国際融合科学論/先端融合科学論

LECTURE 05
Quantum Mechanics II: Quantum Machine Learning

Dr. Suyong Eum

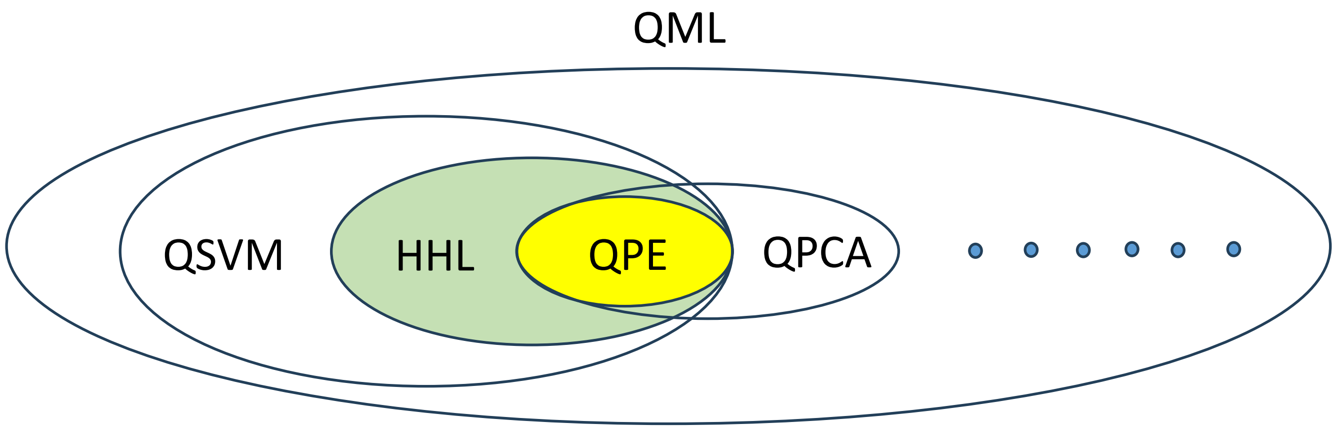
OSAKA UNIVERSITY

Lecture Outline

1) Two key building blocks of quantum machine learning (QML)
   A. Quantum Phase Estimation (QPE)
   B. Harrow-Hassidim-Lloyd (HHL)
2) a brief introduction to
   A. Quantum SVM (QSVM)

Quantum Machine Learning: why QPE and HHL?

- QPCA and QSVM are the quantum counterparts of PCA and SVM.
- The HHL algorithm is essential for comprehending QSVM.
- The QPE algorithm is essential for comprehending both the HHL algorithm and QPCA.
- These are versatile and powerful tools in quantum computing, enabling a range of applications.



Quantum Phase Estimation (QPE)

Quantum Phase Estimation: beginning

- "Quantum Phase Estimation (QPE)" is an algorithm for estimating the eigenvalues λ of a **unitary matrix U** using a quantum computer.

$$U|\psi\rangle = \lambda|\psi\rangle$$

- Assuming the matrix U is a unitary matrix,

$$\langle\psi|U^{\dagger}U|\psi\rangle = \langle\psi|\lambda * \lambda|\psi\rangle$$

$$\langle\psi|\psi\rangle = |\lambda|^2\langle\psi|\psi\rangle$$

$$|\lambda|^2 = 1$$

$$\lambda = \cos(2\pi\emptyset) + i\sin(2\pi\emptyset) = e^{2\pi i\emptyset}$$

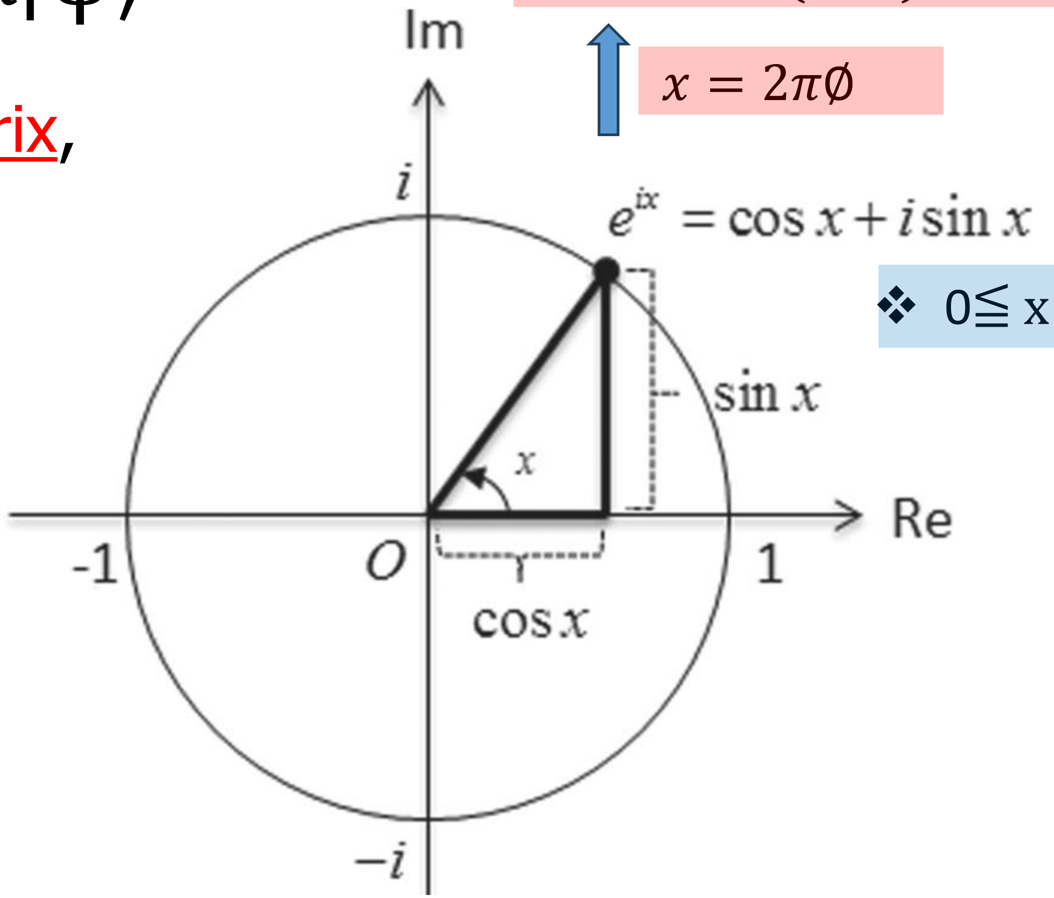
Euler's formula

- $0 \leqq \emptyset \leqq 1$

$$e^{2\pi i\emptyset} = \cos(2\pi\emptyset) + i\sin(2\pi\emptyset)$$

$$x = 2\pi\emptyset$$

- $0 \leqq x \leqq 2\pi$



Quantum Phase Estimation: beginning

- Thus, the previous expression can be written as follows:

$$U|\psi\rangle = \lambda|\psi\rangle \quad \longrightarrow \quad U|\psi\rangle = e^{2\pi i \emptyset}|\psi\rangle$$

- The phase, $\emptyset$, is in the range between 0 and 1, which has a decimal format ($\emptyset$).
- QPE is to estimate the phase, $\emptyset$, using qubits which has a binary format($\emptyset_n$).
- Thus, it would be convenient to express a decimal format as a binary format.

$$\emptyset = 0.\emptyset_1\emptyset_2 \ldots \emptyset_n = \sum_{k=1}^{n} \emptyset_k 2^{-k}$$

where $0 \leqq \emptyset \leqq 1$, and $\emptyset_n \in \{0,1\}$

$$0.11_2 = 0.75_{10}$$

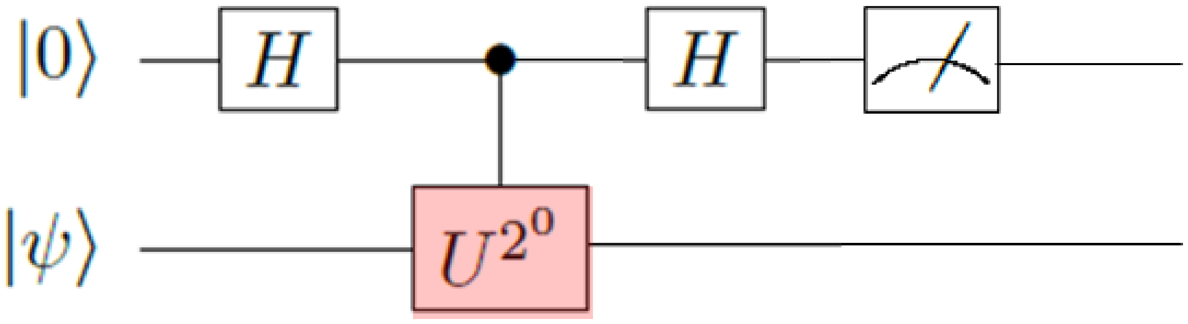
- In the above, when $\emptyset_1\emptyset_2 \ldots \emptyset_n \{0,1\}$ are known, the phase $\emptyset$ can be obtained.

$\emptyset_1\emptyset_2 \ldots \emptyset_n \{0,1\}$: 0.11_2 — the phase $\emptyset$: 0.75_{10}

Quantum Phase Estimation: toy example

Toy example

Quantum Phase Estimation: toy example



- We want to know how much phase is made due to this unitary matrix "U", given the eigen vector |ψ⟩.

$$U|\psi\rangle = \lambda|\psi\rangle \longrightarrow U|\psi\rangle = e^{2\pi i \emptyset}|\psi\rangle$$

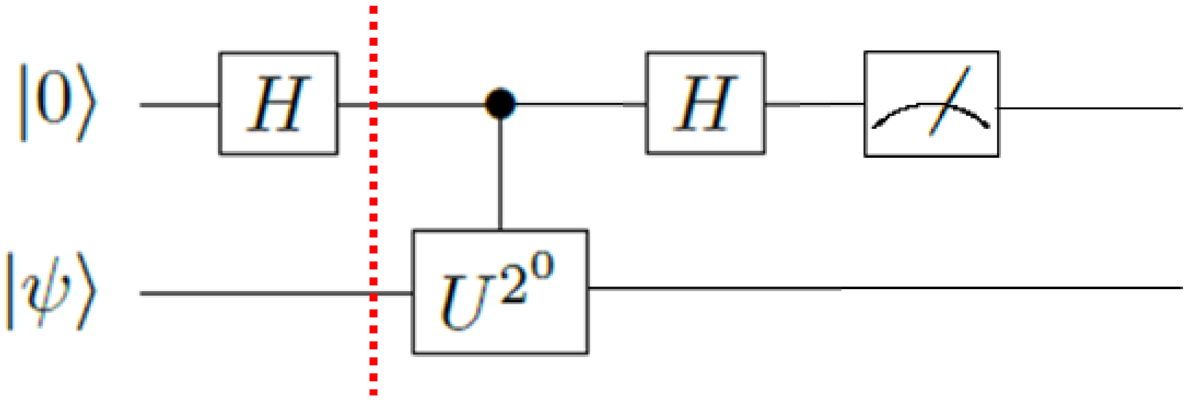
Eigen value (λ)

Phase (∅)

$$U = e^{2\pi i \emptyset}$$

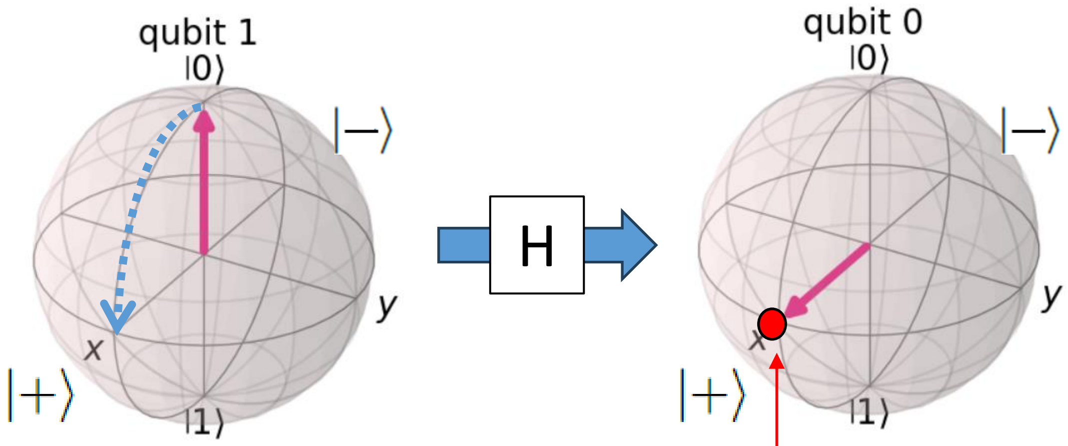
Please, remember this.
We are going to use it.

Quantum Phase Estimation: toy example



$$|+\rangle \otimes |\psi\rangle$$
$$= |0\rangle|\psi\rangle + |1\rangle|\psi\rangle$$

We temporarily do not write down "$1/\sqrt{2}$" for convenience.

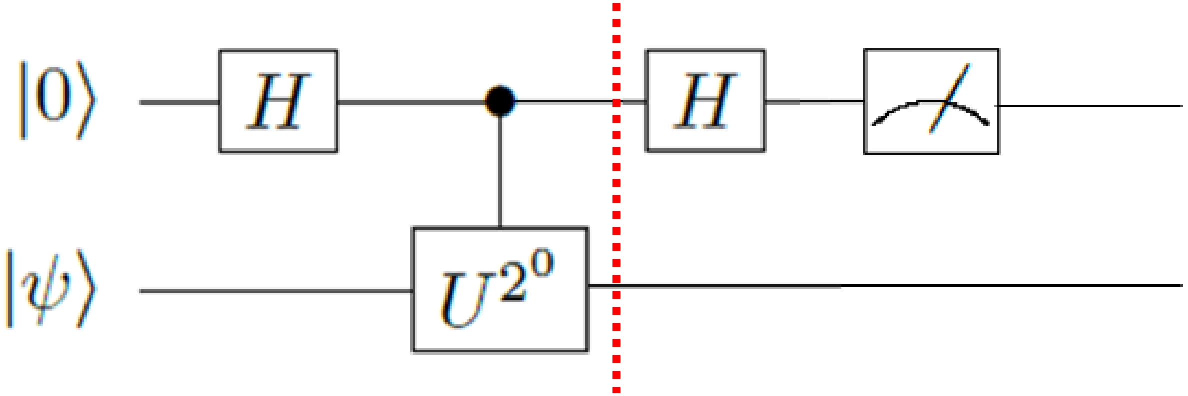


equal superposition of the two basis states

$$|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

$$|-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

Quantum Phase Estimation: toy example



- control qubit
- target qubit

$$|+\rangle \otimes |\psi\rangle$$

$$= |0\rangle|\psi\rangle + |1\rangle|\psi\rangle$$

$$|0\rangle|\psi\rangle + |1\rangle U|\psi\rangle$$

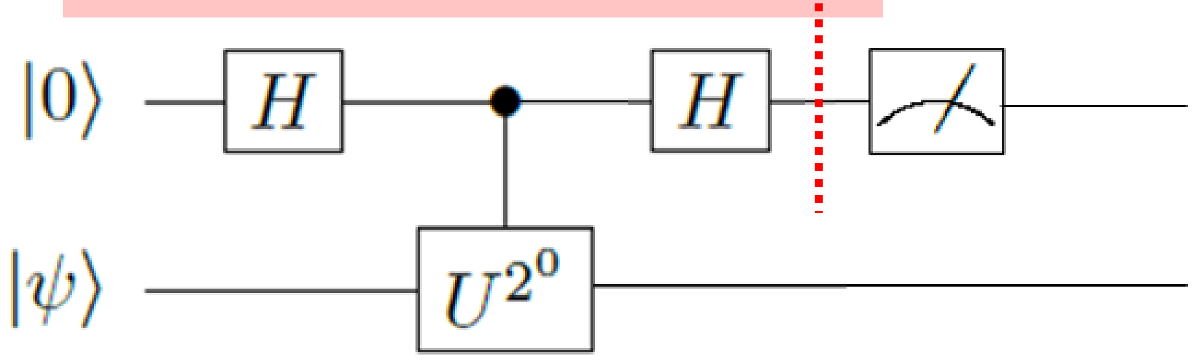
$$= |0\rangle|\psi\rangle + e^{2\pi i 0.\phi_1}|1\rangle|\psi\rangle$$

$$= (|0\rangle + e^{2\pi i 0.\phi_1}|1\rangle) \otimes |\psi\rangle.$$

- The phase of U is encoded in the top qubit. "Kick back"

Quantum Phase Estimation: toy example

$(1 + e^{2\pi i 0.\phi_1})\,|0\rangle + (1 - e^{2\pi i 0.\phi_1})|1\rangle$



$$H(|0\rangle + e^{2\pi i 0.\phi_1}|1\rangle)$$

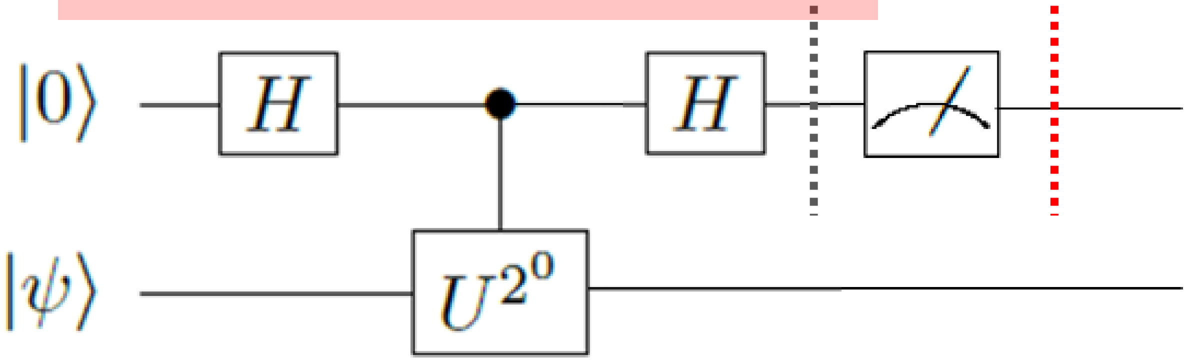
$$= H|0\rangle + H|1\rangle e^{2\pi i 0.\phi_1}$$

$$= (|0\rangle + |1\rangle) + (|0\rangle - |1\rangle)\, e^{2\pi i 0.\phi_1}$$

$$= (1 + e^{2\pi i 0.\phi_1})\,|0\rangle + (1 - e^{2\pi i 0.\phi_1})|1\rangle$$

Quantum Phase Estimation: toy example

$(1+e^{2\pi i 0.\phi_1})\,|0\rangle + (1-e^{2\pi i 0.\phi_1})\,|1\rangle$



1) If we measure $|0\rangle$
   - ϕ_1 must be 0,

   $\Rightarrow (1+e^{2\pi i 0.0})\,|0\rangle + (1-e^{2\pi i 0.0})\,|1\rangle$

   $= 2|0\rangle \Rightarrow |0\rangle$

   Please, remember that the coefficient ½ in front of each term is being omitted.

2) If we measure $|1\rangle$
   - ϕ_1 must be 1.

   $\Rightarrow (1+e^{2\pi i 0.1_2})\,|0\rangle + (1-e^{2\pi i 0.1_2})\,|1\rangle$

   $= (1+e^{2\pi i\, 0.5_{10}})\,|0\rangle + (1-e^{2\pi i\, 0.5_{10}})\,|1\rangle$

   $= 2|1\rangle \Rightarrow |1\rangle$

- ❖ The phase becomes either 0 or ½,
- ❖ The eigen value becomes either 1 or -1

$$e^{2\pi i\emptyset} = \cos(2\pi\emptyset) + i\sin(2\pi\emptyset)$$

Quantum Phase Estimation: general quantum circuit

General Quantum Circuit for QPE

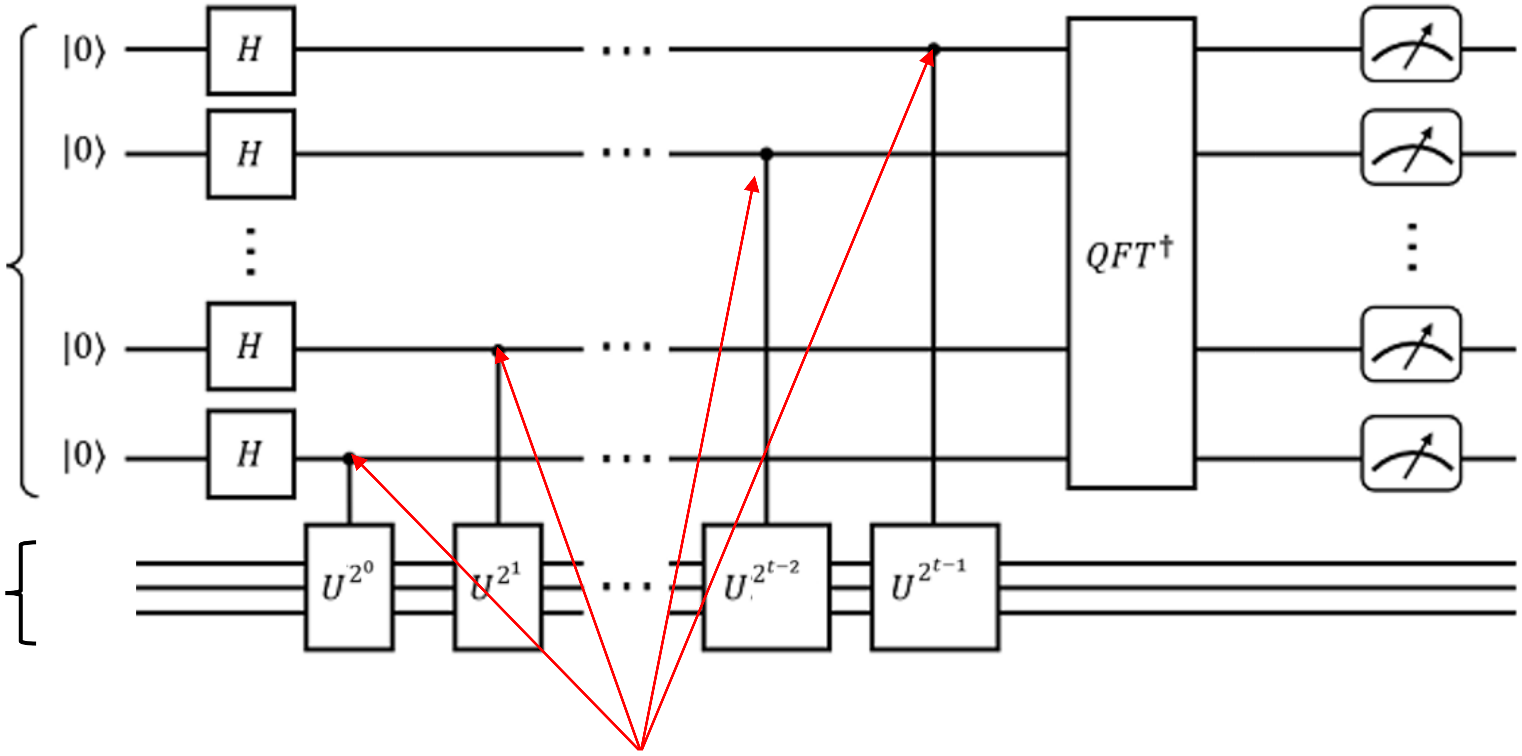
Quantum Phase Estimation: general quantum circuit

<u>Counting register</u>

“t” input qubits

“t” determines
the accuracy of
the estimation

<u>Second register</u>



<u>The phase of U matrix is “kickback” to *t* qubits</u>

- The quantum phase estimation algorithm uses phase <u>kickback</u> to write the phase of U to the t qubits in the counting register.

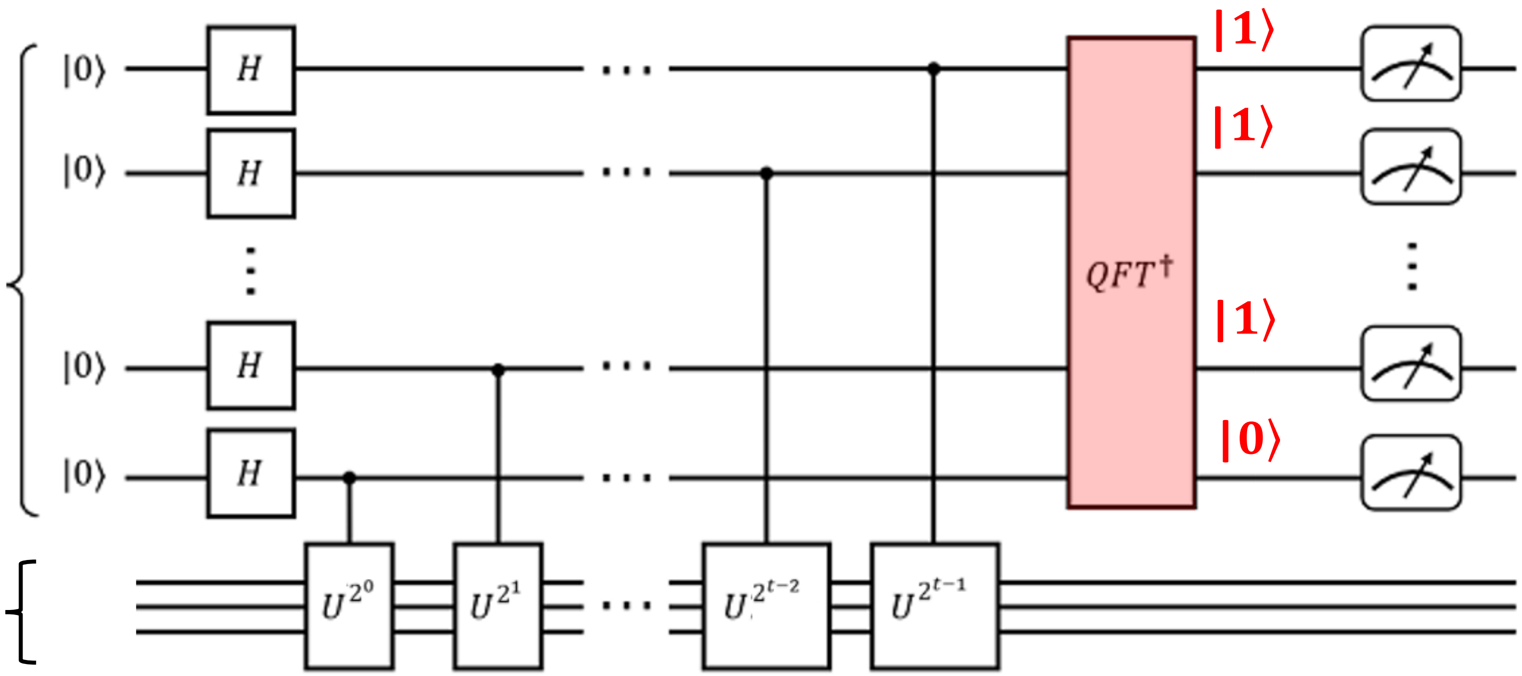
Quantum Phase Estimation: general quantum circuit

Counting register

"t" input qubits

"t" determines the accuracy of the estimation

Second register



- Inverse Quantum Fourier transform (QFT): ($QFT^\dagger$), which is a process to read out the output and produce $|0\rangle$ or $|1\rangle$

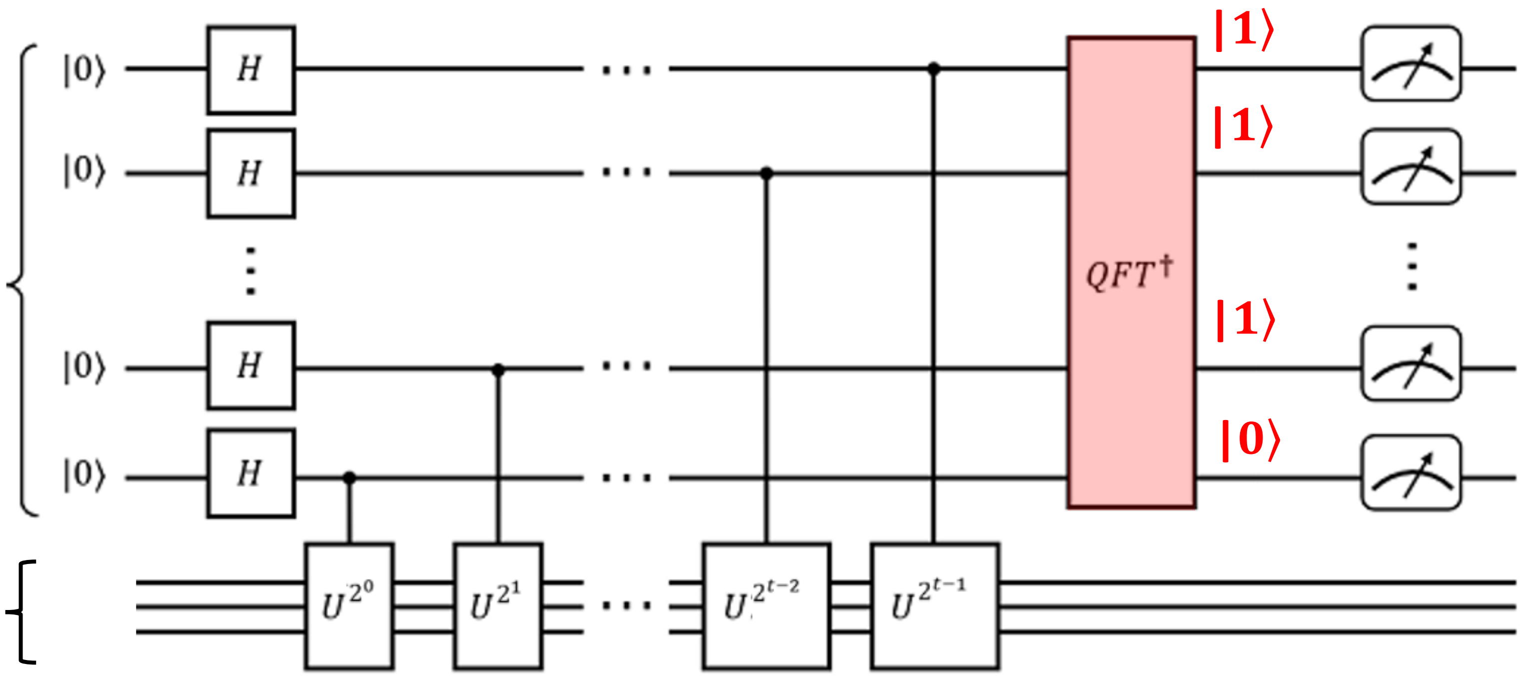
Quantum Phase Estimation: general quantum circuit

<u>Counting register</u>

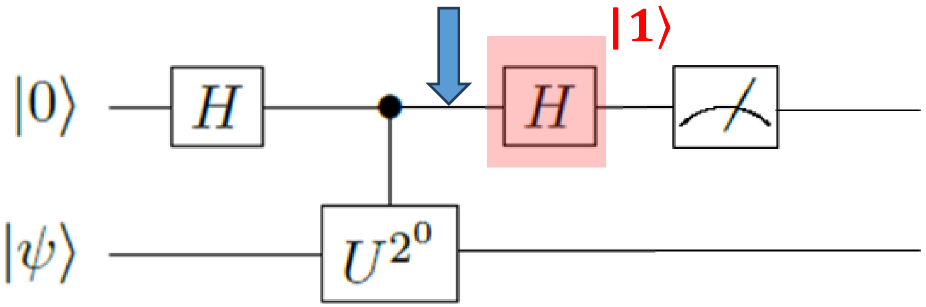
"t" input qubits

"t" determines the accuracy of the estimation

<u>Second register</u>



$(|0\rangle + e^{2\pi i 0.\phi_1}|1\rangle)$



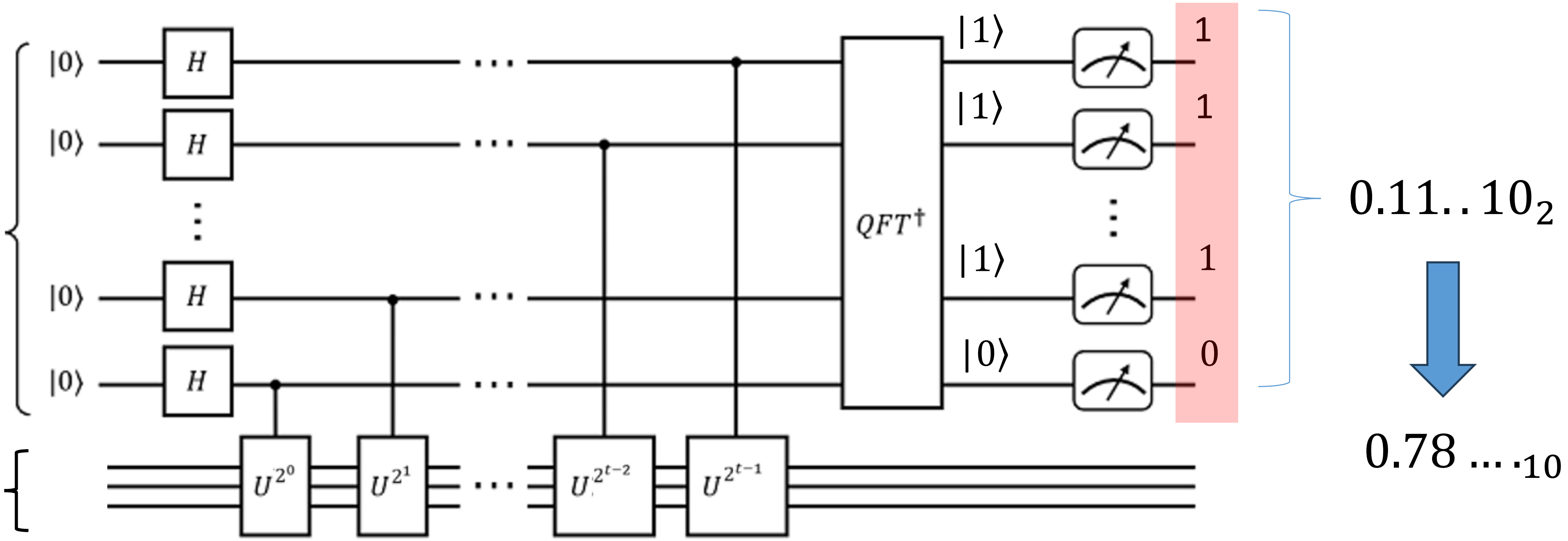
Quantum Phase Estimation: general quantum circuit

<u>Counting register</u>

"t" input qubits

"t" determines the accuracy of the estimation

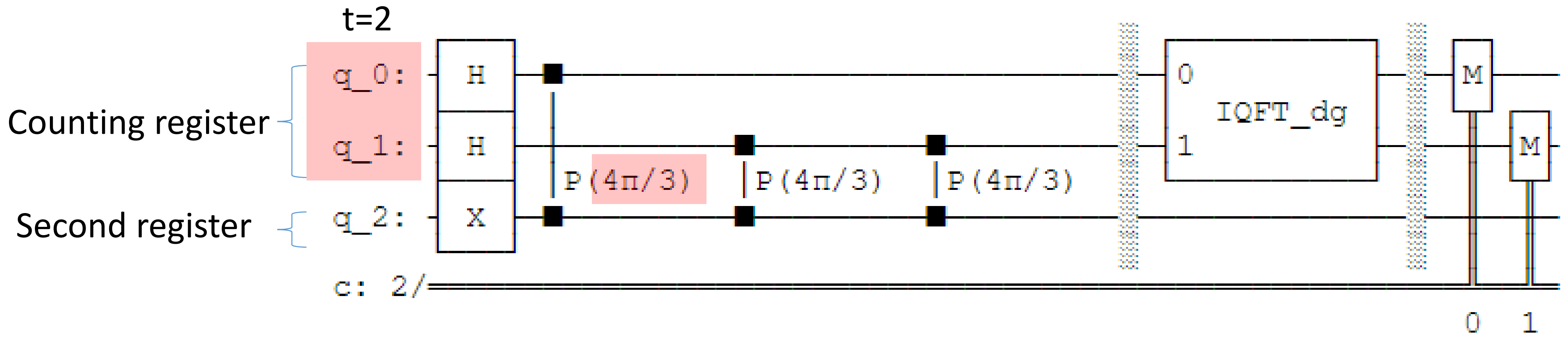
<u>Second register</u>



- Measurement is carried out, and the phase is encoded in binary format, e.g., $0.11..10_2$
- Next, it is converted to decimal format, e.g., $0.78\ldots_{10}$

Implementation

Quantum Phase Estimation: Qiskit implementation (t=2)



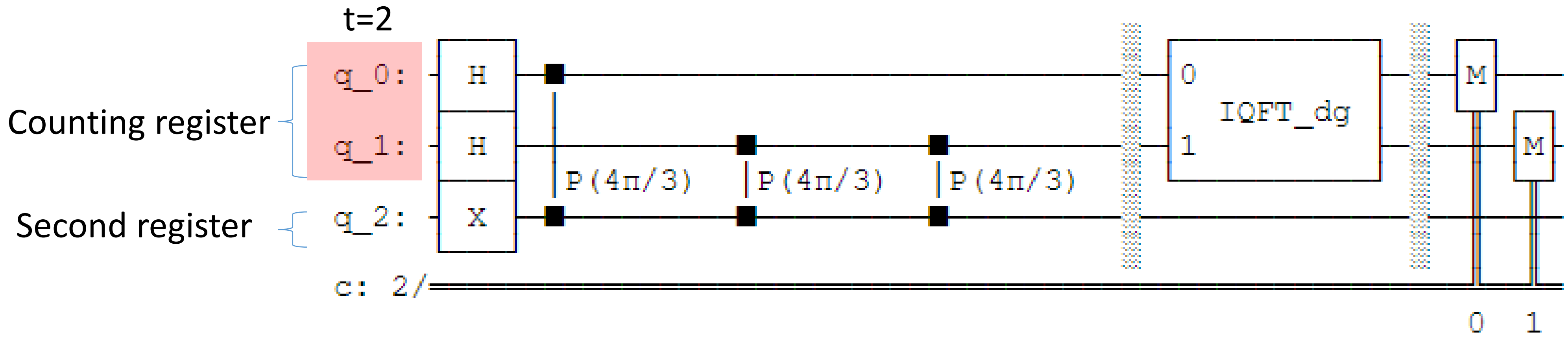
- Creating the circuit above to estimate the phase of a unitary operator U which is equivalent to estimate θ below.

$$U|\psi\rangle = e^{2\pi i\theta}|\psi\rangle$$

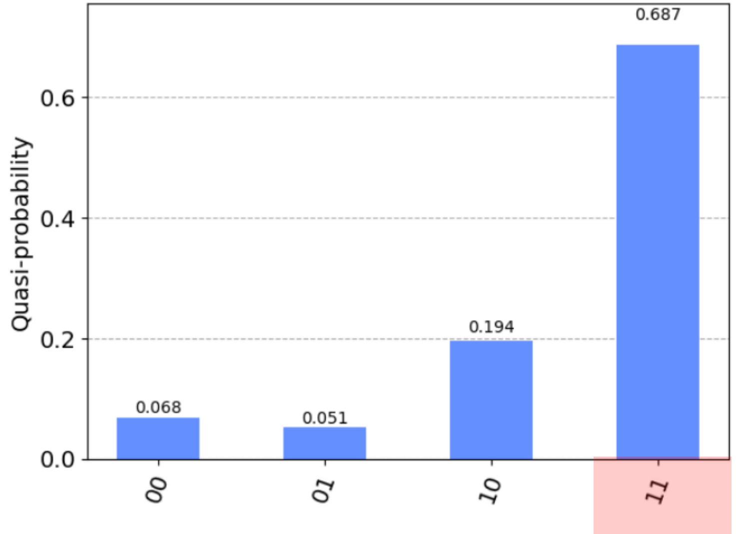
- Assume that the phase of the unitary matrix U is $4\pi/3$. In other words, the quantum phase estimation algorithm will find the value θ below.

$$2\pi\theta = 4\pi/3 \longrightarrow \theta = 4/6 \longleftarrow \text{The answer we expect}$$

Quantum Phase Estimation: Qiskit implementation (t=2)



- The exact solution is "θ =4/6 ($4\pi/3$)" in decimal number.
- The result is approximately "11", which corresponds to 3/4 in decimal form.



$$\sum_{k=1}^{n} \emptyset_k \, 2^{-k}$$

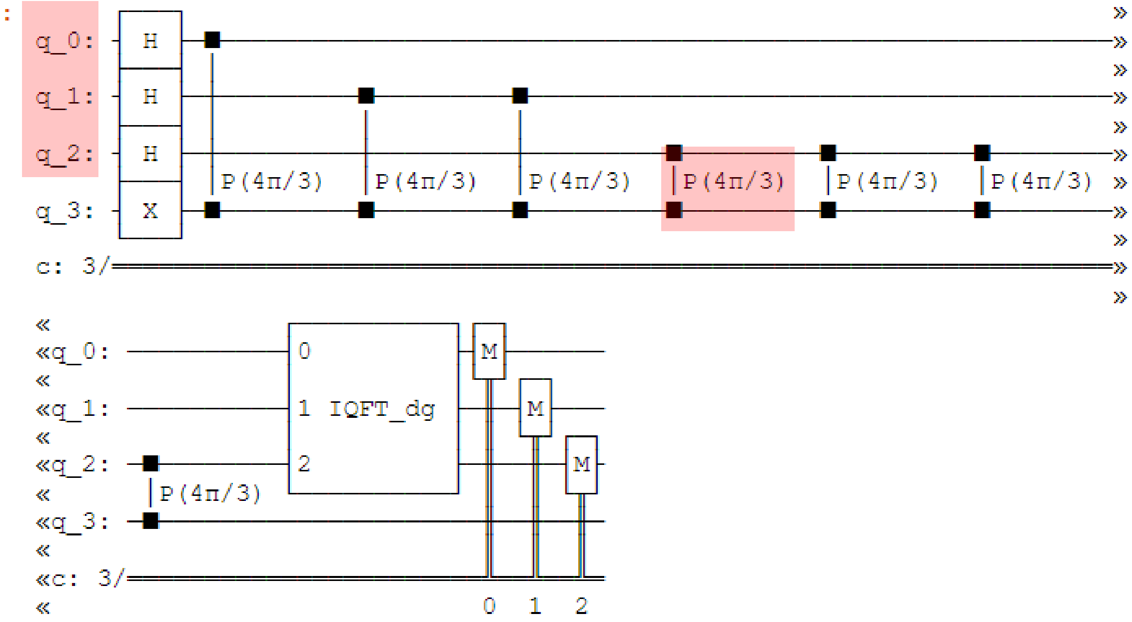
$\emptyset_k$: each digit in binary

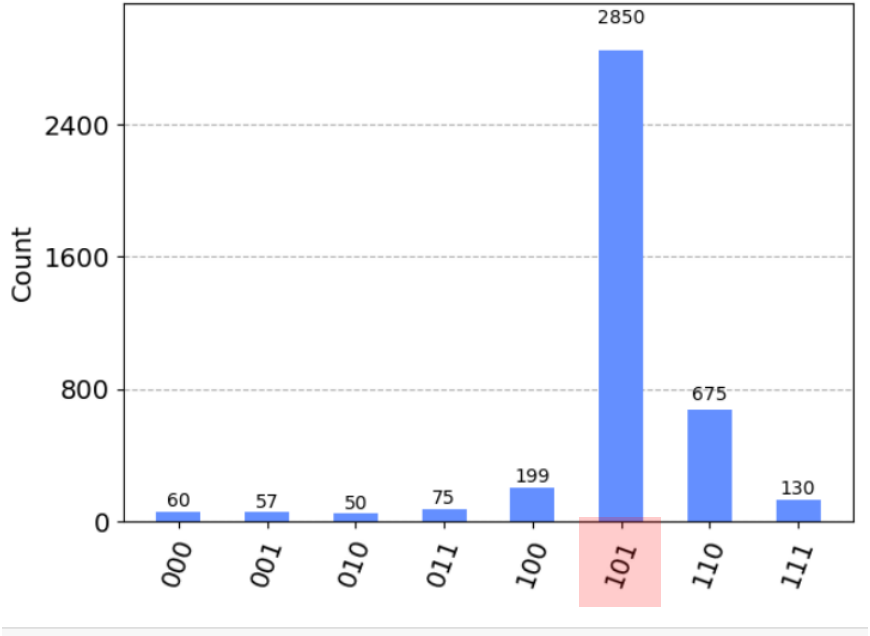
$$\theta = 0.11_2 = 0.75_{10}$$

$1*2^{-1} + 1*2^{-2} = 3/4$

Quantum Phase Estimation: Qiskit implementation (t=3)

t=3



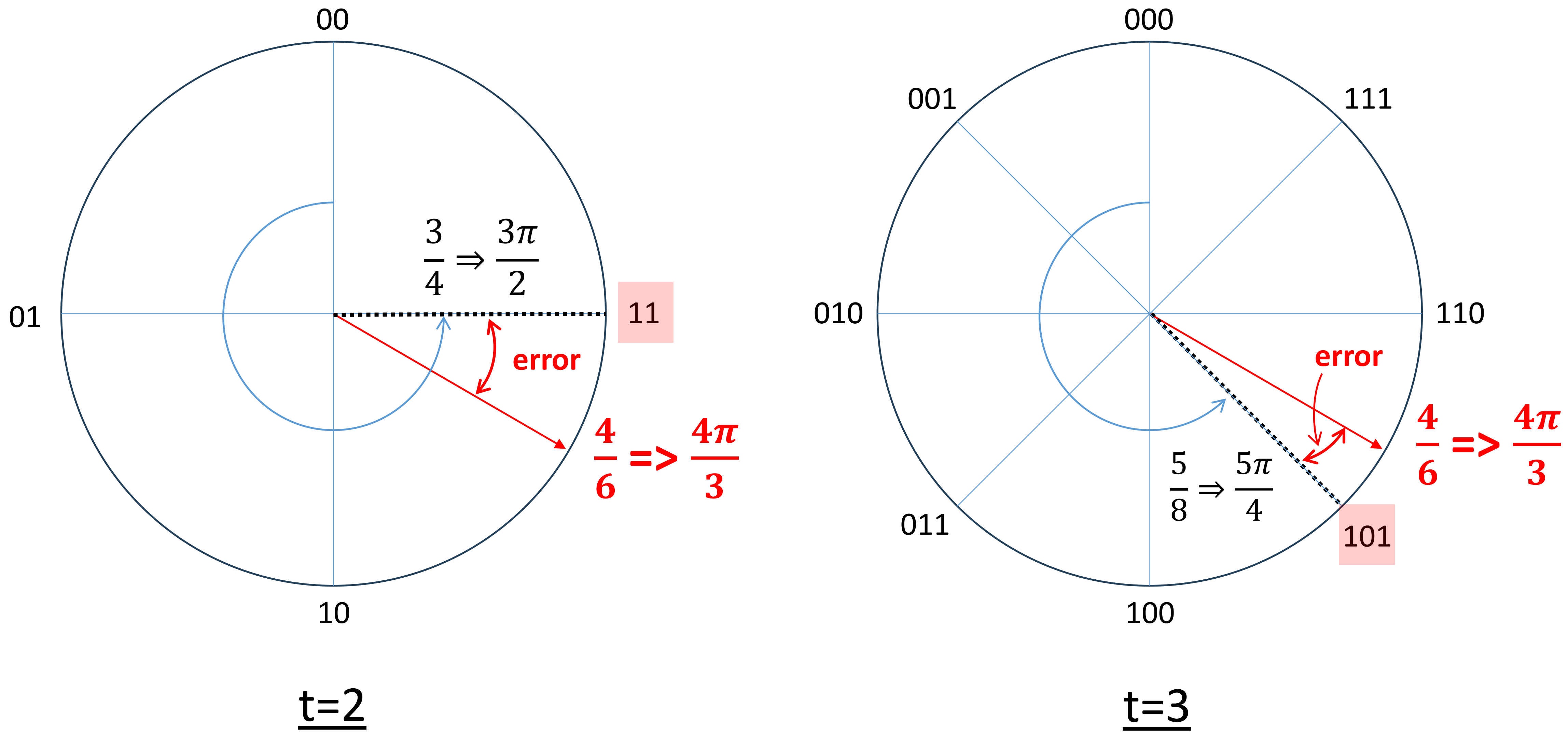


$\theta = 0.101_2 = 0.625_{10}$

$1*2^{-1} + 0*2^{-2} + 1*2^{-3} = 5/8$

- ❑ What is the reason for using more qubits in the counting register?

Quantum Phase Estimation: Comparison (t=2) vs (t=3)



Harrow-Hassidim-Lloyd (HHL)

Harrow-Hassidim-Lloyd (HHL)

- The HHL is for solving linear systems of equations, developed by Aram Harrow, Avinatan Hassidim, and Seth Lloyd (HHL) in 2009.

$$A\vec{x} = \vec{b} \qquad \begin{bmatrix} 1 & -1/3 \\ -1/3 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

- Theoretically speaking, the HHL algorithm achieves an exponential improvement compared to the classical algorithm to solve the problem.
  - Quantum algorithm (HHL)

    $O(\log(N)\, s^2\kappa^2/\varepsilon)$
    - s is the sparsity: the maximum number of non-zero elements in any row
    - κ is the condition number: the ratio of the largest and the smallest eigenvalues
    - ε the precision (error)
  - Classical algorithm (Gaussian elimination)

    $O(N^3)$

Harrow-Hassidim-Lloyd (HHL)

- The linear system of equation is presented in the quantum domain through a process called "state preparation".

$$A\,\vec{x} = \vec{b} \quad \Rightarrow \quad A|x\rangle = |b\rangle$$

- We would like to obtain $|x\rangle$, so

$$|x\rangle = A^{-1}|b\rangle$$
$$= \sum_{j=0}^{N-1} 1/\lambda_j |u_j\rangle\langle u_j|\;|b\rangle$$
$$= \sum_{j=0}^{N-1} 1/\lambda_j |u_j\rangle\langle u_j| \sum_{j=0}^{N-1} b_j |u_j\rangle$$
$$= \sum_{j=0}^{N-1} 1/\lambda_j b_j |u_j\rangle$$

- $|u_j|=1$
- Inner product of two same vectors $\langle u_j|\,|u_j\rangle$ is $|u_j|^2$

Harrow-Hassidim-Lloyd (HHL)

- So what does it mean?

$$|\mathrm{x}\rangle = \sum_{j=0}^{N-1} 1/\lambda_j \mathrm{b}_j |u_j\rangle$$

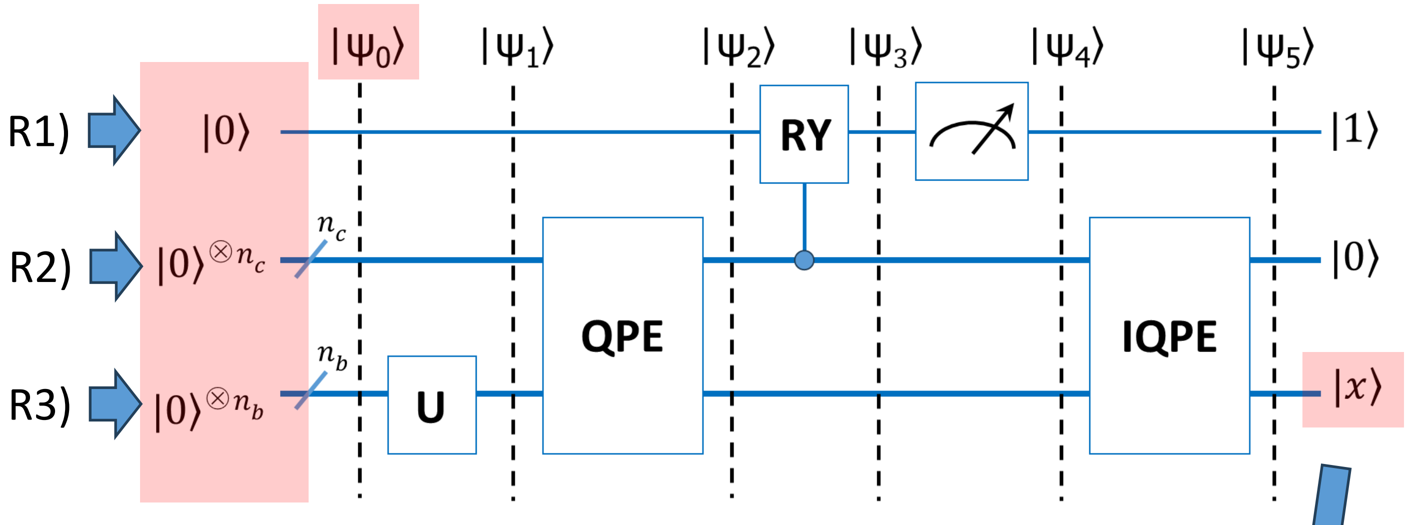
- It means that the solution $|\mathrm{x}\rangle$ is the amplitudes of the eigen vector $|u_j\rangle$.
- The things that you need to remember to understand the following slides.
  1) We need "$1/\lambda_j$": inverse of the eigenvalue,
  2) $|\mathrm{b}\rangle = \sum_{j=0}^{N-1} \mathrm{b}_j |u_j\rangle$: the vector $|\mathrm{b}\rangle$ can be represented using eigen vectors $|u_j\rangle$,
  3) The sum of the squares of the coefficients of $|\mathrm{x}\rangle$ equals 1.

$$\sum_{j=0}^{N-1} \left[\frac{b_j}{\lambda_j}\right]^2 = 1$$

General Quantum Circuit for HHL

Harrow-Hassidim-Lloyd (HHL): general quantum circuit

- There are three registers
  - R1) Ancilla qubit
    - a single qubit
  - R2) the eigenvalues of A; (N x N)
    - n_c = N qubits
  - R3) the encoded value of $|b\rangle$
    - $n_c = \log_2 N$ qubits

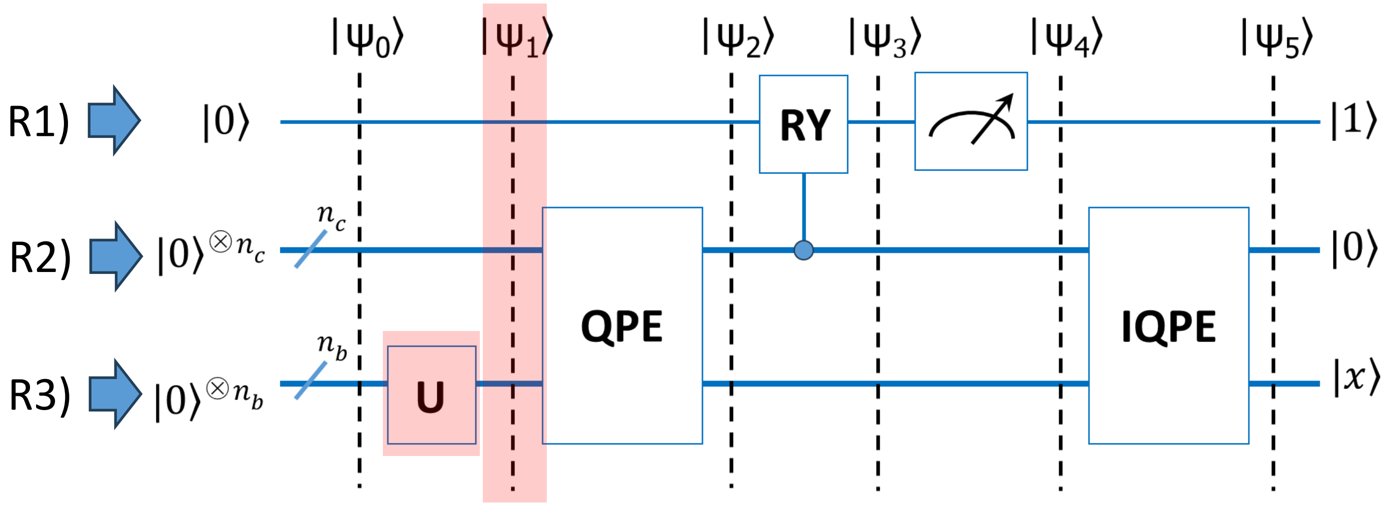


$$|\psi_0\rangle = |0\rangle^{\otimes n_b} |0\rangle^{\otimes n_c} |0\rangle$$

$$|x\rangle = \sum_{j=0}^{N-1} 1/\lambda_j b_j |u_j\rangle$$

Harrow-Hassidim-Lloyd (HHL): general quantum circuit

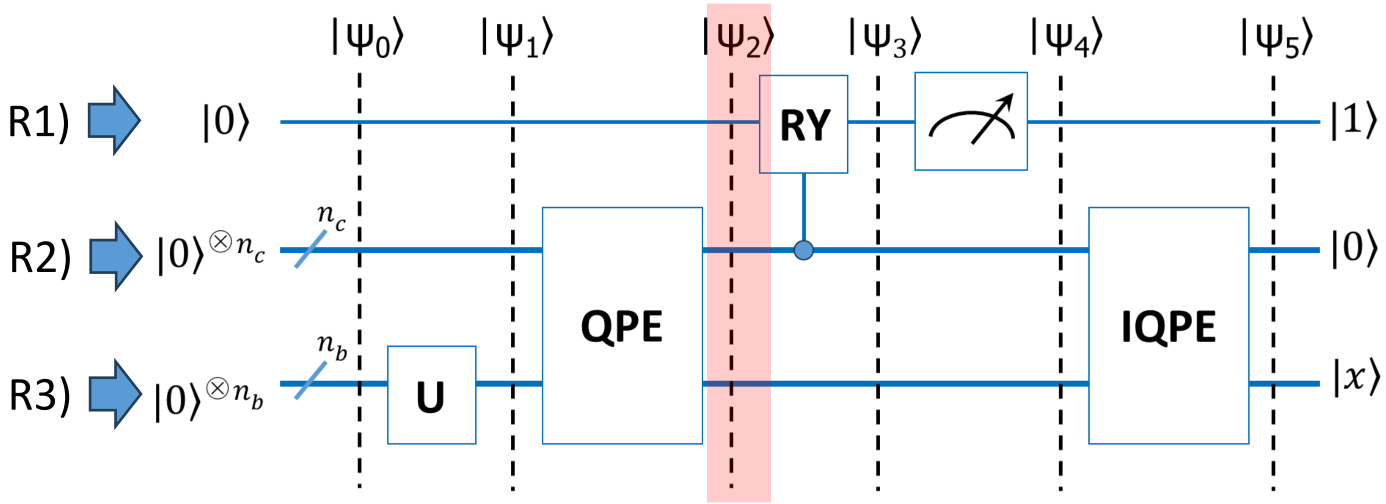
- U: state preparation
  - amplitude encoding: encoding a vector as a quantum state, e.g.,
    - $\vec{b} \Rightarrow |b\rangle$



$$|\psi_1\rangle = |b\rangle^{\otimes n_b} |0\rangle^{\otimes n_c} |0\rangle$$

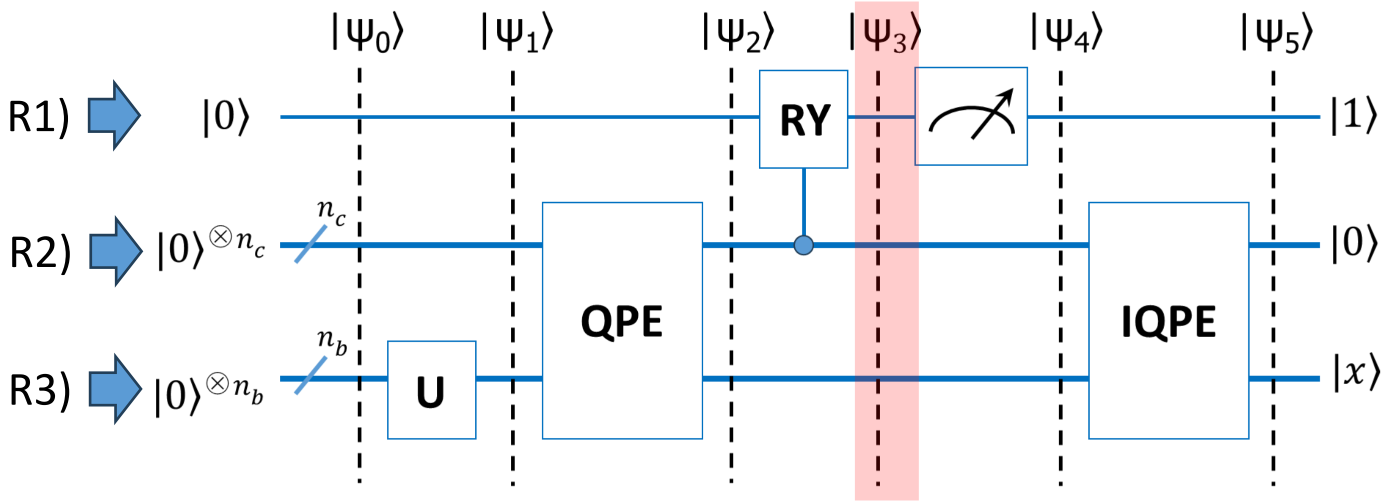
Harrow-Hassidim-Lloyd (HHL): general quantum circuit

- After QPE, we obtain the eigen value $\tilde{\lambda}_j$ which is encoded in R2 register.
- Then, $|\psi_2\rangle$ becomes …



$$|\psi_2\rangle = |b\rangle^{\otimes n_b} |\tilde{\lambda}_j\rangle^{\otimes n_c} |0\rangle$$

- RY gate
  - Encode the amplitudes of the quantum state based on the eigen values from QPE



- Then, $|\psi_3\rangle$ becomes as follows;

$$|\psi_3\rangle = |b\rangle^{\otimes n_b} \, |\tilde{\lambda}_j\rangle^{\otimes n_c} \left(\sqrt{1 - \frac{C^2}{\lambda_j^2}} |0\rangle + \frac{C}{\lambda_j} |1\rangle \right)$$

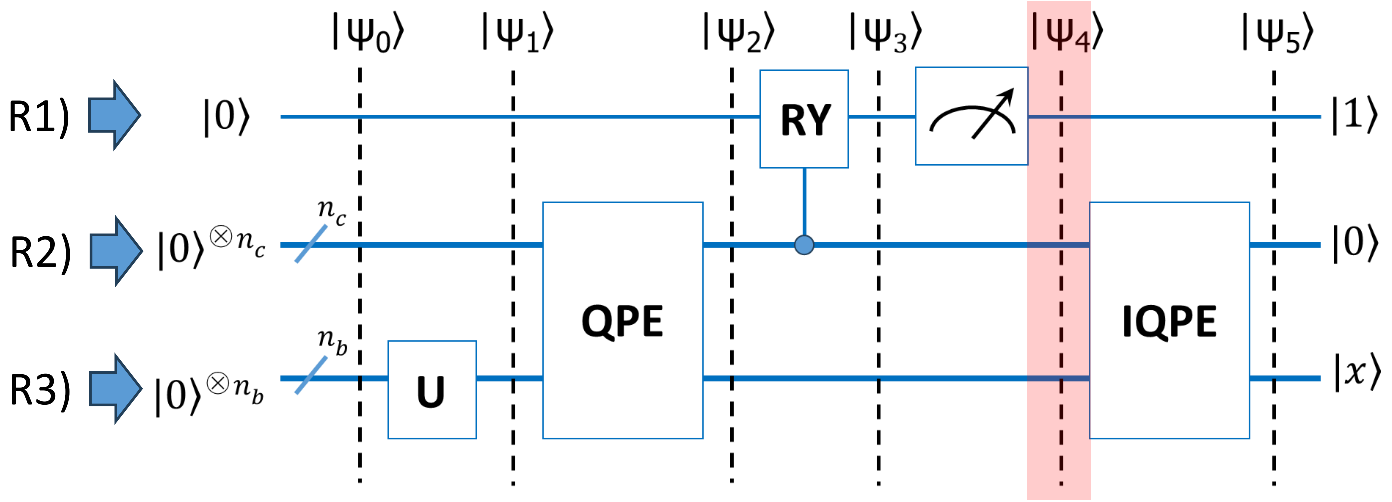
$$= \underbrace{\sum_{j=0}^{N-1} b_j |u_j\rangle}_{} \, \underbrace{|\tilde{\lambda}_j\rangle}_{} \left(\sqrt{1 - \frac{C^2}{\lambda_j^2}} |0\rangle + \frac{C}{\lambda_j} |1\rangle \right)$$

$|b\rangle$ is expressed using eigen vector $|u_j\rangle$ basis

eigen values from QPE

Harrow-Hassidim-Lloyd (HHL): general quantum circuit

- ❑ Only when the outcome is $|1\rangle$, the output is considered,
- ❑ Then, $|\psi_4\rangle$ becomes as follows;



$$|\psi_3\rangle = \sum_{j=0}^{N-1} b_j |u_j\rangle\, |\widetilde{\lambda_j}\rangle \left(\sqrt{1-\frac{C^2}{\lambda_j^2}}\,|0\rangle + \frac{C}{\lambda_j}|1\rangle\right)$$

$$|\psi_4\rangle = \frac{1}{\sqrt{\sum_{j=0}^{N-1}\left[\frac{b_j C}{\lambda_j}\right]^2}} \sum_{j=0}^{N-1} b_j |u_j\rangle |\widetilde{\lambda_j}\rangle \left(\frac{C}{\lambda_j}|1\rangle\right)$$

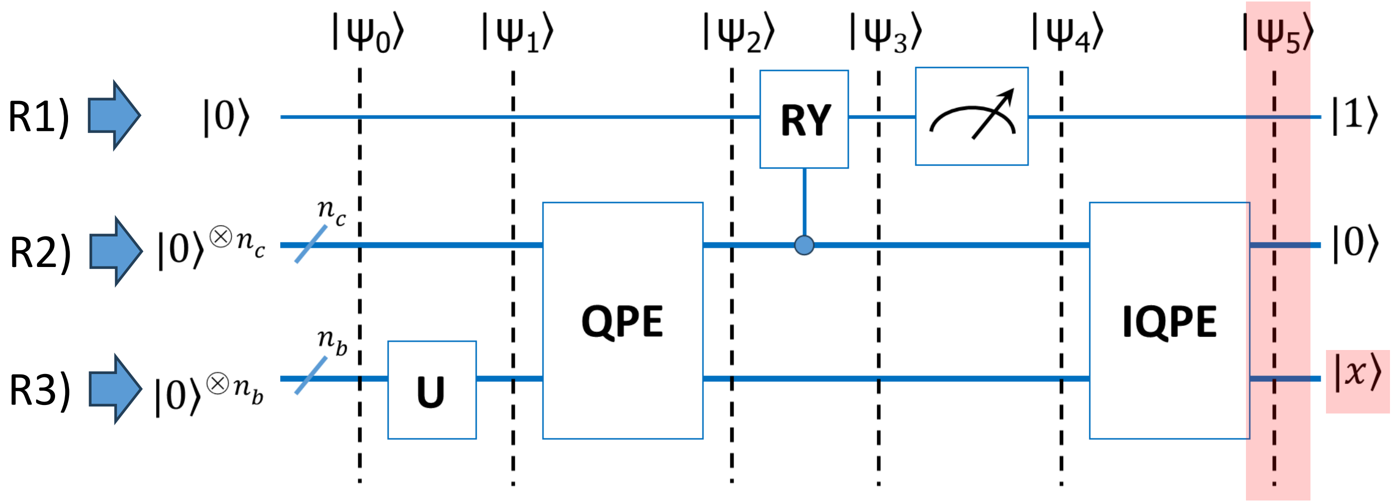
$$= \sum_{j=0}^{N-1} 1/\lambda_j b_j |u_j\rangle |\widetilde{\lambda_j}\rangle\, |1\rangle$$

$$|x\rangle = \sum_{j=0}^{N-1} 1/\lambda_j b_j |u_j\rangle$$

$$\sum_{j=0}^{N-1}\left[\frac{b_j}{\lambda_j}\right]^2 = 1$$

Harrow-Hassidim-Lloyd (HHL): general quantum circuit

- IQPE is applied, which finally returns $|x\rangle$ at R3) register



- Then, $|\psi_5\rangle$ becomes as follows;

$$|\psi_4\rangle = \sum_{j=0}^{N-1} 1/\lambda_j b_j |u_j\rangle |\widetilde{\lambda_j}\rangle |1\rangle$$

Back to original qubit state; QPE => IQPE

$$|\psi_5\rangle = \sum_{j=0}^{N-1} 1/\lambda_j b_j |u_j\rangle |0\rangle^{\otimes n_c} |1\rangle$$

$|x\rangle$ <u>We confirm that it produces $|x\rangle$ at the end.</u>

Quantum Support Vector Machine (QSVM)

Quantum Support Vector Machine (QSVM) with HHL

PRL **113**, 130503 (2014) PHYSICAL REVIEW LETTERS week ending 26 SEPTEMBER 2014

Quantum Support Vector Machine for Big Data Classification

Patrick Rebentrost,[1,*] Masoud Mohseni,[2] and Seth Lloyd[1,3,†]
[1]*Research Laboratory of Electronics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA*
[2]*Google Research, Venice, California 90291, USA*

- ❑ A key idea of the paper is to employ the least-squares reformulation of the SVM that avoids the quadratic programming and obtains the parameters from the solution of a linear equation system.

$$F\begin{pmatrix} b \\ \vec{\alpha} \end{pmatrix} \equiv \begin{pmatrix} 0 & \vec{1}^T \\ \vec{1} & K+\gamma^{-1}\mathbb{1} \end{pmatrix}\begin{pmatrix} b \\ \vec{\alpha} \end{pmatrix} = \begin{pmatrix} 0 \\ \vec{y} \end{pmatrix}. \quad (5)$$

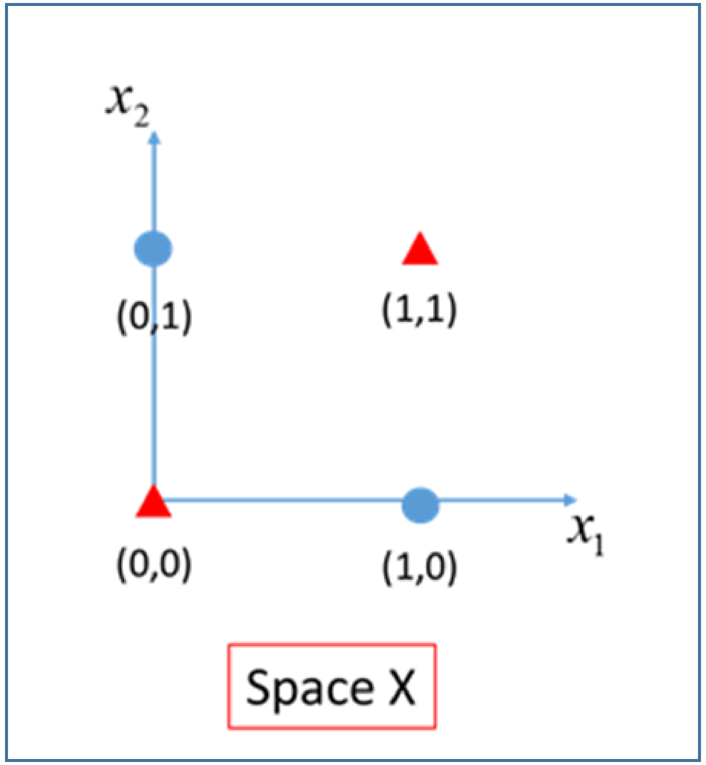
  - ➢ Then, we can apply the Harrow-Hassidim-Lloyd (HHL) algorithm to handle SVM, which is called "QSVM"!!

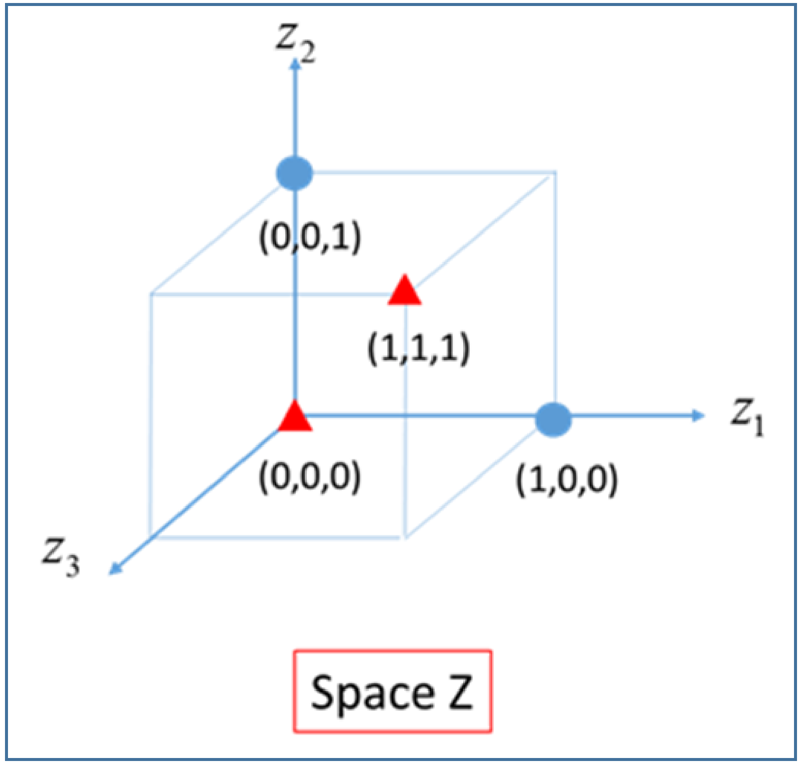
Quantum Support Vector Machine (QSVM) with QKernel

- We formulated SVM as a quadratic programming before…

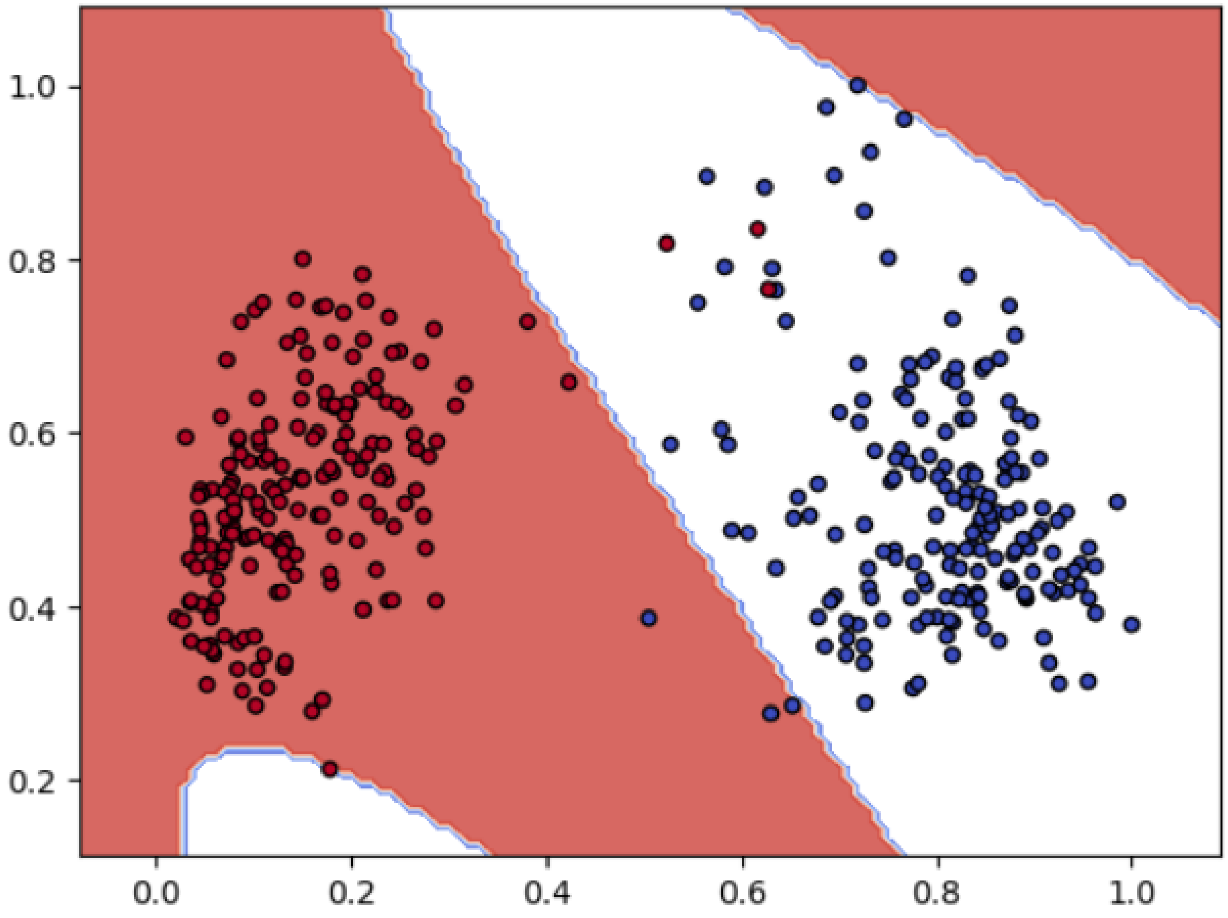
$$\min_{\lambda} \ L(\lambda) = \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} t_n t_m \lambda_n \lambda_m \mathrm{K}(\mathrm{x}_n^T \mathrm{x}_m) - \sum_{n=1}^{N} \lambda_n$$

$$s.t. \quad \lambda \geq 0, \quad t^T \lambda = 0$$

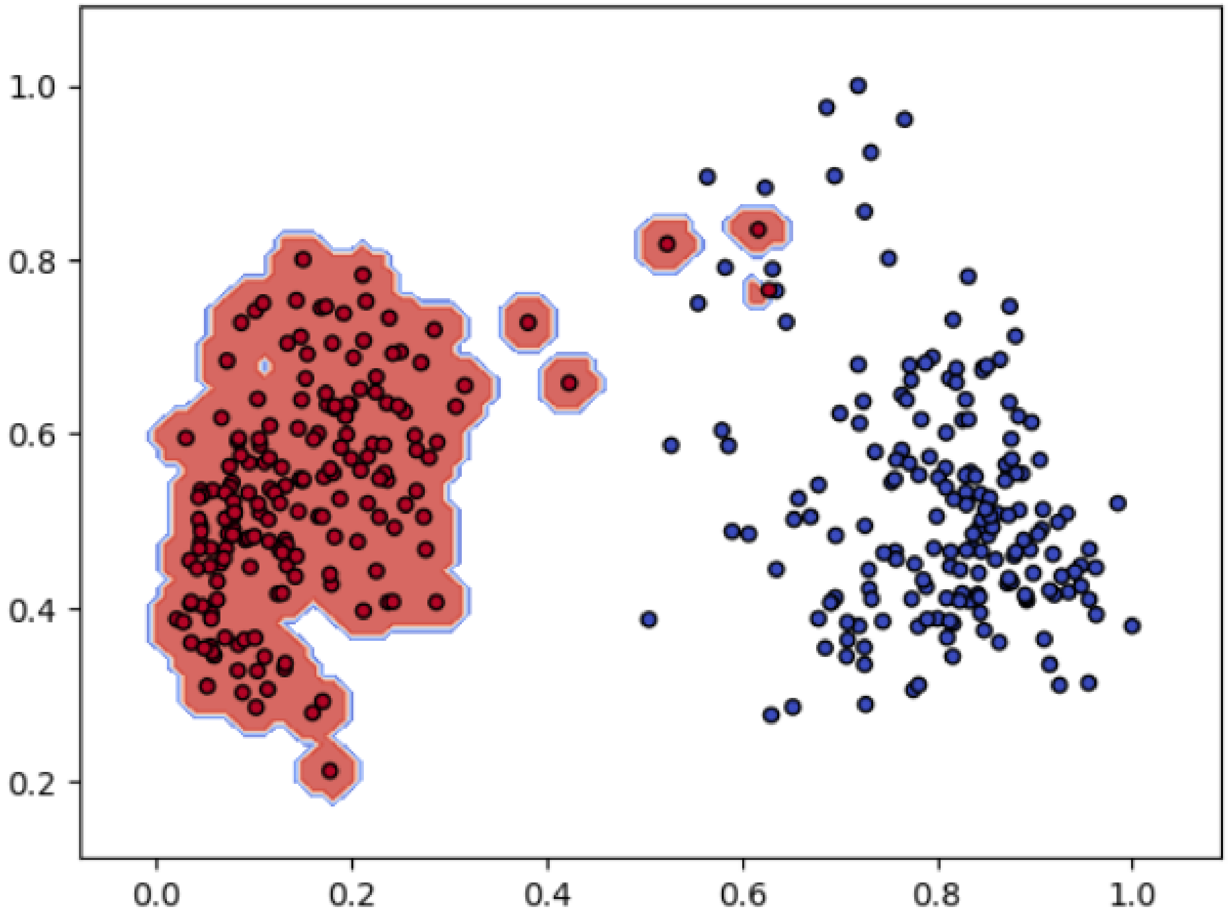




Quantum Support Vector Machine (QSVM)



Quantum Kernel result



RBF Kernel result

Summary

- Two main quantum algorithms—namely QPE and HHL—were explained in detail.
- These algorithms are the building blocks of many quantum applications, making it essential to understand their operations.
- QSVM was briefly introduced to demonstrate how QPE and HHL can serve as such building blocks.
- In the last two lectures, we have only just begun to explore the surface of quantum mechanics. I hope you have gained a solid foundation to explore this topic further on your own in the future.