国際融合科学論/先端融合科学論

LECTURE 05
Quantum Mechanics II: Quantum Machine Learning

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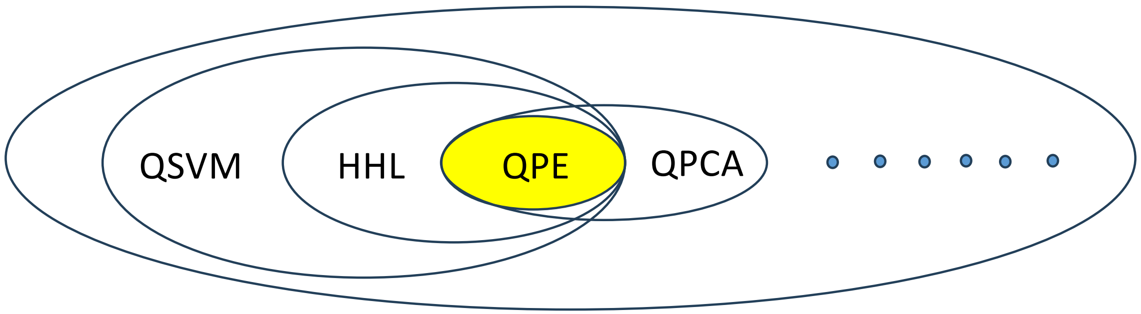
Lecture Outline

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

Quantum Machine Learning: why QPE?

- QPCA and QSVM are the quantum counterparts of PCA and SVM.
- The QPE algorithm is a fundamental building block for many quantum algorithms, including QPCA and QSVM.
- The QPE algorithm is a versatile and powerful tool in quantum computing, enabling a wide 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.

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

- Eigen vector
- Eigen value

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.

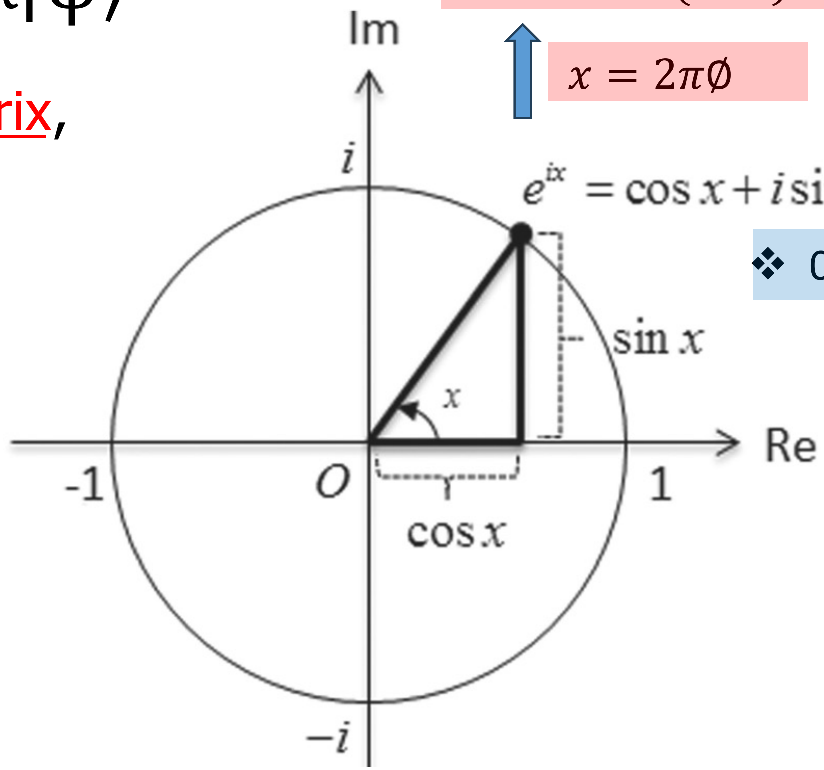
$$U|\psi\rangle = \lambda|\psi\rangle$$

❖ $0 \leqq \emptyset \leqq 1$

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

$x = 2\pi\emptyset$

❖ $0 \leqq x \leqq 2\pi$



- 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

Quantum Phase Estimation: beginning

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

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

- The phase, ∅, is in the range between 0 and 1, which has a decimal format (∅).
- QPE is to estimate the phase, ∅, 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 $\emptyset_n \in \{0,1\}$

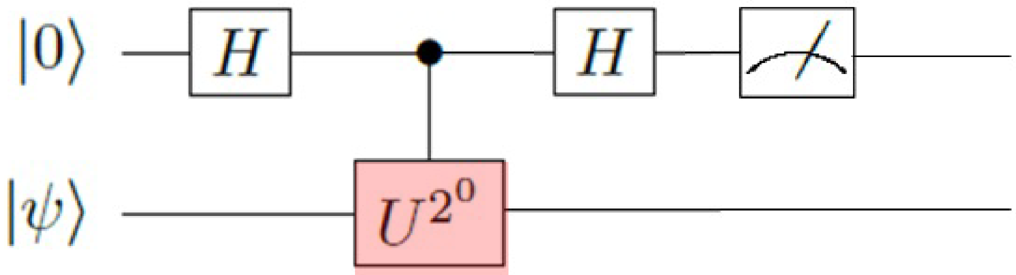
$$0.11_2 = 0.75_{10}$$

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

0.11_2 $\quad$ 0.75_{10}

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 $|\psi\rangle$.

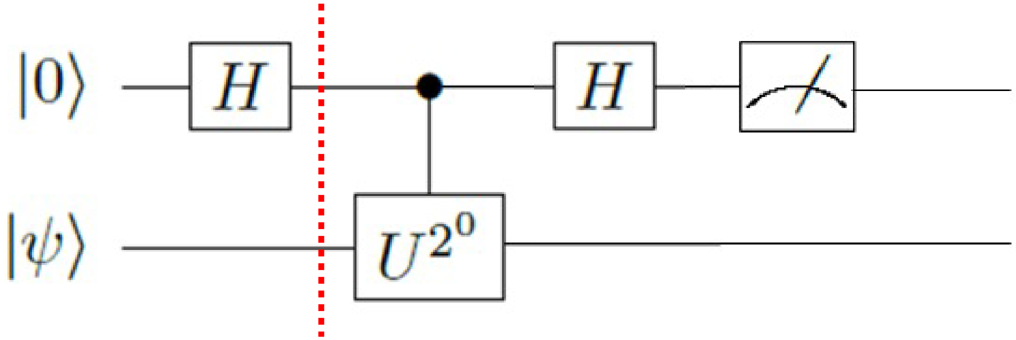
$$U|\psi\rangle = \lambda|\psi\rangle \longrightarrow U|\psi\rangle = e^{2\pi i \emptyset}|\psi\rangle$$

Eigen value (λ) — Phase (∅)

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

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

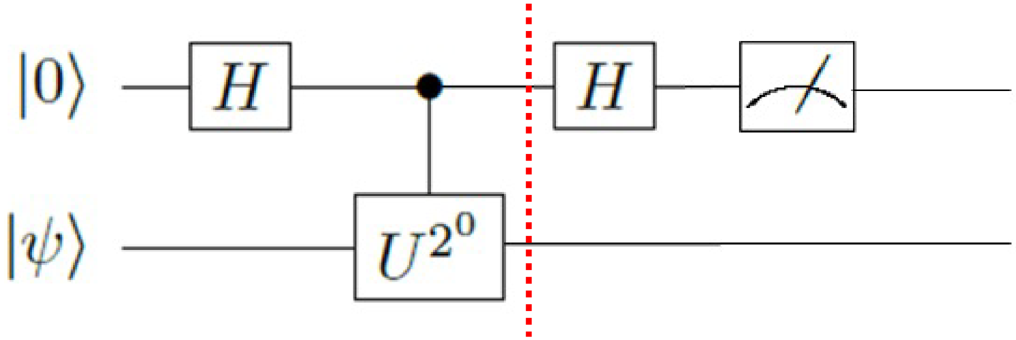
Quantum Phase Estimation: toy example



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

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

Quantum Phase Estimation: toy example



- control qubit
- target qubit

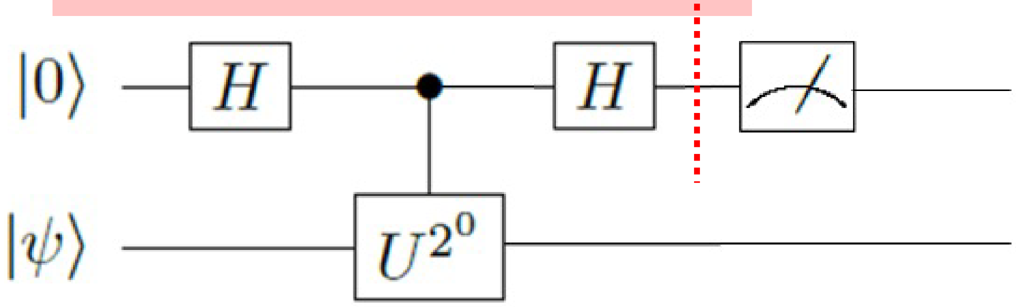
$$|+\rangle \otimes |\psi\rangle$$
$$= |0\rangle|\psi\rangle + |1\rangle|\psi\rangle$$

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

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

Quantum Phase Estimation: toy example

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



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

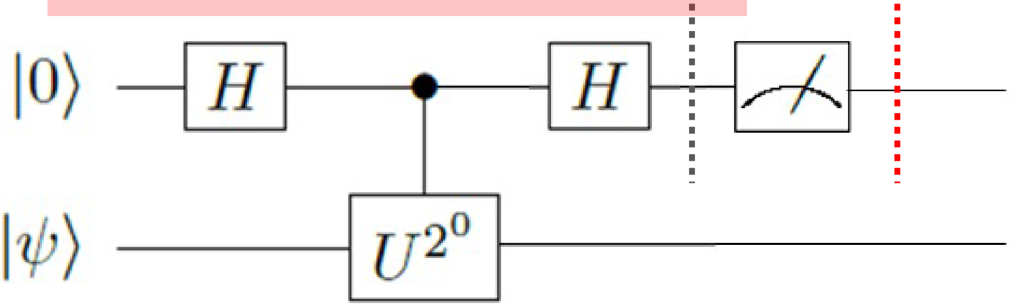
$$= H|0\rangle + H|1\rangle e^{2\pi i 0.\phi_1}$$

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

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

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 ($\emptyset$) becomes either 0 or ½,
- The eigen value ($e^{2\pi i\emptyset}$) becomes either 1 or -1

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

General Quantum Circuit for QPE

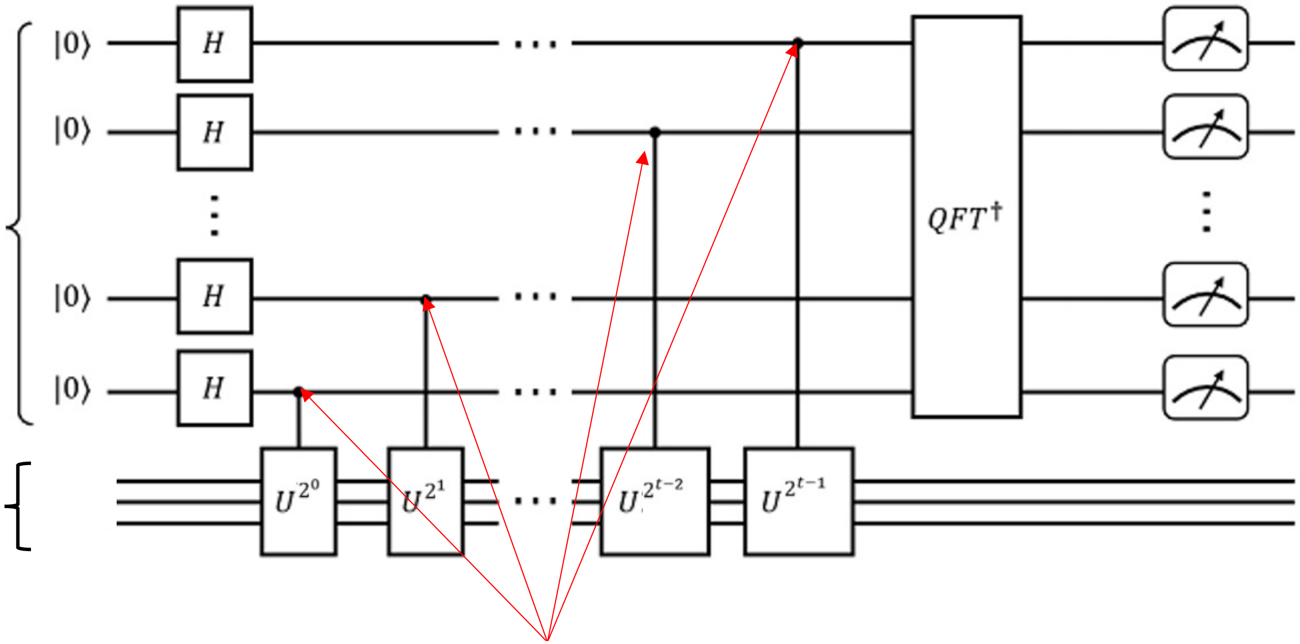
Quantum Phase Estimation: general quantum circuit

Counting register

"t" input qubits

"t" determines the accuracy of the estimation

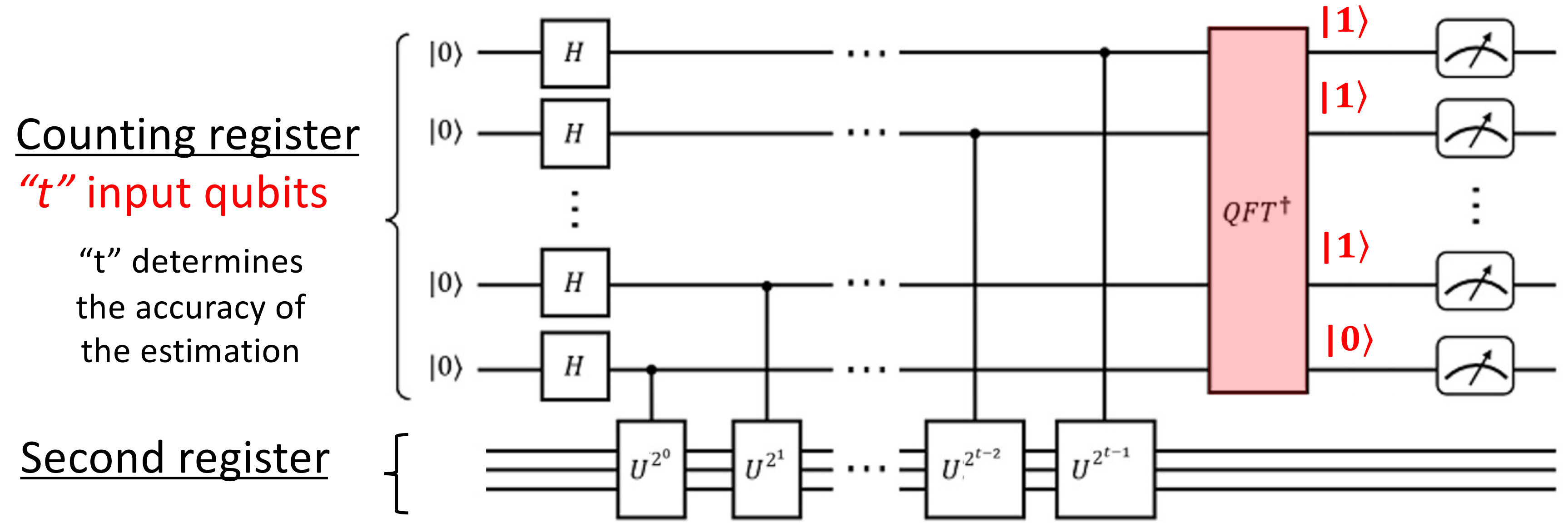
Second register



The phase of U matrix is "kickback" to *t* qubits

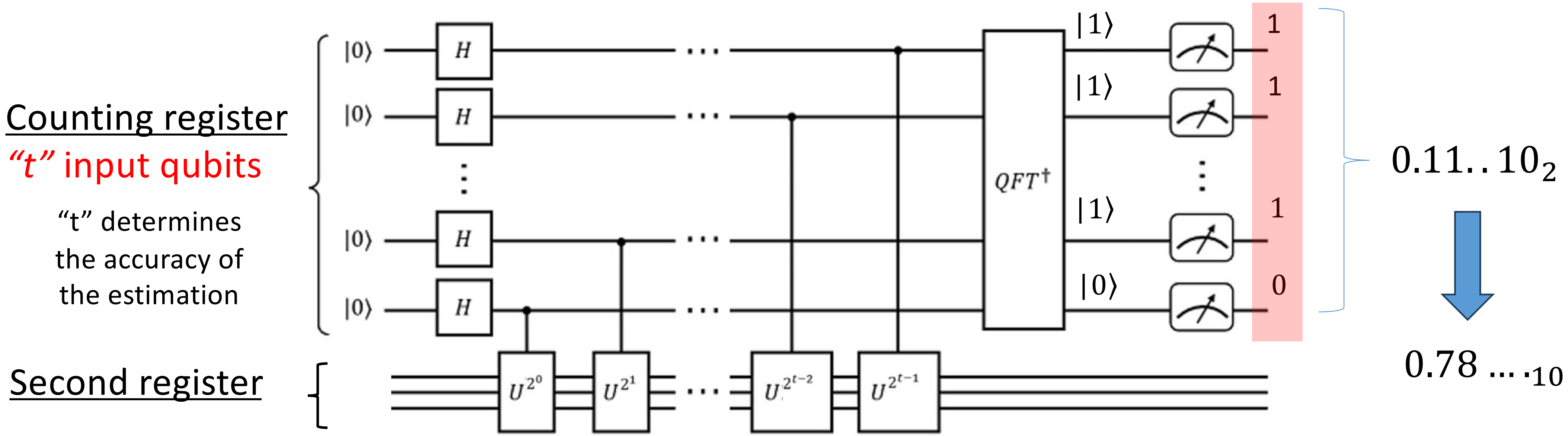
- The quantum phase estimation algorithm uses phase kickback to write the phase of U to the t qubits in the counting register.

Quantum Phase Estimation: general quantum circuit



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

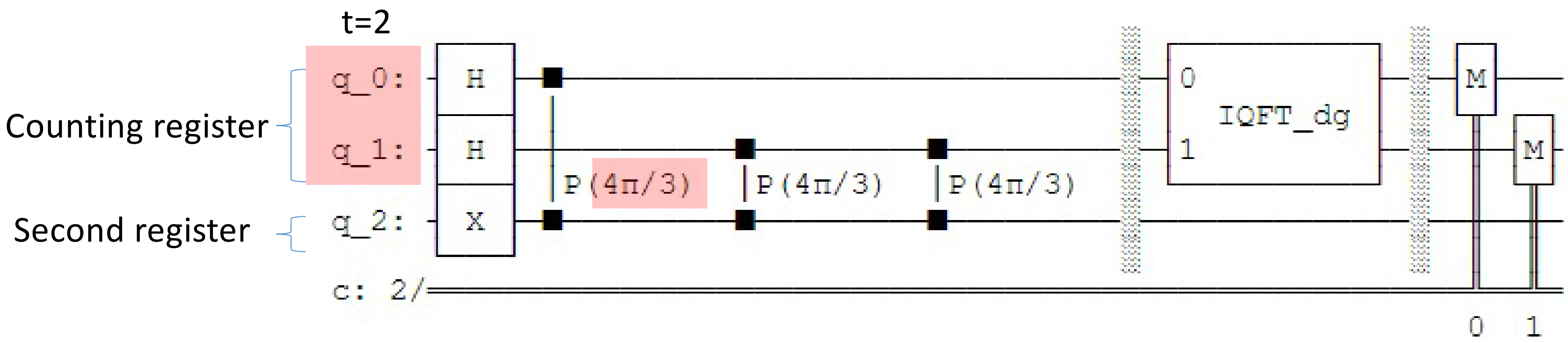
Quantum Phase Estimation: general quantum circuit



- 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)



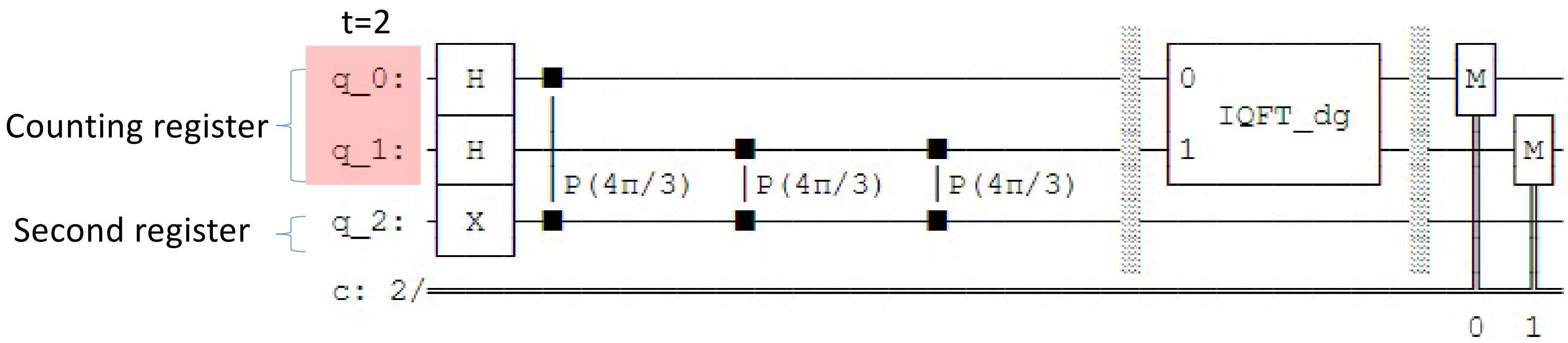
- Creating the circuit above to estimate the phase of a unitary operator U which is equivalent to estimate θ below.

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

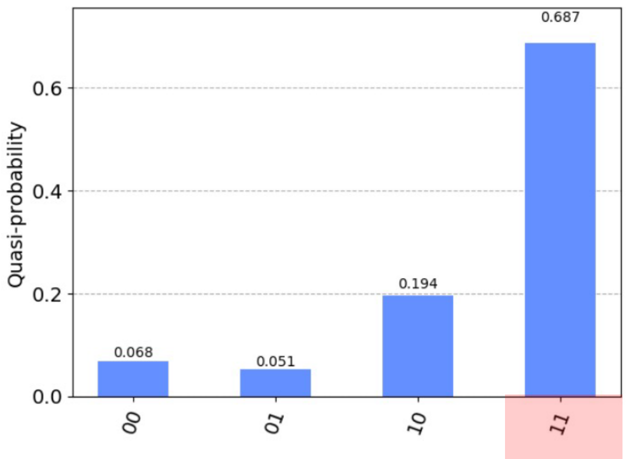
- Assume that the phase of the unitary matrix U is $4\pi/3$. In other words, the quantum phase estimation algorithm will find the value θ below.

$$2\pi\theta = 4\pi/3 \longrightarrow \theta = 2/3 \longleftarrow$$ The answer we expect

Quantum Phase Estimation: Qiskit implementation (t=2)



- The exact solution is "θ =2/3 ($4\pi/3$)" in decimal number.
- The result is approximately "11", which corresponds to 3/4 in decimal form.



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

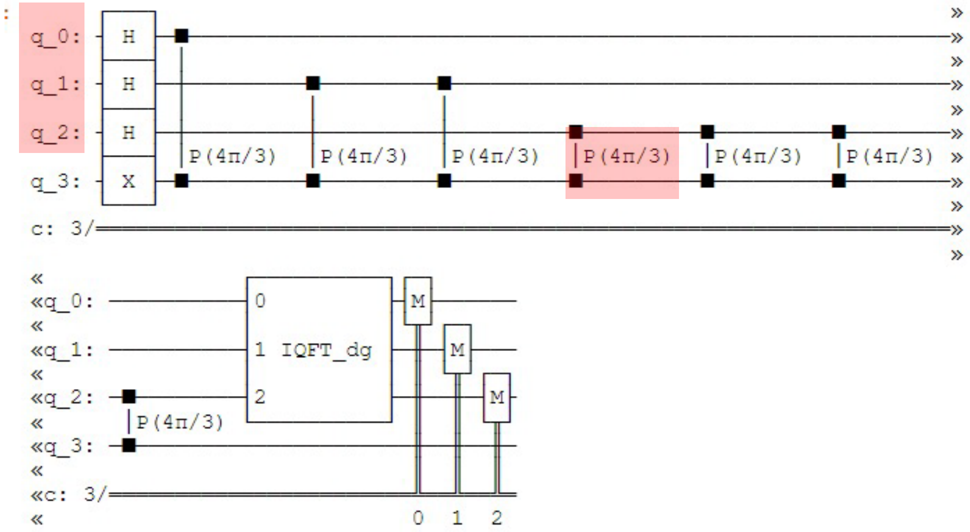
$\emptyset_k$: each digit in binary

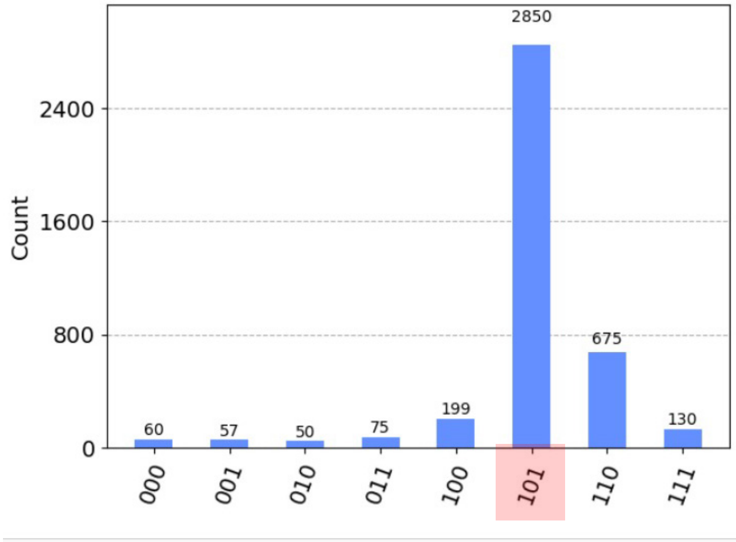
$\theta = 0.11_2 = 0.75_{10}$

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

Quantum Phase Estimation: Qiskit implementation (t=3)

t=3



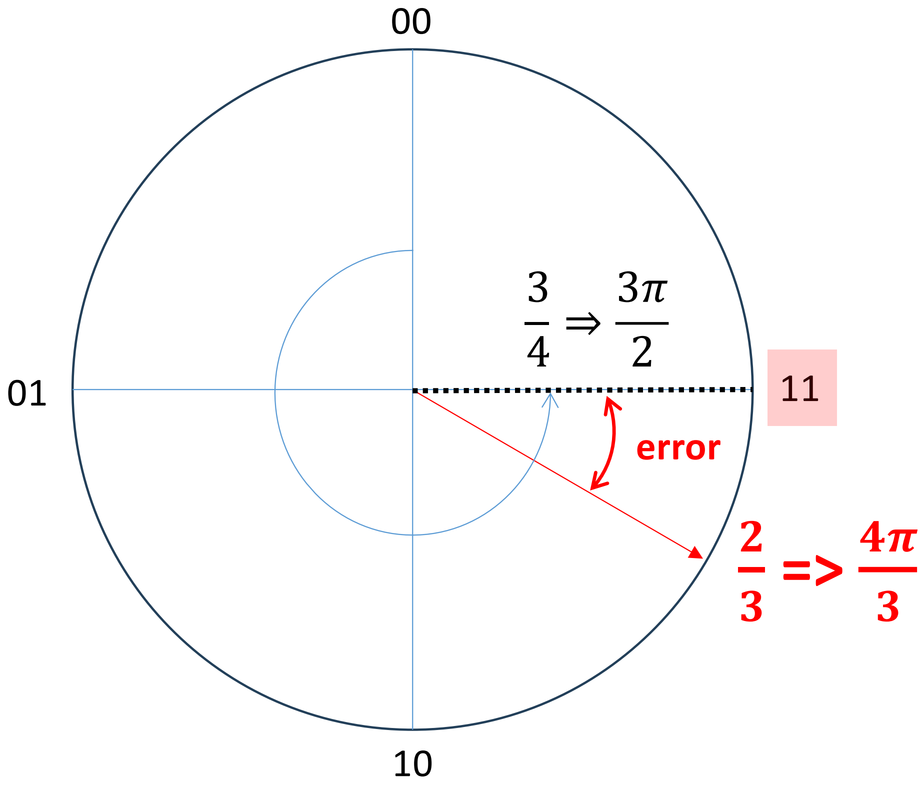


$$\theta = 0.101_2 = 0.625_{10}$$

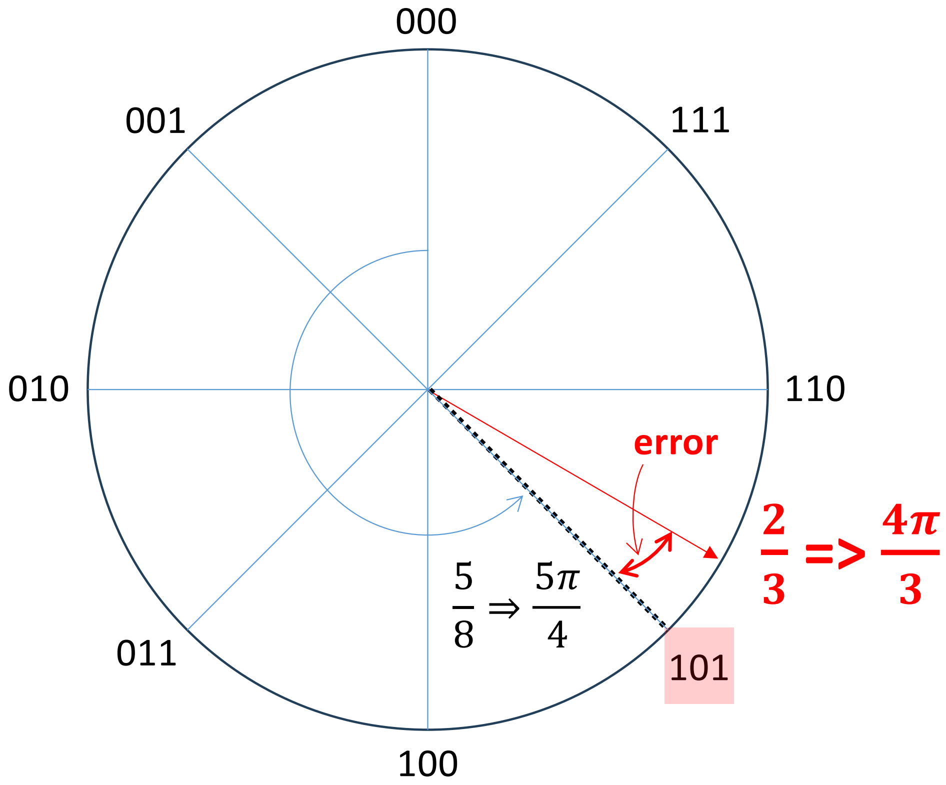
$$1*2^{-1} + 0*2^{-2} + 1*2^{-3} = 5/8$$

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

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



t=2



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.

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

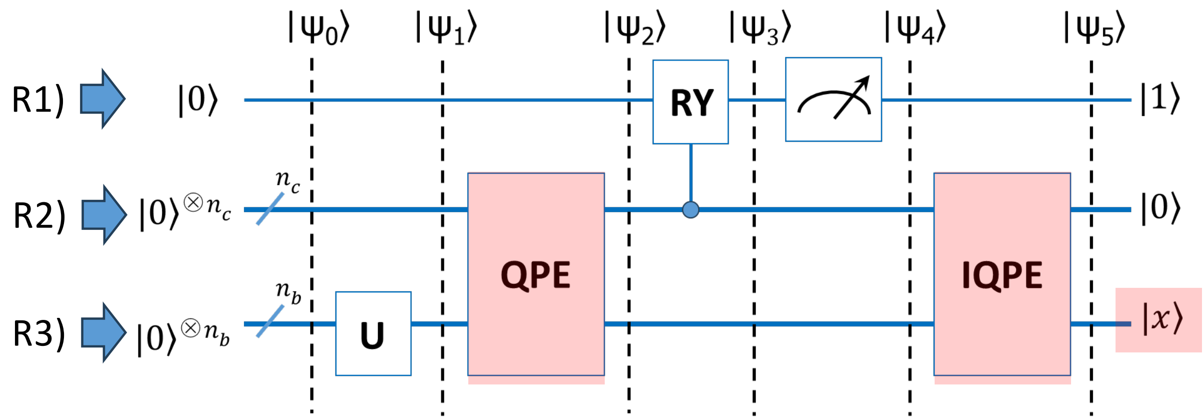
- Theoretically speaking, the HHL algorithm achieves an exponential improvement compared to the classical algorithm to solve the problem.
  - Quantum algorithm (HHL)

    $O(\log(N)\, s^2\kappa^2/\varepsilon)$
    - 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): 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



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

Quantum Support Vector Machine (QSVM)

Quantum Support Vector Machine (QSVM) with HHL

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Quantum Support Vector Machine for Big Data Classification

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[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.

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

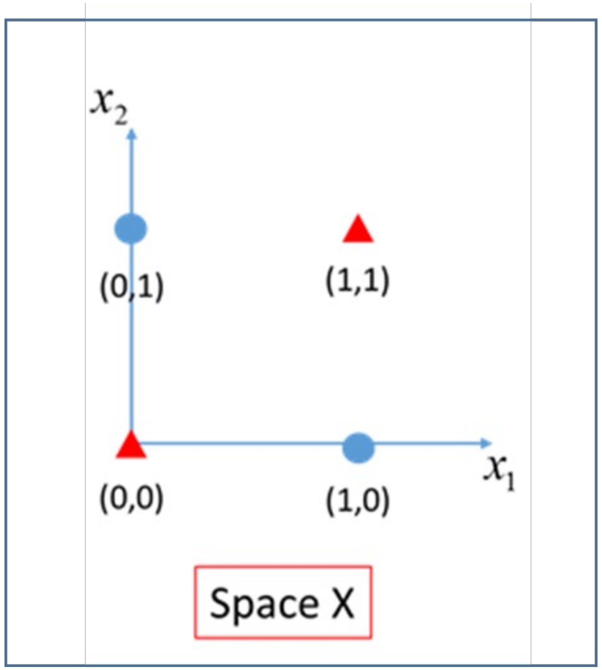
  - Then, we can apply the Harrow-Hassidim-Lloyd (HHL) algorithm to handle SVM, which is called "QSVM"!!

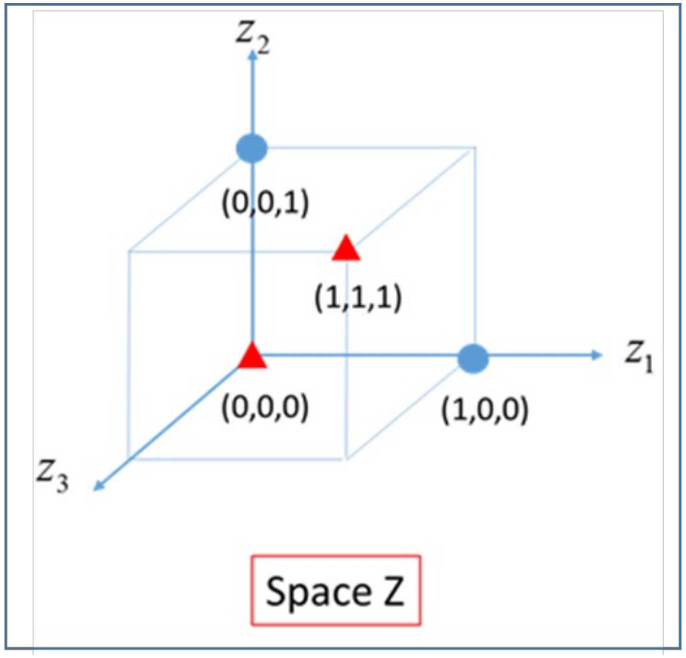
Quantum Support Vector Machine (QSVM) with QKernel

- We formulated SVM as a quadratic programming before…

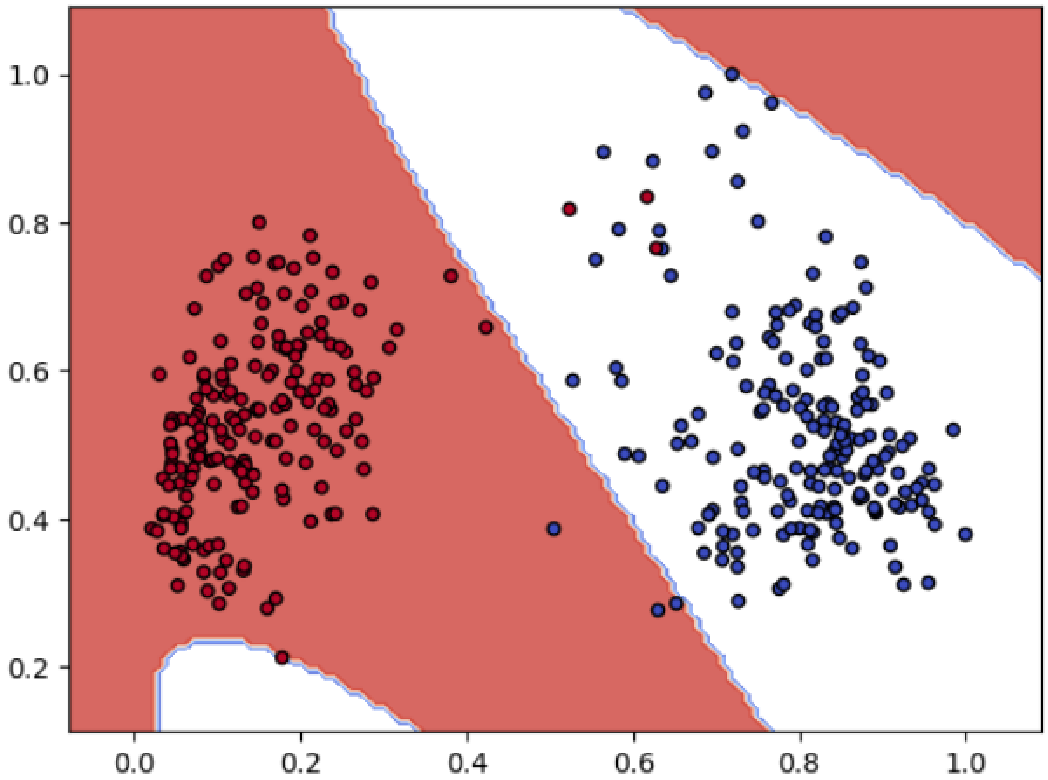
$$\min_{\lambda} \quad L(\lambda) = \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} t_n t_m \lambda_n \lambda_m \mathrm{K}(\mathrm{x}_n^T \mathrm{x}_m) - \sum_{n=1}^{N} \lambda_n$$

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

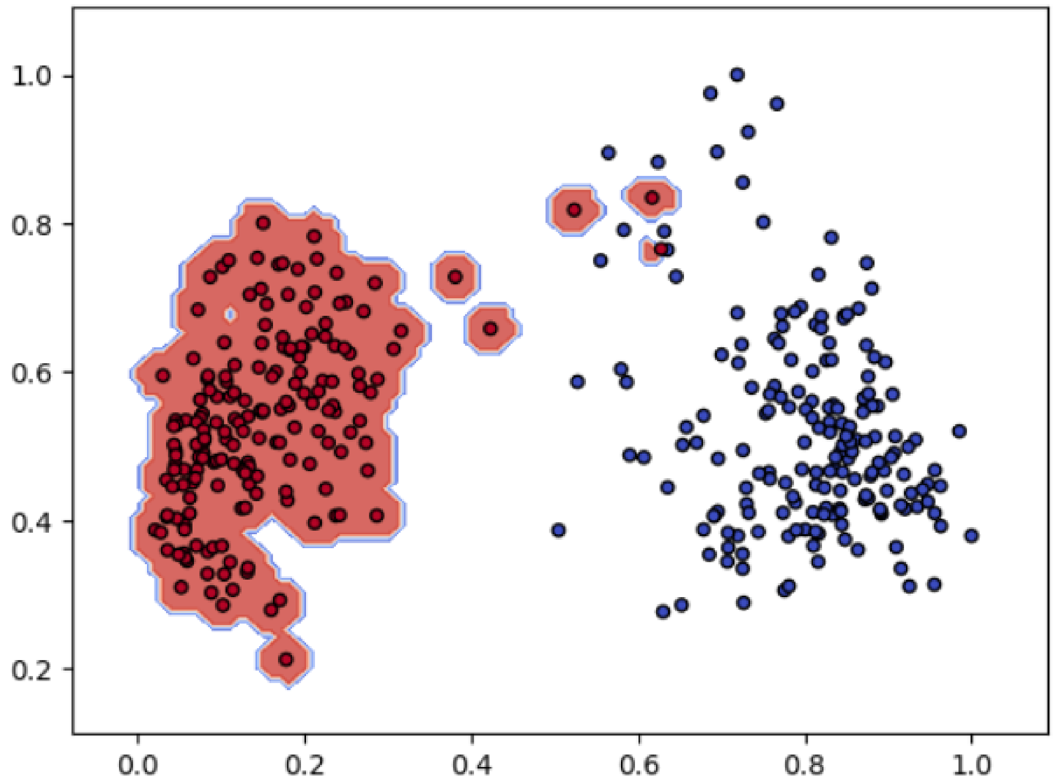




Quantum Support Vector Machine (QSVM)



Quantum Kernel result



RBF Kernel result

Summary

- The QPE was explained in detail.
- It is the building block 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.