sqrt{2}}(|0\rangle|-\rangle + |1\rangle R_x(\pi)|-\rangle) = \frac{1}{\sqrt{2}}(|0\rangle|-\rangle + i|1\rangle|-\rangle) = \frac{1}{\sqrt{2}}(|0\rangle + i|1\rangle)|-\rangle$$

$$= \frac{1}{\sqrt{2}}(|0\rangle + e^{2\pi i\cdot 1\times 0.25}|1\rangle)|-\rangle = \frac{1}{\sqrt{2}}\sum_{k=0}^{1} e^{2\pi i\cdot k\times 0.25}|k\rangle|-\rangle = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ i\frac{1}{\sqrt{2}} \end{bmatrix} \otimes |-\rangle.$$

$F_2^{-1}|x\rangle = H\begin{bmatrix} \frac{1}{\sqrt{2}} \\ i\frac{1}{\sqrt{2}} \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 1+i \\ 1-i \end{bmatrix}$. Measuring this will give you half a chance of 0 and 1.

1.3.2 2-Qubit Register

Let us increase the number of qubits to 2 and see if it gives a better approximation.

Case $n = 2, \;\; U = R_x(\pi), \;\; N = 2^n = 4$.

U and $|\psi\rangle$ have not changed, so we can recall: $\Theta_+ = 0.75 = [0.11]$ and $\Theta_- = 0.25 = [0.01]$.

$|x\rangle$ was initialised to $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$. We omit $|\psi\rangle$ here but please be reminded that R_x is on $|\psi\rangle$, not on $|1\rangle$.

When $|\psi\rangle = |+\rangle$:

$$|x\rangle = (c_1 R_x(2\pi))\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes (c_0 R_x(\pi))\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \otimes \frac{1}{\sqrt{2}}(|0\rangle - i|1\rangle)$$

$$= \frac{1}{\sqrt{4}}\left(|0\rangle + e^{2\pi i \cdot 2\times 0.75}|1\rangle\right) \otimes \left(|0\rangle + e^{2\pi i \cdot 1\times 0.75}|1\rangle\right) = \frac{1}{\sqrt{4}}\sum_{k=0}^{3} e^{2\pi i \cdot k \times 0.75}|k\rangle = \frac{1}{\sqrt{4}}\begin{bmatrix}1\\-i\\-1\\i\end{bmatrix}.$$

$F_4^{-1}|x\rangle = \frac{1}{\sqrt{4}}\begin{bmatrix}1&1&1&1\\1&-i&-1&i\\1&-1&1&-1\\1&i&-1&-i\end{bmatrix}\frac{1}{\sqrt{4}}\begin{bmatrix}1\\-i\\-1\\i\end{bmatrix} = \begin{bmatrix}0\\0\\0\\1\end{bmatrix}$. Measuring this will give you $|11\rangle$ with certainty, which means $\Theta = 0.75 = [0.11]$.

When $|\psi\rangle = |-\rangle$:

$$|x\rangle = (c_1 R_x(2\pi))\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes (c_0 R_x(\pi))\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \otimes \frac{1}{\sqrt{2}}(|0\rangle + i|1\rangle)$$

$$= \frac{1}{\sqrt{4}}\left(|0\rangle + e^{2\pi i \cdot 2\times 0.25}|1\rangle\right) \otimes \left(|0\rangle + e^{2\pi i \cdot 1\times 0.25}|1\rangle\right) = \frac{1}{\sqrt{4}}\sum_{k=0}^{3} e^{2\pi i \cdot k \times 0.25}|k\rangle = \frac{1}{\sqrt{4}}\begin{bmatrix}1\\i\\-1\\-i\end{bmatrix}.$$

$F_4^{-1}|x\rangle = \frac{1}{\sqrt{4}}\begin{bmatrix}1&1&1&1\\1&-i&-1&i\\1&-1&1&-1\\1&i&-1&-i\end{bmatrix}\frac{1}{\sqrt{4}}\begin{bmatrix}1\\i\\-1\\-i\end{bmatrix} = \begin{bmatrix}0\\1\\0\\0\end{bmatrix}$. Measuring this will give you $|01\rangle$ with certainty, which means $\Theta = 0.25 = [0.01]$.

1.4 "Recovery" of Θ from $|x\rangle$

Now, let us see if $F_N^{-1}|q\rangle = \frac{1}{\sqrt{N}}\sum_{k=0}^{N-1} e^{-2\pi i \cdot k(q/N)}|k\rangle$ would recover Θ.

A recap on QFT:

Given $\omega_n = e^{2\pi i/N}$, $\boxed{y_k = \frac{1}{\sqrt{N}}\sum_{j=0}^{N-1} x_j \omega_n^{jk}}$ and $\omega^{jk} = \omega^{kj}$, we have $|y\rangle = F_N|x\rangle$, $F_N^{-1}|y\rangle = |x\rangle$, and $\boxed{x_j = \frac{1}{\sqrt{N}}\sum_{k=0}^{N-1} y_k \omega_n^{-jk}}$.

This makes sense as $y_k = \frac{1}{\sqrt{N}}\sum_{j=0}^{N-1}\left(\frac{1}{\sqrt{N}}\sum_{k'=0}^{N-1} y_{k'}\omega_n^{-jk'}\right)\omega_n^{jk} = \frac{1}{N}\sum_{k'=0}^{N-1} y_{k'}\left(\sum_{j=0}^{N-1}\omega_n^{-jk'}\omega_n^{jk}\right) = \frac{1}{N}\sum_{k'=0}^{N-1} y_{k'}\left(\sum_{j=0}^{N-1}\omega_n^{j(k-k')}\right)$.

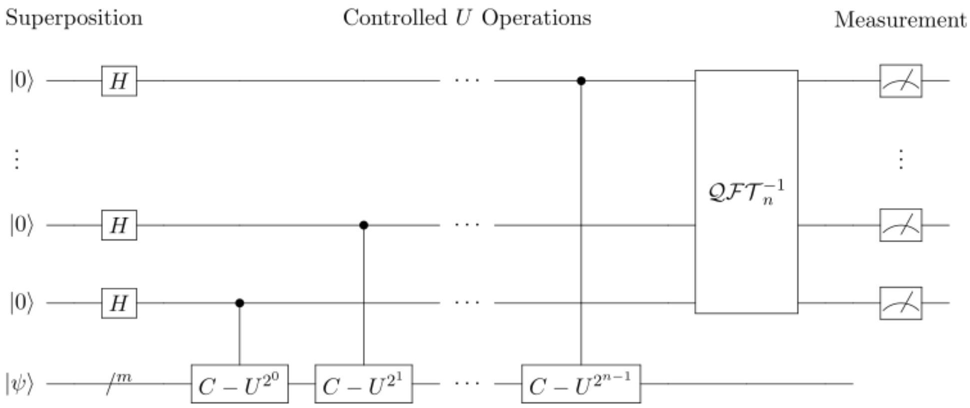
The ω_n terms will add up to zero when $k \neq k'$, and add up to N when $k = k'$. So $y_k = \frac{1}{N} y_k N = y_k$.

...

Given $|x\rangle = \frac{1}{\sqrt{N}}\sum_{j=0}^{N-1} e^{2\pi i \cdot j\Theta}|j\rangle$, we can express $|x\rangle = \frac{1}{\sqrt{N}}\sum_{j=0}^{N-1} x_j|j\rangle$, where $x_j = e^{2\pi i \cdot j\Theta}$.

$|y\rangle = \frac{1}{\sqrt{N}}\sum_{k=0}^{N-1} y_k|k\rangle$, where $y_k = \frac{1}{\sqrt{N}}\sum_{j=0}^{N-1} x_j\omega_n^{jk}$.

Here is the circuit from Wikipedia. The top line is the MSB.

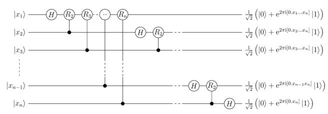


https://upload.wikimedia.org/wikipedia/commons/thumb/a/a5/PhaseCircuit-crop.svg/750px-PhaseCircuit-crop.svg.png

---

The QFT_n^{-1} (Inverse Quantum Fourier Transform) on the right is as following.

Note: R_n gates in QFT_n are phase shift by $2\pi/2^n$. In QFT_n^{-1}, the phase shift is negative, i.e. $\exp\left(-2\pi i\,[0.\overbrace{0..1}^{n}]\right)$. So R_2 is $S^\dagger$, R_3 is $T^\dagger$ and so on.



https://upload.wikimedia.org/wikipedia/commons/thumb/6/61/Q_fourier_nqubits.png/1050px-Q_fourier_nqubits.png