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Original Article

Quantum Clustering Algorithm using the Wheel of Tomography

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Abstract - *A quantum k-means clustering algorithm is introduced by integrating the quantum paradigm to enhance the efficiency of the classical k-means algorithm. Firstly, each vector and k cluster centers are prepared to be in a quantum superposition, then utilized to compute the similarities in parallel. Secondly, the quantum amplitude estimation is applied to convert the similarities into the quantum bit. Finally, the most similar center of the vector is obtained from the qubits by using the quantum algorithm with the help of tomography to determine the minimum distances. Using the IBMQ simulator, completed the performance analysis for air pollution, which involved a two-dimensional dataset. The paper discussed a qk-means quantum clustering algorithm, which first maps the classical data into quantum states and performs distance calculation and updation using the quantum circuits. The paper proposed a general, parallelized, and competitive version of qk-means clustering, observing the outcomes of this performance analysis for multiple combinations of quantitative data series. Results show that the IBMQ simulator can overcome the classical k-means clustering problem of completion time and accuracy.*

Keywords - *Quantum Clustering, Quantum Machine Learning, Incremental Learning, Quantum Incremental learning, qk-means Algorithm.*

1. Introduction

Artificial Intelligence (AI) is a wide-range domain of Computer Science that makes machines act like a human brain. AI is apart from programming a Computer, but also about training it. Suppose there is a room, and a certain sensor is installed. The sensor analyzes the temperature and gives the output as an exact room temperature [1]. This is the way that confirms the system is artificially intelligent. Machine Learning (ML) comes like making ability without explicit programming. The model gives a certain threshold value, which proves the artificial working of the system [2]. In a different situation, where various attributes and aspects may arise, the machine has to do the analysis and provide accurate results. That means the machine can learn from its environment and get trained to work. If the environment has been altered, the model needs to put more attributes to training data. This type of attribute involves further knowledge, learning, and adequate action to enhance the device's intelligence. Certain kind of a structure of an animal comprises its shape, color, and different kind of curvatures in the interior. First, it should be attempted to discover features before their extraction, which may count on an individual's learning [2].

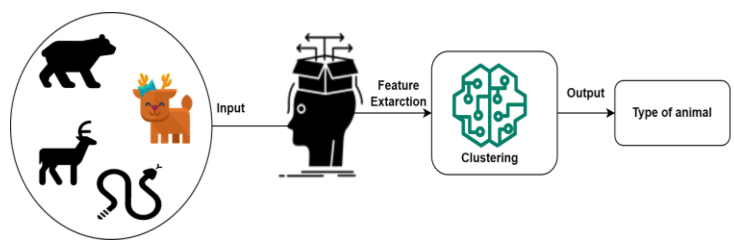

Fig. 1 Intelligent process using AI and ML for clustering the animals

ML offers solutions to several classes of problems intractable through conventional computing means. For example, solutions to classification problems and regression of large datasets based on ML techniques are more powerful than earlier solutions. These algorithms suffer in that they grow polynomial-wise with the size and dimension of the data, which leads to substantial run times when dealing with large datasets, coined "Big Data ."The capacity of data to be more capably stored and deployed in quantum states has recently led to the proposal of several quantum algorithms for ML [1],[4],[5],[9].

This paper discussed the advancement of a quantum k-means (qk-means) clustering algorithm with the help of tomography to classify clusters in data and compare them with analogous, not required, classical algorithms. The

algorithm counts on a distance measure, which has been taken to be Euclidean square distances. As shown in this paper, this distance can be calculated resourcefully on a quantum simulator to accelerate the algorithm as a whole.
Tasks performed by information processors in ML [1],[10] -

- Sorting
- Assembling
- Assimilating
- Classifying information [2]

In unsupervised learning, the model attempts to discover the concealed pattern in untagged data. The current studies emphasize specifically highlighting complications of large-scale Big Data, where the number of features is large for analysis [11]. Quantum information processors are used to accomplish the following to achieve results in Quantum Machine Learning (QML) -

- ML tasks
- Similarities in complex patterns [3]
- Adequate Learning process [4]
- Feedback Learning for Measurement [5]
- Classifiers [6]
- Quantum Support Vector Machines (QSVM) [8]

Illustration in the proposed paper-This paper shows that:

- QML can provide exponential speedups over classical computers for various learning tasks.
- ML is about deploying and categorizing an enormous size of data.
- Inner product, distance estimation, and sampling between vectors are exponentially hard in classical computers compared to the quantum platform.
- Tomography is used to find the correct state at the time of measurement to improve the accuracy of a cluster [4],[16].
- The problem of assigning N-dimensional vectors to the cluster of C states takes time O(log(MCN)) on a quantum simulator.
- QML can offer an exponential speedup for problems concerning big quantum data.
- Quantum version of k-means using adiabatic algorithm analyze V vectors into C clusters in O(ClogCVN).

Algorithm Implementation of the algorithm through quantum circuits can offer improved outcomes on the IBM quantum simulator. Considering the difficulty of execution, it is measured as the total number of quantum gates that are essential for circuit building [3]-[4]. The proposed paper discovers the quantum implementation of k-means clustering on the IBM Q simulator. This paper proposes the following contributions:

1) An algorithm calculates distances from a combination of quantum gates and updates the clusters as per the requirement.
2) Cluster assignment is done with the quantum circuit. And measurement is analyzed by the look of tomography to achieve high efficiency and accuracy.
3) The result shows that the tomography is also useful for achieving a benchmark completion time of the quantum algorithms.

2. Background

2.1. Quantum Computing Basics

Every qubit is initialized in a $|0\rangle$ state. Applying operations to process initial state quantum has various single and two-qubit gates. The measurement is required to fetch the results. The measurement interacts with a quantum simulator which has classical input/output, and then it throws the output as a bit string [12]. The block sphere is used to represent qubit as a vector which can be at any point on the block sphere [18]. The quantum gates can be used to rotate the qubits on the block sphere. The basic principle of quantum mechanics is a superposition (also known as a linear combination of quantum states) which is represented by Dirac notation (See Equation (1)).

$$|\psi\rangle = A|0\rangle + B|0\rangle \text{ ------------- } (1)$$

Where $|\psi\rangle$ is an arbitrary state vector in Hilbert space. A and B are probability amplitude (See Equation (2)). The basis state is $|0\rangle$ and $|1\rangle$. $|0\rangle$ state represents the spin up, and $|1\rangle$ state represents the spin down.

$$|\psi\rangle = |A|^2 + |B|^2 \text{ ---------- } (2)$$

Where Equation (2) shows probabilities ($|A|^2$ and $|B|^2$) of quantum measurement for coming to a state, due to the quantum mechanics principle, any particle can be in a single state or multiple states simultaneously. The following (See Equation (3)) probability amplitude in the matrix represents a qubit.

$$\begin{bmatrix} A \\ B \end{bmatrix} \text{ ---------------------------- } (3)$$

A Series of qubits can be shown in the following form (see Equation (4))

$$\begin{bmatrix} A1 \\ B1 \end{bmatrix} \begin{bmatrix} A2 \\ B2 \end{bmatrix} \begin{bmatrix} A3 \\ B3 \end{bmatrix} \text{-------} \begin{bmatrix} An \\ Bn \end{bmatrix} \text{ ------------ } (4)$$

Moreover, the state $|0\rangle|1\rangle$ can represent by bit form in a matrix (See Equation (5))

$$|0\rangle = \begin{bmatrix}1\\0\end{bmatrix} \quad |1\rangle = \begin{bmatrix}0\\1\end{bmatrix} \text{----------(5)}$$

The 00101101eight bit string can be represented in the following way (See Equation (6))

$$\begin{bmatrix}1\\0\end{bmatrix}\begin{bmatrix}1\\0\end{bmatrix}\begin{bmatrix}0\\1\end{bmatrix}\begin{bmatrix}1\\0\end{bmatrix}\begin{bmatrix}0\\1\end{bmatrix}\begin{bmatrix}0\\1\end{bmatrix}\begin{bmatrix}1\\0\end{bmatrix}\begin{bmatrix}0\\1\end{bmatrix} \text{-----------(6)}$$

2.2. Quantum Machine Learning

Use of Machine Learning in the extensive fields-

- The cumulative accessibility of data sets and the prerequisite of extracting patterns from data that has propagated the advantage of learning in the extensive fields [19].
- Its comprehensive mathematical foundations have accepted the expansion of dependable applications in diverse problems, in academic and commercial applications.

Benefits of Quantum methods application-

- The merging of learning algorithms with quantum models has highlighted extensive applications in every sector [18].
- Some recent works have analyzed quantum methods' provision of alternative learning representations.
- The computational speedup of the ML algorithm gives accurate predictions [20]. Fig2 and Fig3 show the workflow of stages of models. Classical ML and Quantum ML have different modes of input data. The Quantum model needs to have a compatible data format. The quantum data is to be preferred by the QML model. Then the input data is allocated to the quantum state and processed on a quantum circuit. But starting phase in most models followed a downgrading of the computational complexity.

These different types map to quantum processes in general and the suitability of each kind of learning to different environments [5],[7], [9][22],. There have been a lot of works in that I used classical ML to solve certain challenging quantum problems. For example, in quantum chemistry, the trained graph neural networks predict the property of a molecule, resulting in 105 times speedups. In quantum physics, solving the ground state of local Hamiltonian using the restricted Boltzmann machine. Classical ML is used to forecast and simulate the chaotic behavior that results in billion times of speedup. However, all the works are mostly heuristic to apply classical ML to the quantum data and then analyze the results. The Quantum model has input x on the classical vector. Encode x into the quantum state, then apply unitary applications. After applying unitary operations, measure some observables [22]. It is a model that takes a classical vector and produces a real number as an output. This corresponds to all the computations that can be done on quantum platforms. Fig3 process shows the theory of knowledge discovery phases of the QML model from Encoding to Measurement.

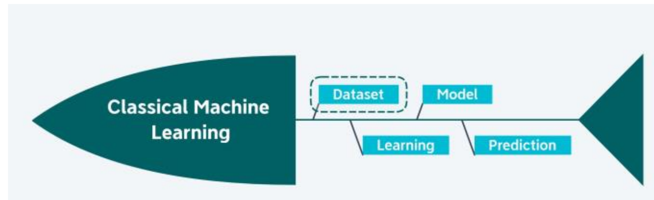

Fig. 2 Workflow of classical machine learning model

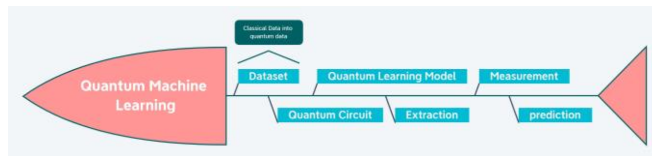

Fig. 3 Workflow of quantum machine learning model

2.3. Quantum Clustering

The field of Quantum Information Processing (QIP) comprises an extensive process known as Quantum Clustering [23],[29]. Purpose of introducing Physics intention of Quantum and accomplishment of quantization of the classical clustering algorithm made efficient clusters. The idea is to process the classical data in a classical-quantum hybrid way to achieve the clustering in the benchmarking time. The paper shows the dynamic data is analyzed with the help of a quantum model to know the hidden patterns.
Function of the QC method [21],[26][31]

- Schrödinger equation for clustering of high dimensional data.
- Grover search algorithm from the collection of the quantum algorithm has the potential to speed up the overall performance of the QC.

The fundamental idea of this mapping-

- The distance between the data point and the random cluster is calculated using the unitary operations.
- The quantum system's state is signified by a function ψ (x) that rests on the value x to analyze the results. [29].

Two additional advantages of the probabilistic approach –

1) To observe the cluster probability to identify the outliers.
2) QC is to be correlated with the Jaccard Score method to assess the unsupervised structure of the data.
3) A Quantum algorithm analyzes the high-dimensional data with fewer qubits with the help of quantum logic operations. Following Figure 4 gives the methodology details of the three different mythology conceptual papers [12],[18],[22].

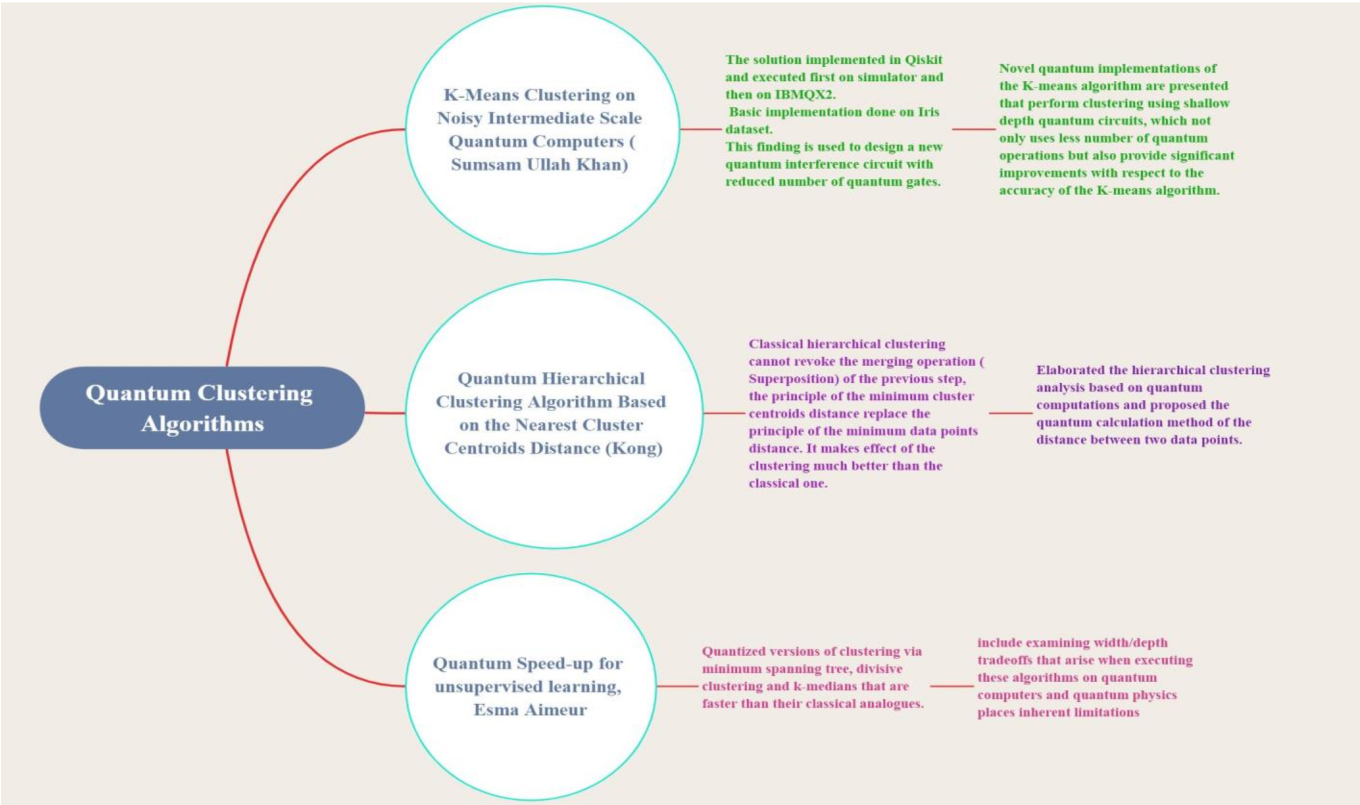

Fig. 4 The sketch shows three types of Unsupervised Quantum Clustering algorithms. The quantum version of Hierarchical, k-means, nearest neighbor is briefly explained

3. Experimental Implementation

This section talks about implementation, calculating the distance measured between arbitrary-dimensional feature vectors in the proposed clustering algorithm, and comparing to similar classical algorithms using the open-source IBMQ simulator (qasm simulator) for creating and running quantum circuits. The results achieved this stage by utilizing the Python module Qiskit developed by IBMQ, injecting it into a rudimentary k-means algorithm, and coding a modular quantum algorithm for distance calculation and cluster updation. The Qiskit module offers the ability to execute circuits on quantum computers operated by IBM built with superconducting transmon qubits and Josephson junctions and on IBM's high-performance quantum simulator Designed for the accurate simulation of typical noisy transmons. As in [29], the experimental error associated with remotely executing circuits on the real devices offered by IBMQ was too high to extract significant results. Due to this, along with qubit restrictions and long queue times, executed the proposed algorithm on the simulator to analyze its performance in an unrestricted and less noisy environment, similar to [20] and [30]. Note that while using a superconducting processor, additional qubit devices demonstrate promise for ML applications, such as optical systems [21] and trapped-ion processors [32]. Quantum simulators are optimized with gates, topology, and error rate, and finally, the schedules come into the picture to build a qasm program. Following are the quantum simulators advances compared to the classical platform [33]-[34]:

- Quantum circuit: User Input
- Pulse schedule: User Input + Device Scheduling
- Processors: Device Scheduling + Processor specific compilation

Table 1. The generalized stages of the quantum circuit to calculate distance between data point and centroid

Step 1: Initial Stage $\|0\rangle\|\theta1\rangle\|\theta2\rangle$
Step 2: Apply Hadamard gate, $H = \left(\frac{\|0\rangle + \|1\rangle}{\sqrt{2}}\right)\|\theta1\rangle\|\theta2\rangle$ $H = \frac{\|0\rangle\|\theta1\rangle\|\theta2\rangle + \|1\rangle\|\theta1\rangle\|\theta2\rangle}{\sqrt{2}}$
Step 3: Apply SWAP $SWAP = \frac{\|0\rangle\|\theta1\rangle\|\theta2\rangle + \|1\rangle\|\theta2\rangle\|\theta1\rangle}{\sqrt{2}}$
Step 4: Again, apply the H gate,

$$H = \frac{\frac{|0\rangle+|1\rangle}{\sqrt{2}}|\theta1\rangle|\theta2\rangle+\frac{|0\rangle-|1\rangle}{\sqrt{2}}|\theta2\rangle|\theta1\rangle}{\sqrt{2}}$$

$$H = \frac{|0\rangle(|\theta1\rangle|\theta2\rangle+|\theta2\rangle|\theta1\rangle)+|1\rangle(|\theta1\rangle|\theta2\rangle-|\theta2\rangle|\theta1\rangle)}{2}$$

Step5: After that, apply measurement,

It performs the inner product between P_0 and P_1, Where P_0 and P_1 are of getting $|0\rangle$ State and $|1\rangle$ state. Where P_0 is the outcome of Mod Square of all the states except $|0\rangle$ State and P_1 is the outcome of Mod Square of all the states except $|0\rangle$ State.

$$P_0 = \left|\frac{(|\theta1\rangle|\theta2\rangle+|\theta2\rangle|\theta1\rangle)}{2}\right| * \left|\frac{(|\theta1\rangle|\theta2\rangle+|\theta2\rangle|\theta1\rangle)}{2}\right|$$

$$P_0 = \frac{(1+\langle\theta1|\theta2\rangle\ \langle\theta2|\theta1\rangle)}{2}$$

$$\langle\theta1|\theta2\rangle = \sqrt{2P_0 - 1}$$

Finally, remove P_0 from $\sqrt{2P_0 - 1}$, so the output is the inner product $|\theta1\rangle|\theta2\rangle$. i.e. $\langle\theta1|\theta2\rangle$

Table 1concisely outlines the used approach of distance calculation using the quantum method. One of the new quantum clustering algorithms is discussed in [29]-[31]. The implementation uses the following subroutines to perform the qk-means clustering as follows:

- Swap Test
- Distance Calculation
- Tomography: The idea of tomography is that, rather than measurements directly, first see how the state overlaps with many different states that create a form of basis state. Then use those output statistics to reconstruct the original state.

Purpose/Process:

- To accomplish optimization and implement the qk-means algorithm.
- A swap Test [9] calculates the distance between vectors or data points.
- The assignment of clusters stage uses the wheels of quantum gates and assigned data points to clusters.
- The mod square of all the vectors is used to find the exact probability of the result (i.e., exact quantum state)

The distance calculation is performed using the inner products of the two probabilities. The (See Fig5) shows the quantum circuit used to perform the inner product. The Hadamard gate and SWAP test are applied to the $|0\rangle$ state. $\theta1$And$\theta2$ are the features of the data points which helps to calculate the accuracy to maintain the efficiency of the given data points. The measurement of the inner product of $\theta1\theta2$and throws the nearest value from the selected centroid point. The operation is shown in Table and Figure (See Fig5) is performed throughout the experiment on the data point and specified centroid.

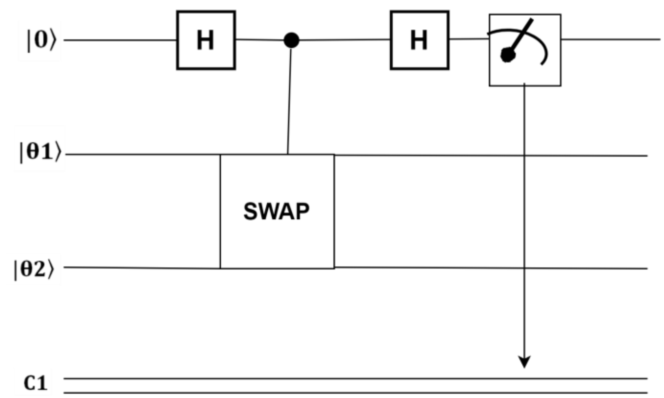

Fig. 5 Pictorial representation of quantum circuit using Hadamard gate and SWAP gate to calculate distance between $\theta1\theta2$ and

Verification process-

- The random air pollution dataset aids in the verification of the execution of the qk-means clustering algorithm available in this paper.
- Two dimensions randomly generated 100 input vectors with 2 dimensions.
- In the initial stage, input vectors are subjectively allocated to a respective group.
- Then there is the standardization of the dataset to have unit variance, and zero mean.
- Pre-processing is a subsequent step to control the input data into an encoding phase.
- The discussed technique is used in a learning model where the two input vectors are vital to discriminate between diverse clusters.

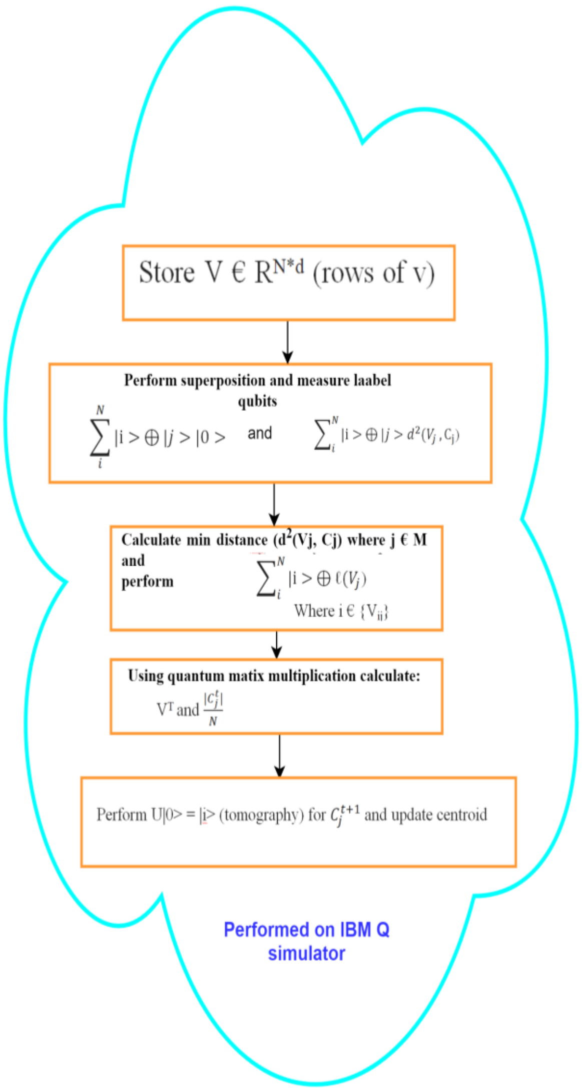

Fig. 6 Cloud structure shows the qk-means algorithm steps using the tomography

3.1. IBM Qiskit: Simulator

Quantum computing requires quantum hardware to produce the measurement. IBM Quantum Experience various types of quantum simulators are available. Qiskit grants access to all IBM's quantum simulators on a cloud service and local device or classical computer. For experimental purposes, the Qasm simulator has been used without adding the noise into the simulator [12],[22][34]. Qasm simulator provides ideal results while running quantum circuits because of their noise-free quality. The addition of a noise model provides the potential for a quantum computer in a quantum simulator to mimic. Noise-free simulators help check the imprecision in the output, which leads to knowing whether the circuit implementation is correct and not exactly checking the noise in the quantum simulator [32]. The measured probabilities of the quantum simulator are the theoretical predictions of the result from the noise-free quantum simulator [27].

4. Result and Discussion

A Quantum algorithm requires the coordination of classical and quantum parts of the computation. The execution phase involves a quantum algorithm, transforming the algorithm into the executable format, running the simulation or experiment, and finally analyzing the outcome. The basic implementation is performed using the standard classical k-means algorithm with k=2. The random air pollution dataset is used (with 100 data points) to test the performance for implementation purposes. The result shows the formation of two clusters as defined (k=2), which has an expected result for centroid C. The simulation results of classical k-means and qk-means algorithms are shown in the table (See Table2). As shown (See Fig7 and Fig8), the quantum circuit performed efficiently and accurately in two clusters that match the theoretical predictions and are superior to the classical k-means algorithm. The implementation starts with using the 20 data points, and every time it adds new data series to check the accuracy of the qk-means algorithm. Showing simulation results as up to the mark, the accuracy of the clusters from the qasm simulator are 60.45%, 98.30%, 97.67%, and 93.70% for 20, 50, 80, and 100 data points, respectively. Coherence time is advantageous to the number of vectors for the assignment of cluster 0. The qubit collapsed to its $|0\rangle$state when the coherence time was over, which ultimately made it difficult to reach the higher probability for cluster 1. The estimating distance for the proposed algorithm is executed using the quantum SWAP gate, which shows identical results for the execution of the qk-mean algorithm.

Table 2. Completion time of the classical k-means and qk-means using the number of data points. 8219 shots are used to execute the quantum circuit

Data points	Completion time (k=2)	
	Classical Platform	**Quantum platform (shots= 8219)**
20	1.2ms	0.23ms
50	2.3ms	0.3ms
80	2.5ms	0.367ms
100	2.9ms	0.5ms
120	2.9ms	0.58ms

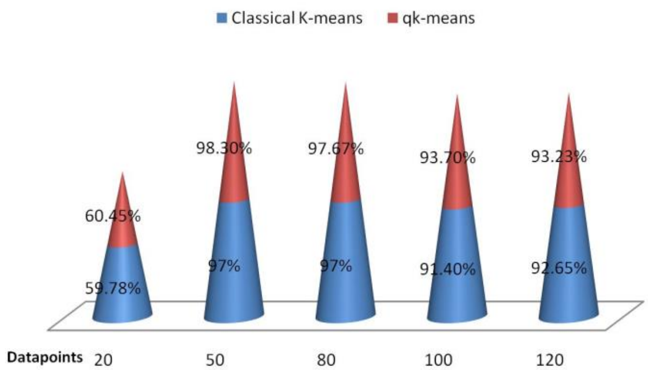

Fig. 7 The accuracy of the classical k-means and qk-means incrementally increases as the number of data points increases

The quantum algorithms start with the conversion of classical data into quantum data. In the execution, amplitude encoding techniques have been used to convert classical input data into quantum input data. The completion time of the qk-means algorithm includes the encoding stage of the input data. The quantum circuit passes the amplitude values, and the SWAP test performs the distance calculation between the data point and the centroids. Finally, measurement is done to see the cluster assignment of the processed data point. It is shown that when the appropriate ML algorithm is used with exact quantum circuit depth, it ultimately leads to getting higher prediction accuracy (See Table 2 and Fig7).

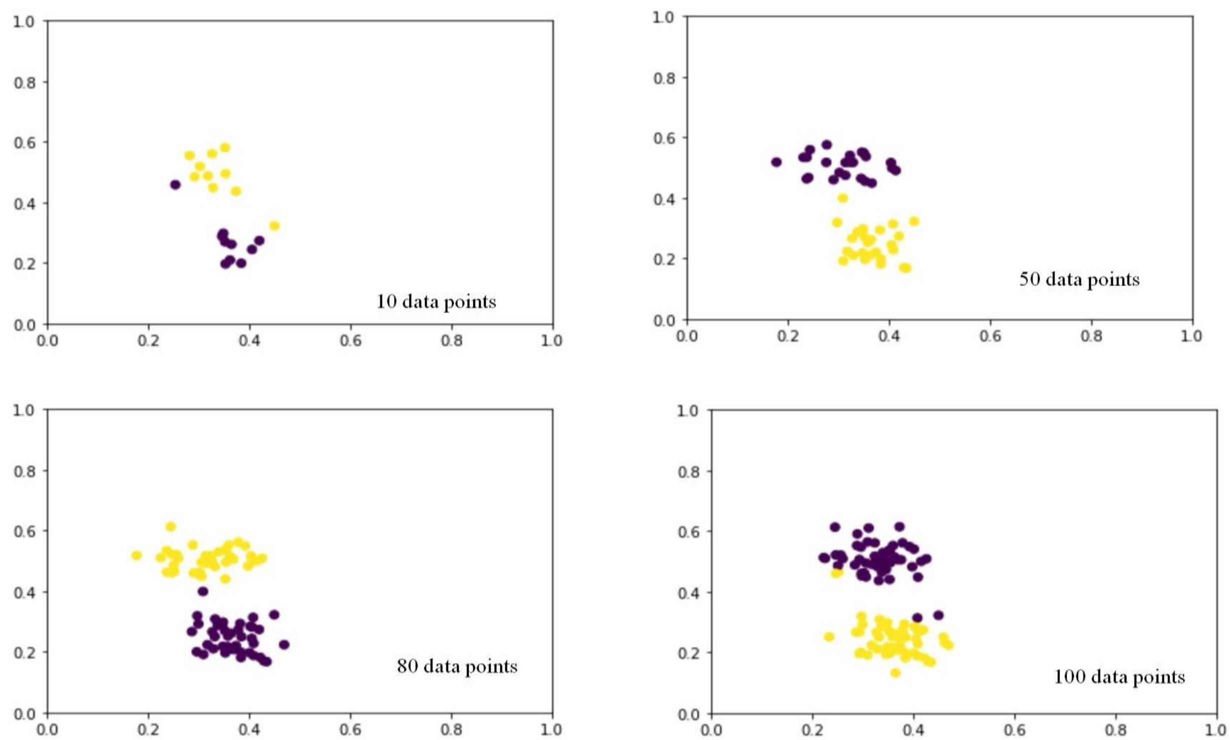

Fig. 8 Result of quantum clustering using the qk-means algorithm on various data point combinations

5. Conclusion

The proposed paper is acquainted with a quantum algorithm for k-means clustering. It is grounded on the average classical clustering algorithm and a novel quantum technique for the computation of Euclidean distance. The algorithm thoroughly accords with the classical k-means algorithm precision on clustering problems. When run on a quantum simulator, it displays the potential advances in cluster assignment performance. This marks another step in the field of QML in designing and implementing quantum algorithms. They surpass their classical counterparts in accuracy and speed. Quantum computing is in its initial phases of development. The investigation of the prevailing limitations concerning non-trivial problems is vital. Those move beyond fundamental algorithm proofs-of-concept. Countless industrial applications operate clustering and distance estimation expansively. This proves that quantum technology is perpetually rising. Researchers expect that as NISQ-era quantum computers mature, these analyses and industry-driven use-case studies will be obligatory. Those will develop cherished outlooks to bring out their utilization in real-life applications. Though this presented work contributes to enhancing the quantum clustering algorithm with the help of quantum tomography for industrial use-cases, there are still unreciprocated queries. Incremental learning is needed when new data series will arrive so that the advancement in classical and quantum clustering algorithms is the future work. Many algorithms undeniably involve a distance calculation step recurrently. Accordingly, benchmarking their quantum efficiency paves the way toward numerous opportunities such as Quantum Incremental Learning for future work.

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