Quantum Principal Component Analysis

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A report on

Quantum Principal Component Analysis

by,

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Abstract

Principal Component Analysis is a dimension reduction technique. In this project, the quantum version of the technique is studied named Quantum Principal Component Analysis (qPCA). Quantum Singular Value Threshold (qSVT) is a quantum version of Singular Value Threshold, which filters the singular values (eigenvalues) of a given matrix. Thus, with the help of qSVT used as a subroutine, qPCA is performed and depending on the threshold condition, eigenvalues are extracted and filtered. First, qPCA of two different cases of matrix (2x2 and 4x4) are studied and then the method is applied to an 8x8 diagonal matrix.

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Chapter 1

Introduction

In this chapter, a detailed explanation of supporting material is provided. Starting with PCA, SVD and then Phase Estimation and inverse fourier transform to extract eigenvalues. Then a necessary requirement is the Hamiltonian simulation, which can be achieved easily if the matrix is diagonal and with the help of SVD, can be achieved for off-diagonal matrix. At the end of this chapter, various quantum gates that are used in the simulation are mentioned and its decomposition to fundamental quantum gates.

1.1 Principal Component Analysis (PCA)

Principal Component Analysis or PCA is a method used to evaluate the principal component(s) of a given data set. The data set contains values of variables. An nxn correlation matrix is created from the values where n represents total number of variables.

Given a correlation matrix, principal components are the set of unit vectors where the i^{th} vector is orthogonal to the first i-1 vectors. For d dimension, we have d vectors. The vector has a property that it best fits the given data set meaning the average squared distance from the points to the vector is minimized. The vectors are the eigen vectors of the given data set. Higher eigenvalue represents that the corresponding vector has high variance.

Sometimes, vectors with low eigenvalue are discarded because those vectors has less variance.

As an example consider the following case (Figure 1.1): For the given correlation matrix, the two vectors that best fit the given data set are shown. Principal Components are the two vectors v_1 and v_2 with correlation being 5 and 1 respectively. [1]

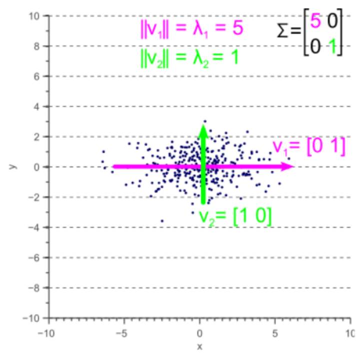


Figure 1.1: Data set and it's principal components

1.2 Singular Value Decomposition (SVD)

SVD is used to compute eigenvalues (singular values) of a given matrix. SVD extract eigen vectors and corresponding eigenvalues of a given matrix. Given a matrix **A**, it's SVD is given as [2]

$$A = UMV^*$$

Where, M is a diagonal matrix with entries are eigenvalues of matrix A and are called singular values. Matrix U and V^* has the following property:

$$U^*U = I, \quad V^*V = I$$

If matrix is a square matrix with dimension m by n, then matrix U has dimension m by m, M has dimension m by n and V has the dimension of n by n.

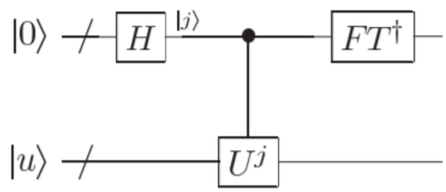
1.3 Phase Estimation and Inverse QFT

Let $|\psi\rangle$ be eigenvector of operator A with eigenvalue λ. Thus, $A|\psi\rangle = \lambda|\psi\rangle$. Thus, $e^{iAt}|\psi\rangle = e^{i\lambda t}|\psi\rangle$.

After performing Inverse Fourier Transform, λ upto a certain approximation will be in the state $|\frac{\lambda t}{2\pi}\rangle$. To get $|\lambda\rangle$ t is taken as 2π. [3]

Now, if $\lambda = \lambda_1\lambda_2...\lambda_t$, in binary then for $U = e^{2\pi i A/2^t}$, so that the corresponding eigenvalue will be $e^{2\pi i\lambda/2^t} = e^{2\pi i 0.\lambda_1\lambda_2...\lambda_t}$.

Complete Phase Estimation process is shown below:
In the figure above, for example let's say there 3 qubits are required to store the eigenvalues. And the form of k^{th} eigenvalue in binary is $\lambda_k = \lambda_1\lambda_2\lambda_3$. And the operator U has eigenvalue $e^{2\pi i\lambda/2^3} = e^{2\pi i 0.\lambda_1\lambda_2\lambda_3}$. Then the operators U^2 and U^4 has eigenvalues $e^{2\pi i\lambda/2^2} = e^{2\pi i 0.\lambda_2\lambda_3}$ and $e^{2\pi i\lambda/2} = e^{2\pi i 0.\lambda_3}$ respectively.



If the 3 qubits $|q_0q_1q_2\rangle$ are controlled qubits with operator U, U^2 and U^4 respectively then. after applying phase estimation procedure, $|q_0q_1q_2\rangle$ will have the form:

$|q_0q_1q_2\rangle = (|0\rangle + e^{2\pi i 0.\lambda_1\lambda_2\lambda_3}|1\rangle) \otimes (|0\rangle + e^{2\pi i 0.\lambda_2\lambda_3}|1\rangle) \otimes (|0\rangle + e^{2\pi i 0.\lambda_3}|1\rangle)$.

After applying inverse fourier transform depending on the orientation of qubits, the state will be: $|q_0q_1q_2\rangle = |\lambda_3\lambda_2\lambda_1\rangle$.

1.4 Decomposition and matrix exponentiation

Any 2x2 unitary matrix A can be decomposed as, $A = e^{i\theta_1}R_z(\theta_2)R_y(\theta_3)R_z(\theta_4)$, [4]

$$A = \begin{pmatrix} e^{i\theta_1} & 0 \\ 0 & e^{i\theta_1} \end{pmatrix} \begin{pmatrix} e^{\frac{-i\theta_2}{2}} & 0 \\ 0 & e^{\frac{i\theta_2}{2}} \end{pmatrix} \begin{pmatrix} cos\frac{\theta_3}{2} & -sin\frac{\theta_3}{2} \\ sin\frac{\theta_3}{2} & cos\frac{\theta_3}{2} \end{pmatrix} \begin{pmatrix} e^{\frac{-i\theta_4}{2}} & 0 \\ 0 & e^{\frac{i\theta_4}{2}} \end{pmatrix}$$

If matrix A is only diagonal matrix, then it's exponentiation e^{kA} (k is constant) is [6],

$$A = \begin{pmatrix} a_1 & 0 & \dots & 0 \\ 0 & a_2 & \dots & 0 \\ \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \dots & a_n \end{pmatrix}, \text{ then } e^{kA} = \begin{pmatrix} e^{ka_1} & 0 & \dots & 0 \\ 0 & e^{ka_2} & \dots & 0 \\ \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \dots & e^{ka_n} \end{pmatrix}$$

For any square matrix A, A can be decomposed as $A = QMQ^{-1}$, where M is a diagonal matrix with entries are eigenvalue of matrix A and matrix Q's i^{th} column is the i^{th} eigenvector of matrix A.

If a matrix A has off diagonal elements, then it's eigenvalue decomposition is $A = QMQ^{-1}$ and [5]

$$e^{kA} = e^{kQMQ^{-1}}$$

$$e^{kA} = 1 + kQMQ^{-1} + \frac{(kQMQ^{-1})^2}{2!} + \frac{(kQMQ^{-1})^3}{3!} + \dots$$

$$e^{kA} = 1 + kQMQ^{-1} + \frac{(kQMQ^{-1})(kQMQ^{-1})}{2!} + \frac{(kQMQ^{-1})(kQMQ^{-1})(kQMQ^{-1})}{3!} + \dots$$

$$e^{kA} = 1 + kQMQ^{-1} + \frac{Qk^2M^2Q^{-1}}{2!} + \frac{Qk^3M^3Q^{-1}}{3!} + \dots$$

$$e^{kA} = Q(1 + kM + \frac{k^2M^2}{2!} + \frac{k^3M^3}{3!} + \dots)Q^{-1}$$

$$e^{kA} = Qe^{kM}Q^{-1}$$

1.5 QASM Simulator

The simulation is performed on QASM Simulator. The simulator emulates the given circuit like on a real device and returns result with certain error. The noisy simulator is used because the real quantum computers don't perform on 100 % fedility.

1.6 General way to initialize a quantum state for desired probabilities

This method output state $|\psi_2\rangle$ from a state $|\psi_1\rangle$ for n qubits, where $|\psi_1\rangle = |00...0\rangle$ and $|\psi_2\rangle = \sum_i \sqrt{p_i}|i\rangle$, where i $\in \{0,1\}^n$.

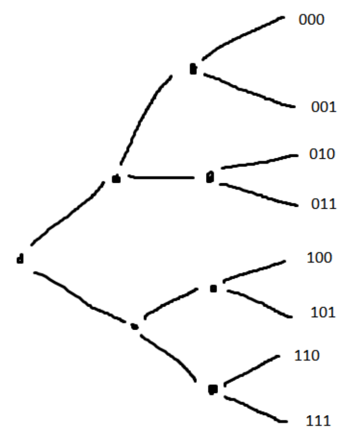


Figure 1.2: Initialization to superposition of quantum states

The main gate that is used is $R_y(\theta)$, where $R_y(\theta) = \begin{pmatrix} cos\frac{\theta}{2} & -sin\frac{\theta}{2} \\ sin\frac{\theta}{2} & cos\frac{\theta}{2} \end{pmatrix}$

$R_y(\theta)|0\rangle = cos\frac{\theta}{2}|0\rangle + sin\frac{\theta}{2}|1\rangle$.

$R_y(\theta)|1\rangle = -sin\frac{\theta}{2}|0\rangle + cos\frac{\theta}{2}|1\rangle$.

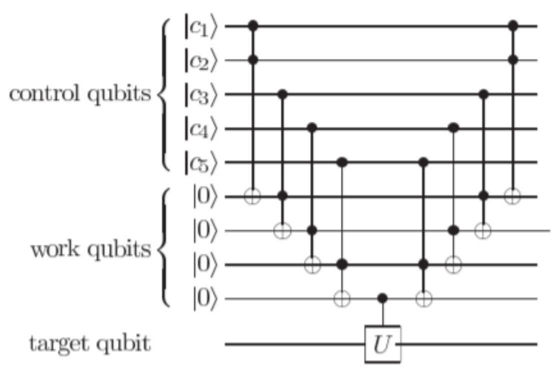
So, if the initial state is $|00...0\rangle$, then by applying successive rotations on Y axis with different angles, one can get the superposition with desired probabilities. The condition is that the probability of the parent branch is the sum of the probabilities of the states that emerge from that.

Consider for example of 3 qubits initialized as 000. After applying rotation about Y axis on the leftmost qubit, the state will split into 000 and 100 with certain probabilities.

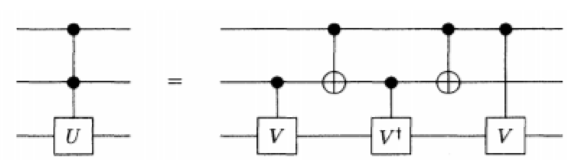
So, the probabilities of the two states should be equal to the probabilities of the parent branch that is 1.

1.7 Various Quantum Gates used and it's qiskit implementation

1. X gate, qiskit.x(q)
2. Controlled-X, qiskit.cx(c,t)
3. Controlled Controlled X (Toffoli Gate), qiskit.ccx(c1,c2,t)
4. Hadamard gate, qiskit.h(q)
5. Phase gate: $R(\theta) = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\theta} \end{bmatrix}$, qiskit.p($\theta$,qubit)
6. Controlled-$R_x(\theta)$=qiskit.cu3(θ,-$\pi/2$,$\pi/2$,c,t)
7. Controlled-$R_y(\theta)$=qiskit.cu3(θ,0,0,c,t)
8. Controlled-Z gate, Z=HXH, C-Z=$(I \otimes H)(C \otimes X)(I \otimes H)$
9. Multi qubit controlled X gate. There is no default implementation of this gate. This gate can be decomposed into 2 qubit gates as follows: (Where U=X) [6]



10. Two qubit controlled U gate can be decomposed as ($U = VV^\dagger$) [7]:



Chapter 2

Algorithm

The algorithm studied [8] is an exact algorithm meaning upon performing it gives an exact result rathar then approximate result, which is an improvement over algorithm represented in [9] this paper. Both algorithms are based on Quantum Singular Value Threshold (qSVT).

Both algorithms only differ in the initialization matrix and controlled operation. Algorithm in section 2.1 is just for reference and algorithm in section 2.2 is studied thoroughly and examples in chapter 3 are based on algorithm mentioned in section 2.2 only.

2.1 Improved algorithm for qPCA (only qSVT part) [9]

For a matrix A_0 whose singular value decomposition is $A_0 = UMV = \sum_{k=1}^{T} \sigma_k u_k v_k$, where σ_k is eigenvalue of A_0, u_k and v_k are left and right singular value vectors. Let $A = A_0^2$, then the SVD of A is $A = \sum_{k=1}^{T} \sigma_k^2 u_k u_k$.

The complete algorithm as in the paper:

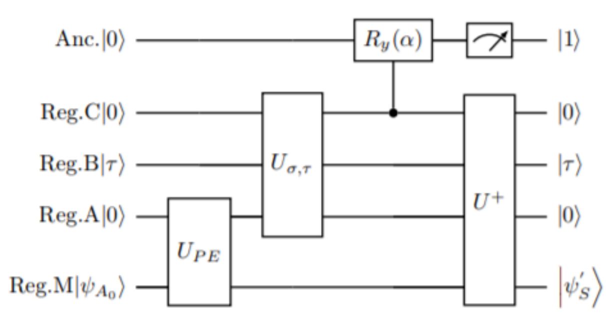


Figure 2.1: qSVT part

- Input: Quantum state $|\psi_{A_0}\rangle$, threshold constant τ and unitary operation $U_{PE} = e^{iAt}$, where $A = A_0 A_0^\dagger$.
- Output: Quantum State $|\psi_4\rangle$.

1. Preparing quantum state: $|\psi_1\rangle = (a|0\rangle + b|1\rangle)|00\rangle|\psi_A\rangle$.

   If the top qubit is 0, then qSVT is performed. qSVT method is described as follows:

2. Phase Estimation U_{PE}: $|\psi_2\rangle = |00\rangle \sum_{k=1}^{T} \sigma_k|\sigma_k^2\rangle|u_k\rangle|v_k\rangle$. (Total eigenvalues are T.)

3. Unitary Operation $U_{\sigma,\tau}$ (where τ is threshold for eigenvalues):
   $|\psi_3\rangle = |0\rangle \sum_{k=1}^{r} \sigma_k|y_k\rangle|\sigma_k^2\rangle|u_k\rangle|v_k\rangle$.

   Where, $|y_k\rangle = |1 - \frac{\sigma_k}{\tau}\rangle$, and for negative values, $|y_k\rangle = |0\rangle$.

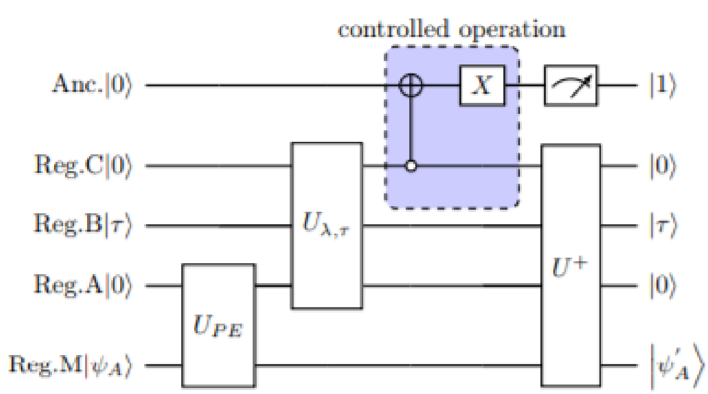
4. Applying Controlled Rotation
   $R_y(\alpha)$: $|\psi_4\rangle = \sum_{k=1}^{r} \sigma_k[sin(y_k\alpha|1\rangle) + cos(y_k\alpha)|0\rangle]|u_k\rangle|v_k\rangle$.

5. After inverse unitary operation and if after measurement of top qubit is 1 then, $|\psi_4\rangle = \sum_{k=1}^{r} \sigma_k sin(y_k\alpha)|u_k\rangle|v_k\rangle$.

2.2 Exact algorithm for qPCA [8]

The given algorithm has main 4 parts, 1st part is to initialize the given matrix into quantum state. 2nd part is the phase estimation part, where the eigenvalues of the initialized quantum state are extracted. 3rd part is Unitary Operation $U_{\sigma,\tau}$, changing eigenvalues to 0 if they are less than the given threshold and remains same if they are greater than the threshold. 4th, last step is the controlled rotation. In this step with the help of an ancillary qubit, the qubit is changed to 1 if there are non zero eigenvalues and remains 0 otherwise.

The complete algorithm as in the paper:



- Input: Quantum State: $|\psi_A\rangle$, threshold τ and Unitary operation $U_{PE} = e^{iAt}$

- Output: $|\psi_7\rangle$

1. Initialization: $|\psi_1\rangle = |000\rangle|\psi_A\rangle$. (Where A is a correlation matrix.)
2. Phase Estimation U_{PE}: $|\psi_2\rangle = |00\rangle \sum_{k=1}^{T} \lambda_k|\lambda_k\rangle|u_k\rangle|u_k\rangle$. (Total eigenvalues are T.)
3. Unitary Operation $U_{\lambda,\tau}$ (where τ is threshold for eigenvalues):
   $|\psi_3\rangle = |0\rangle \sum_{k=1}^{r} \lambda_k|y_k\rangle|\lambda_k\rangle|u_k\rangle|u_k\rangle \ + \ |0\rangle \sum_{k=r+1}^{T} \lambda_k|y_k\rangle|\lambda_k\rangle|u_k\rangle|u_k\rangle$.
   After the 3rd step, the eigenvalues which are lower than threshold τ will be 0.
4. Controlled Operation:
   $|\psi_4\rangle = \sum_{k=1}^{r} \lambda_k|1\rangle|y_k\rangle|\lambda_k\rangle|u_k\rangle|u_k\rangle \ + \sum_{k=r+1}^{T} \lambda_k \ |0\rangle|0\rangle|\lambda_k\rangle|u_k\rangle|u_k\rangle$.

   Where, $|y_k\rangle$=$|1 - \frac{\lambda_k}{\tau}\rangle$.
5. Inverse unitary operation:
   $|\psi_5\rangle = \sum_{k=1}^{r} \lambda_k|1\rangle|u_k\rangle|u_k\rangle \ + \sum_{k=r+1}^{T} \lambda_k \ |0\rangle|u_k\rangle|u_k\rangle$.
6. Measurement: When the measurement of the 1st qubit is 1, the state will collapse to $|\psi_6\rangle = \sum_{k=1}^{r} \lambda_k|u_k\rangle|u_k\rangle$.
7. After phase estimation: $|\psi_7\rangle = \sum_{k=1}^{r} \lambda_k|\lambda_k\rangle|u_k\rangle|u_k\rangle$

The circuit of $U_{\lambda,\tau}$ is quite complicated and lengthy because it outputs $|\lambda_k$ to $|1 - \frac{\lambda_k}{\tau}\rangle$. To achieve this, circuits of addition and multiplication are needed. One other way to achieve this is to simply map the $|\lambda_k\rangle$ to $|0\rangle$ if the eigenvalues are less than threshold constant if the eigenvalues are greater than threshold.

Chapter 3

Running algorithm on QASM Simulator

In this chapter, quantum circuit is created for each case and it is run on QASM simulator. In result section, result from qiskit and result from classical pca is little bit different because QASM simulator gives result upto certain error.

3.1 Implementation of a 2x2 matrix

The correlation matrix A = $\begin{pmatrix} 1.5 & 0.5 \\ 0.5 & 1.5 \end{pmatrix}$. A total of 5 qubits are required to perform qPCA.

3.1.1 Initialization (Step 1)

2 qubits are required to initialize the matrix as a quantum state. Qubits q_3 and q_4 are taken to initialize. Here, in the pair q_4 is the most significant qubit. The normalized state can be written as:

The order in the initialization state of quantum circuit can be written as:
$|\psi_S\rangle = |q_4 q_3\rangle$.

$|\psi_S\rangle = \frac{1}{\sqrt{5}}(1.5|00\rangle + 0.5|01\rangle + 0.5|10\rangle + 1.5|11\rangle) = [0.6708,\ 0.2236,\ 0.2236,\ 0.6708]$.
$|00\rangle$, before doing anything.

The complete circuit for initialization is shown in fig 3.1.
$\frac{1}{\sqrt{2}}(|00\rangle + |10\rangle)$, after applying hadamard gate to 2nd qubit.

Now, from the 1st state $0.707|00\rangle$, states $0.6708|00\rangle + 0.2236|01\rangle$ can be created with the help of R_y gate. $0.707(I \otimes R_y)(\theta)|00\rangle = 0.707 * cos(\frac{\theta}{2})|00\rangle + 0.707 * sin(\frac{\theta}{2})|01\rangle$. Angle $\theta = 0.643$ (in radians) can be found by comparing the co-efficient. To peform a controlled gate, 1st qubit is zero and $cR_y(\theta, c, t) = cU3(\theta, 0, 0, c, t)$

Similarly, $0.2236|10\rangle + 0.6708|11\rangle$, can be obtained, with $\theta = 2.5$ radians.

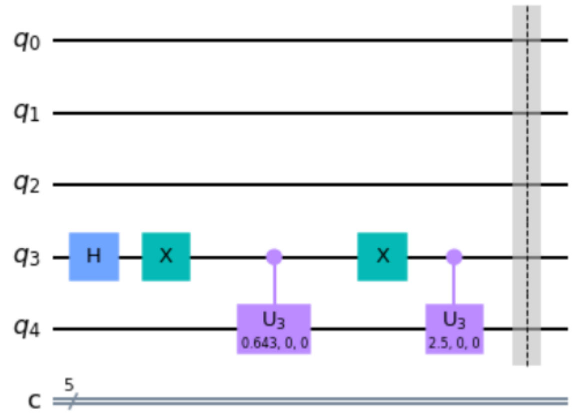


Figure 3.1: Circuit of state initialization

3.1.2 Phase Estimation (Step 2)

Eigenvectors and eigenvalues of the matrix A are:

$|u_1\rangle = \begin{pmatrix} -1 \\ 1 \end{pmatrix}$, $\lambda_1 = 1$ and $|u_2\rangle = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$, $\lambda_2 = 2$, so total 2 qubits are required to represent eigenvalues (01_2 and 10_2).

As mentioned above, for controlled-U operation, $U = e^{\frac{2\pi i A}{4}}$. For 2 qubits $U_1 = U$ and $U_2 = U^2 = e^{\frac{2\pi i A}{2}}$ gates are required.

From eigenvalue decomposition, matrix A can be decomposed as:

$$A = QMQ^{-1} = \begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix} \begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix}^{-1}$$

Exponentiation of A to get U_1 and decomposition of U_1

Exponentiation:

$$U_1 = e^{\frac{2\pi i A}{4}} = Qe^{\frac{2\pi i M}{4}}Q^{-1} = \begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} e^{\frac{2\pi i}{4}} & 0 \\ 0 & e^{\frac{4\pi i}{4}} \end{pmatrix} \begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix}^{-1}$$

$$U_1 = \begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} i & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix}^{-1} = \frac{-1}{2} \begin{pmatrix} 1-i & 1+i \\ 1+i & 1-i \end{pmatrix}$$

Unitary Decomposition of U_1: As mentioned above, U_1 can be written as (after finding 4 θ's):

$$U_1 = \begin{pmatrix} e^{i\frac{3\pi}{4}} & 0 \\ 0 & e^{i\frac{3\pi}{4}} \end{pmatrix} \begin{pmatrix} e^{-i\frac{\pi}{4}} & 0 \\ 0 & e^{i\frac{\pi}{4}} \end{pmatrix} \begin{pmatrix} cos\frac{\pi}{4} & -sin\frac{\pi}{4} \\ sin\frac{\pi}{4} & cos\frac{\pi}{4} \end{pmatrix} \begin{pmatrix} e^{i\frac{\pi}{4}} & 0 \\ 0 & e^{-i\frac{\pi}{4}} \end{pmatrix}$$

Exponentiation of A to get U_2

$$U_2 = e^{\frac{2\pi iA}{2}} = Qe^{\frac{2\pi iM}{2}}Q^{-1} = \begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} e^{\frac{2\pi i}{2}} & 0 \\ 0 & e^{\frac{4\pi i}{2}} \end{pmatrix} \begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix}^{-1}$$

$$U_2 = \begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix}^{-1} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

If matrix W is composed of unitary matrices $W = XYZ$, then a controlled-W operation can be performed as controlled-Z then controlled-Y then controlled-X.

If matrix $M = e^{i\theta}I_2$, then controlled-M can be written as $N \otimes I_2$ [6], where

$$M = \begin{pmatrix} e^{i\theta} & 0 \\ 0 & e^{i\theta} \end{pmatrix} \text{ and } N = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\theta} \end{pmatrix}$$

$$\text{controlled-M}=N \otimes I_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & e^{i\theta} & 0 \\ 0 & 0 & 0 & e^{i\theta} \end{pmatrix}$$

Qubits q_1 and q_2 are used to store the eigenvalues. Here, in the pair q_2 is the most significant qubit and q_1 is the least significant qubit. Qubit order is $|q_2q_1\rangle$. The controlling qubit will get the most significant bit after the Inverse Fourier Transform if the controlling gate is U^2. In the circuit below 1st part is Phase Estimation till 1st barrier and inverse Fourier Transform between 1st and 2nd barrier.

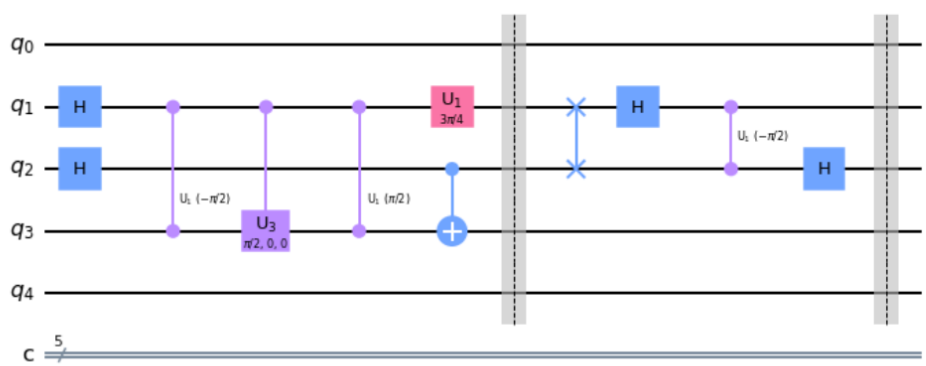


Figure 3.2: Circuit of Phase Estimation

3.1.3 Unitary Operation $U_{\sigma,\tau}$ (Step 3)

Applying operator $U_{\lambda,\tau}$ that is $U_{\lambda,\tau}|0\rangle|\lambda\rangle = |y_k\rangle|\lambda\rangle$, where λ is eigenvalue and $y_k = (1-\frac{\tau}{\lambda})_+ = max(0, 1-\frac{\tau}{\lambda})$ and τ is the threshold value for eigenvalues. Creating this kind of circuit is complex and requires too many gates, instead this circuit can be optimized. Then the function of $U_{\lambda,\tau}$ is change λ to 0 if $\lambda \leq \tau$ and do nothing if $\lambda > \tau$.

In this case $\lambda_1 = 1 = 01_2$ and $\lambda_2 = 2 = 10_2$ and by taking $\tau = 1$, then the task of $U_{\lambda,\tau}$ will be to make $\lambda_1 = 00_2$ and $\lambda_2 = 10_2$. The circuit below do this task.

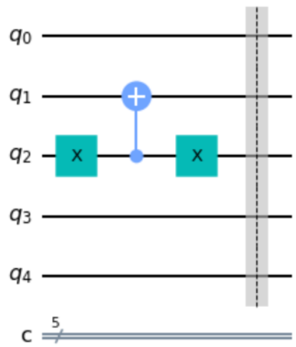


Figure 3.3: Optimized circuit of $U_{\lambda,\tau}$, for $\tau = 1$

3.1.4 Controlled Operation (Step 4)

This part uses one ancillary qubit as follows: Ancillary qubit changes to 1 if eigenvalues are non zero and remains constant if eigenvalues are 0. In the figure below q_0 is the ancillary qubit.

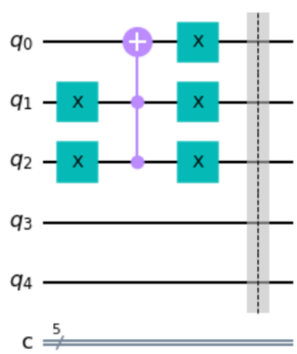


Figure 3.4: Circuit of Controlled Rotation

3.1.5 Result

After running the qPCA circuit, the final result is as follows: that is step 1 + step 2 + step 3 + step 4 + inverse of step 3 + inverse of step 2. From left to right in result, any state is in the order $|q_4q_3q_2q_1q_0\rangle$.

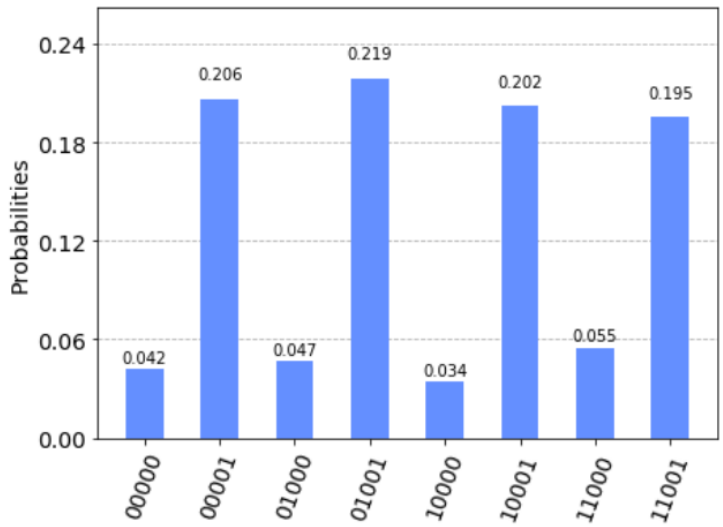


Figure 3.5: Result of qPCA of a 2x2 matrix

Interpretation of results step by step (order is $q_4q_3q_2q_1q_0$):

After the final state can be written as: $|\psi_1\rangle = \frac{\lambda_1}{\sqrt{\lambda_1^2+\lambda_2^2}}|u_1\rangle + \frac{\lambda_2}{\sqrt{\lambda_1^2+\lambda_2^2}}|u_2\rangle$.

Where, $\lambda_1 = 1$, $\lambda_2 = 2$, $|u_1\rangle = [-0.707, 0.707] \otimes [-0.707, 0.707]$ and $|u_2\rangle = [0.707, 0.707] \otimes [0.707, 0.707]$.

In the above results, states with states with probability 20% are eigenstates of eigenvalue 2. Thus, writing only the state with eigenvalue 2:

$|\psi_2\rangle = \sqrt{0.206}|00\rangle + \sqrt{0.219}|01\rangle + \sqrt{0.202}|10\rangle + \sqrt{0.195}|11\rangle$.

Normalizing the above state (i.e. dividing by 0.9066):

$|\psi_3\rangle = 0.5006|00\rangle + 0.5162|01\rangle + 0.4957|10\rangle + 0.4871|11\rangle$.

Classical PCA should yield: $\frac{2}{\sqrt{2^2}}|u_2\rangle|u_2\rangle = |\psi_3\rangle = 0.5|00\rangle + 0.5|01\rangle + 0.5|10\rangle + 0.5|11\rangle$.

3.2 Implementation of 4x4 matrix

The 4x4 matrix $A = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 3 \end{pmatrix}$, with eigenvalues 0, 1, 2 and 3 with eigen vectors are corresponding column vectors of matrix A. Total 8 qubits are required to perform qPCA in this case.

3.2.1 Initialization (Step 1)

There are total 16 entries in the matrix, so total 4 qubits are required to store 16 values. The initialization state can be written as:

$|\psi_S\rangle = \frac{1}{\sqrt{14}}(|0101\rangle + 2|1010\rangle + 3|1111\rangle)$, in the form of $|q_6q_5q_4q_3\rangle$.

Before doing anything qubit's state is $|0000\rangle$.

$I \otimes I \otimes I \otimes X|0000\rangle = |0001\rangle$.

Applying $R_y(2.6)$ on qubit q_6 will yield: $\frac{1}{\sqrt{14}}|0001\rangle + \frac{\sqrt{13}}{\sqrt{14}}|1001\rangle$.

Applying X gate on q_5 if q_6 is 0. Applying $cR_y(1.96)$ on q_5 with controlling qubit q_6 will yield $\frac{1}{\sqrt{14}}|0101\rangle + \frac{2}{\sqrt{14}}|1001\rangle + \frac{3}{\sqrt{14}}|1101\rangle$. The final state can be obtained after applying controlled x gates.

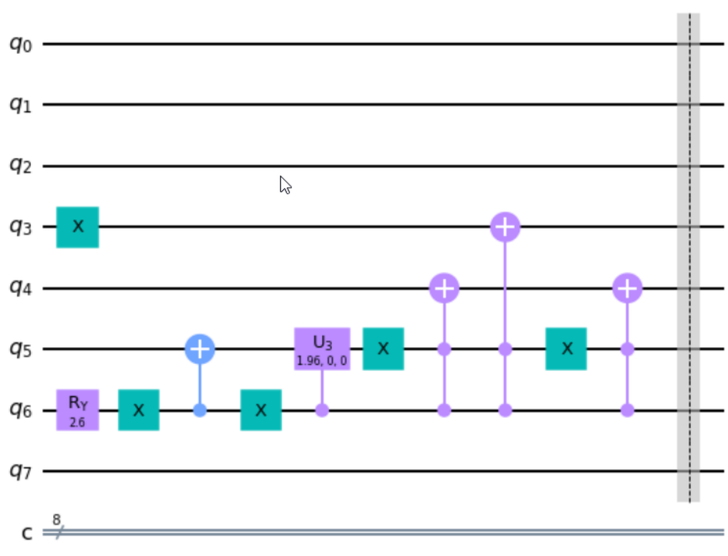


Figure 3.6: Quantum circuit of the initialization state

3.2.2 Phase Estimation (Step 2):

Two qubits are required for three eigenvalues. Qubits $|q_2q_1\rangle$ are used.

Two controlled $U = e^{\frac{2\pi i A}{4}}$ gates are applied. $cU_1 = U$ and $cU_2 = U^2$.

Matrix A is diagonal, so only matrix exponentiation is required.

$$U_1 = e^{\frac{2\pi i A}{4}} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -i \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} = Z \otimes S,\ S = \begin{pmatrix} 1 & 0 \\ 0 & e^{\frac{i\pi}{2}} \end{pmatrix}$$

$$U_2 = e^{\frac{4\pi i A}{4}} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = I \otimes Z.$$

The circuit below summarize the complete Phase Estimation Circuit.

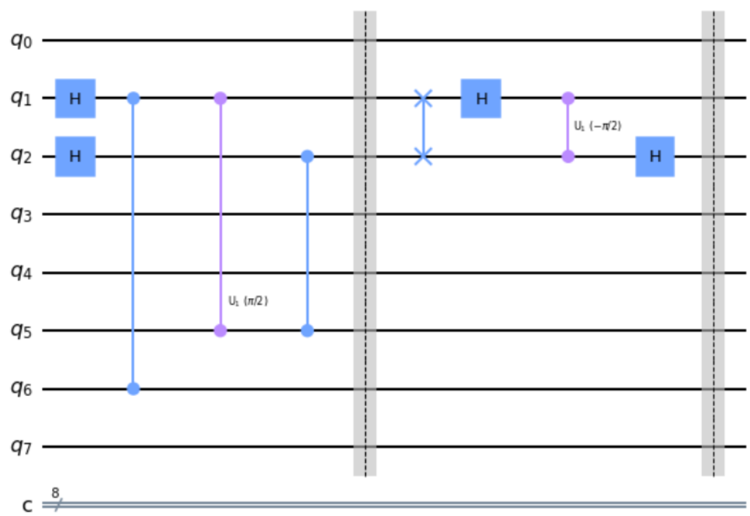


Figure 3.7: Quantum Circuit for Phase Estimation

3.2.3 Unitary Operation $U_{\sigma,\tau}$ (Step 3)

With $\tau = 1.8$, eigenvalue 1 will become 0 and eigenvalues 2 and 3 will remain same. Quantum circuit can be given as below. $|q_7\rangle$ is ancilla qubit. $|q_2q_1\rangle$ is qubit order. Eigenstate $|01\rangle$ will be changed to $|00\rangle$ and eigenstates $|10\rangle$ and $|11\rangle$ will remain same.

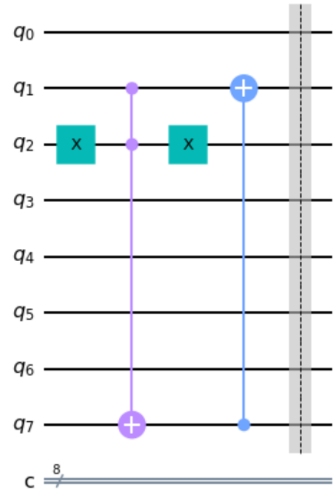


Figure 3.8: Circuit for eigenvalue Unitary Operation $U_{\sigma,\tau}$, for $\tau = 1.8$

3.2.4 Controlled Rotation (step 4)

This part uses one ancillary qubit as follows: Ancillary qubit changes to 1 if eigenvalues are non zero and remains constant if eigenvalues are 0. In the figure below q_0 is the ancillary qubit. So, for $\tau = 1.8$, ancillary qubit changes to 1 when eigenvalues are 11_2 and 10_2.

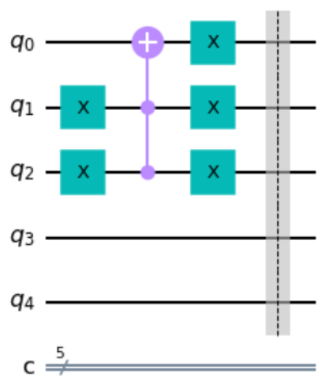


Figure 3.9: Circuit of Controlled Rotation

3.2.5 Result

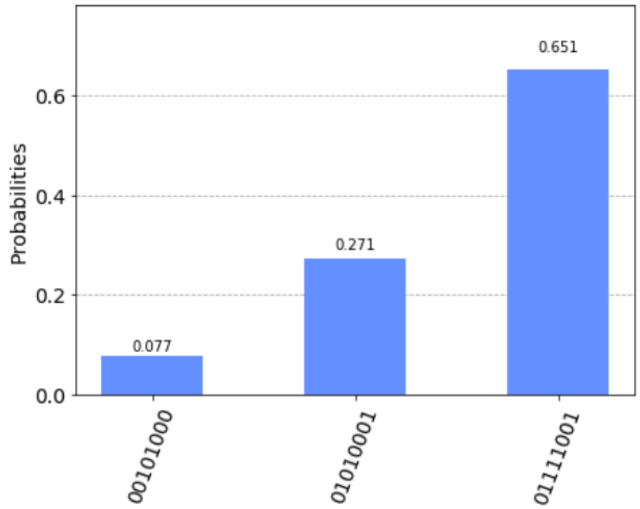


Figure 3.10: Result of qPCA of 4x4 matrix

As shown in 2x2 results, here with threshold being 1.8, thus eigenvalues 2 and 3 are considered. From left to right in result, any state is in the order $|q_7 \dots q_1 q_0\rangle$.

Writing the above result in the state form:
$|\psi_1\rangle = [0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ \sqrt{0.271}\ 0\ 0\ 0\ 0\ \sqrt{0.651}]$

Normalizing the above state (i.e. dividing by 0.9602):
$|\psi_3\rangle = [0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0.5422\ 0\ 0\ 0\ 0\ 0.8403]$

Classical PCA should yield: $\frac{2}{\sqrt{2^2+3^2}}|u_2\rangle|u_2\rangle + \frac{2}{\sqrt{2^2+3^2}}|u_3\rangle|u_3\rangle = |\psi_4\rangle$
$|\psi_4\rangle = [0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0.5547\ 0\ 0\ 0\ 0\ 0.8321]$.

3.3 Implementation of qPCA on 8x8 diagonal matrix

The 8x8 matrix is $A = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 5 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 6 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 7 \end{pmatrix}$ with eigenvalues 0 to 7 and eigenvectors are corresponding column of the matrix. A total of 14 qubits are required to perform particular eigenvalue threshold.

3.3.1 Initialization (Step 1)

A total of 64 states are required to store of which 7 states are non zero 57 states are zero. So, total of 6 qubits are required to store the matrix. Qubits $|q_9q_8q_7q_6q_5q_4\rangle$ are used for this purpose. In this order qubit q_9 is considered as highest value and q_3 has the lowest value.

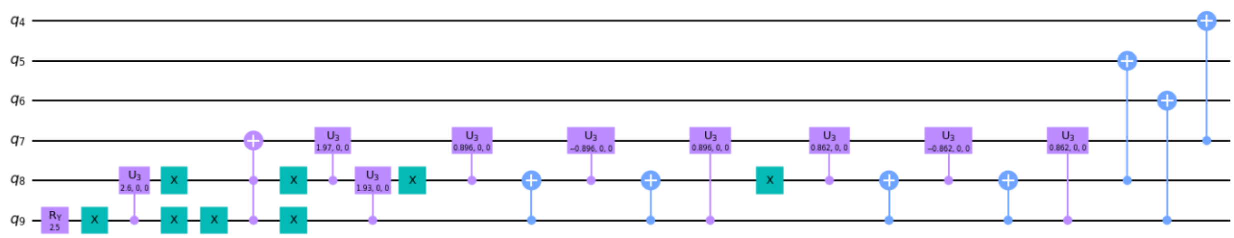


Figure 3.11: State initialization circuit

The required state is: $|\psi_1\rangle = \frac{1}{\sqrt{140}}(|001001\rangle + 2|010010\rangle + 3|011011\rangle + 4|100100\rangle + 5|101101\rangle + 6|110110\rangle + 7|111111\rangle)$, which can be achieved by applying controlled rotations to qubits.

The first rotation is $R_y(2.498)$ on q_9 so that the superposition $\sqrt{\frac{14}{140}}|000000\rangle + \sqrt{\frac{126}{140}}|100000\rangle$ will be created. Then rotating q_8 with certain angle while q_9 is $|0\rangle$ will create further required states. A series of rotations and cnot and toffoli gates will create the required state.

The complete quantum circuit is shown in the above figure.

3.3.2 Phase Estimation (Step 2)

The maximum eigenvalue is 7 which is 111_2 so total 3 qubits are required to store every eigenvalue. For this, the U gate is $U = e^{2\pi i A/2^3} = e^{2\pi i A/8}$.

For 3 controlled rotations, 3 gates are required, which are: U, U^2 and U^4. Which can be constructed as follows:

$$U = e^{2\pi i A/8} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & e^{i\pi/4} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & i & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & e^{i3\pi/4} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -e^{i\pi/4} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -i & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -e^{i3\pi/4} \end{pmatrix},$$

$$U = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi} \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/2} \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix}.$$

$$U^2 = e^{2\pi i A/4} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & i & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -i & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & i & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -i \end{pmatrix},$$

$$U^2 = \begin{pmatrix} 1 & 0 \\ 0 & e^{2\pi i} \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi} \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/2} \end{pmatrix}.$$

$$U^4 = e^{2\pi i A/2} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix},$$

$$U^4 = \begin{pmatrix} 1 & 0 \\ 0 & e^{2\pi i} \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & e^{2\pi i} \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi} \end{pmatrix}.$$

Qubits $q_3q_2q_1$ are used to store eigenvalues. With q_3 being highest value. The complete Phase Estimation circuit is shown in fig 3.12 with inverse quantum fourier transform.

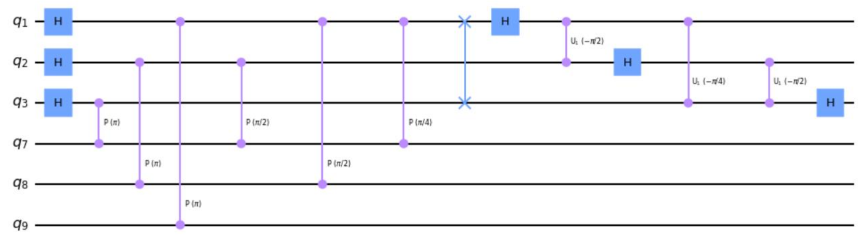


Figure 3.12: Phase estimation circuit

3.3.3 Unitary Operation $U_{\sigma,\tau}$ (Step 3)

The threshold $\tau = 3$ is taken so that the eigenvalues 1,2 and 3 will be mapped to 0 and eigenvalues 4, 5, 6 and 7 will remain constant. The quantum circuit that implements this operation is shown below.

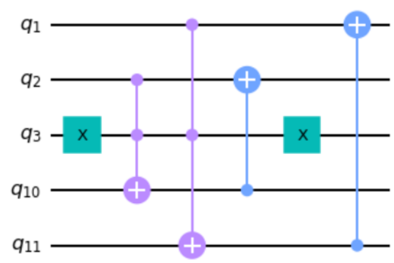


Figure 3.13: Eigenvalue Unitary Operation $U_{\sigma,\tau}$, for $\tau = 3$

3.3.4 Controlled Rotation (Step 4)

Qubit q_0 will change to 1 if eigenvalues are non zero and remain same if eigenvalues are 0. The quantum circuit that implements this operation is shown below. Where qubits $q_{12}q_{13}$ are ancilla qubits.

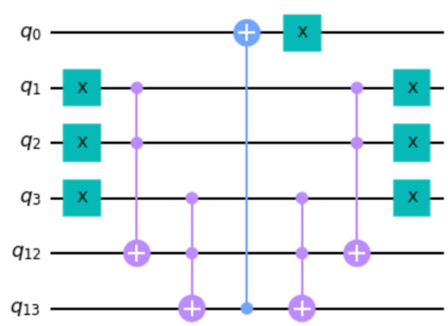


Figure 3.14: Controlled Rotation

3.3.5 Result

The final result is shown below:

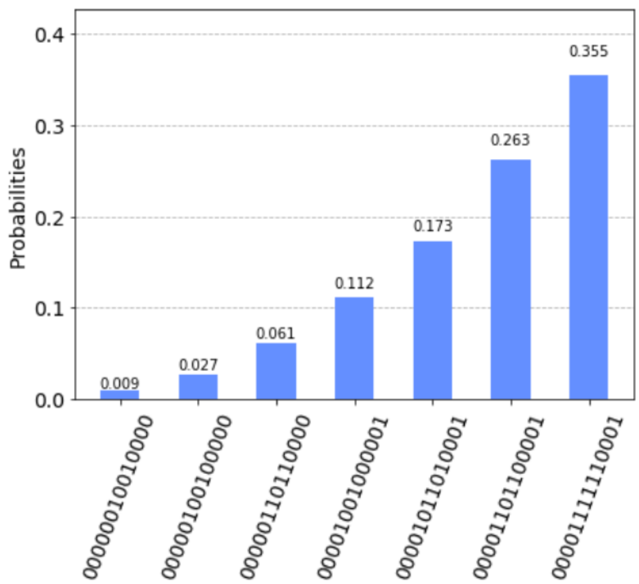


Figure 3.15: Result of qPCA on 8x8 matrix

Only considering quantum states with ancilla qubit 1,
$|\psi_1\rangle = \sqrt{0.112}|100100\rangle + \sqrt{0.173}|101101\rangle + \sqrt{0.263}|110110\rangle + \sqrt{0.355}|111111\rangle$, after normalizing the state,

$|\psi_2\rangle = 0.352|100100\rangle + 0.438|101101\rangle + 0.540|110110\rangle + 0.627|111111\rangle$.

And the expected state is:
$|\psi_3\rangle = \frac{1}{\sqrt{126}}(4|100100\rangle + 5|101101\rangle + 6|110110\rangle + 7|111111\rangle)$.

$|\psi_3\rangle = 0.356|100100\rangle + 0.445|101101\rangle + 0.534|110110\rangle + 0.623|111111\rangle$

Conclusion

In this project, the quantum version of Principal Component Analysis is studied. And the two examples are which were given in the research paper were performed on QISKIT successfully. And later on the algorithm is applied to an 8x8 matrix. The circuits for each case is run on QISKIT's QASM simulator. Because QASM simulator emulates the circuits like they are running on a real quantum computer, sone noise is present while measuring the qubits. So, that's why the final result is little deviated from the classical result. Here classical result means the output is calculated theoretically with 0 error.

The 4x4 and 8x8 matrices that are studied are diagonal, so the Hamiltonian simulation is quite simplified. So, the one can extend this work by simulating for the general case where the Hamiltonian have off diagonal elements.

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