Practical Quantum K-Means Clustering: Performance Analysis and Applications in Energy Grid Classification

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Abstract—In this work, we aim to solve a practical use-case of unsupervised clustering which has applications in predictive maintenance in the energy operations sector using quantum computers. Using only cloud access to quantum computers, we complete a thorough performance analysis of what some current quantum computing systems are capable of for practical applications involving non-trivial mid-to-high dimensional datasets. We first benchmark how well distance estimation can be performed using two different metrics based on the swap-test, using both angle and amplitude data embedding. Next, for the clustering performance analysis, we generate sets of synthetic data with varying cluster variance and compare simulation to physical hardware using the two metrics. From the results of this performance analysis, we propose a general, competitive, and parallelized version of quantum $k$-means clustering to avoid some pitfalls discovered due to noisy hardware and apply the approach to a real energy grid clustering scenario. Using real-world German electricity grid data, we show that the new approach improves the balanced accuracy of the standard quantum $k$-means clustering by 67.8% with respect to the labeling of the classical algorithm.

Index Terms—Quantum clustering, quantum distance estimation, quantum computing, cloud quantum computing.

I. INTRODUCTION

Given the challenging engineering requirements for building and maintaining quantum computers, it is likely that quantum computers will only be accessible through cloud services for the majority of users. Quantum computers, depending on the qubit technology, can require a complex construction and maintenance schedule that make it impractical for the average user to own. Rather than building quantum computers as a hardware product to sell to consumers, large companies like Amazon, Microsoft, and IBM are rather developing cloud-based platforms for online access to their quantum devices. Although these quantum cloud services are currently accessible, the question of how useable are they for practical, industrial use-cases arises. Can these quantum computers produce accurate enough distance estimates for clustering? Can we achieve any speedup with them currently? The focus of this work is therefore to benchmark a simple, common use-case using IBM’s Quantum cloud services.

Clustering algorithms can be used on unlabeled data to find relationships between the data’s various features. To perform clustering, an algorithm introduced by Lloyd in 1982 called $k$-means clustering can be used. The $k$-means algorithm takes as input a collection of unlabeled data points, or feature vectors, and outputs a list of labels, one for each data point. The data points are labeled based on the minimal distance to a particular centroid. During execution, the algorithm improves the centroid locations by running iteratively, updating the location to be the mean of the data points that are determined nearest to them based on a distance metric.

Classically, the usual method for measuring the distance between centroids and data points is to simply compute the Euclidean distance. For feature vectors of $N$ features, computing the Euclidean distance requires $O(N)$ computational steps. With a quantum approach, using quantum amplitude encoding (see [4] for details), one can encode length-$N$ vectors into $O(\log_2 N)$ qubits, an exponential decrease in resources for encoding, assuming one can load quantum states into a quantum random access memory [5]. With this encoding, one can perform what is known as a swap-test using a quantum computer, as described in [5], [6], to compute an estimate for the Euclidean distance between two vectors. Because the swap-test requires a number of operations proportional to the number of qubits used for encoding—needed for swapping two multi-qubit states—in theory this would result in an exponential speedup in runtime complexity. Moreover, the minimum distance to a centroid for each point can be found using a Grover’s search for an additional quadratic speedup. Using a simpler data embedding approach like angle embedding, the theoretical advantage provided by an amplitude embedding is lost, as angle embedding requires a number of qubits directly proportional to the data dimension. However, the benefit of using this alternative embedding is that the depth of the state preparation circuit is constant, whereas with amplitude encoding, the state preparation circuit uses exponentially more non-local gates as the data dimension grows [8], leading to vastly deeper circuits using current approaches.

This result makes quantum clustering and nearest-neighbor classification appear as very attractive use cases for quantum computing, since they both use distance estimation and
therefore can benefit by a theoretical speedup. When put into practice though, there are various challenges to overcome before one can effectively perform distance estimation on a quantum computer. Moreover, a strong assumption of efficient state preparation needs to be made in order to have an exponential speedup using the quantum approach over the classical approach [9]. Nonetheless, with this article, we aim to expand the results related to clustering on real, gate based, quantum hardware, and in particular, to explore how this type of algorithm can be executed on IBM’s quantum cloud computing service. In this work, we use only the software libraries and services available to us with no direct hardware access, aiming to demonstrate how well one can expect quantum clustering to perform using generally available resources.

We begin in Section II by reviewing how we perform data encoding and how we calculate the distance estimation in our quantum algorithm using the cloud service. In Section III we benchmark how well distance estimation can be performed, testing for various Euclidean distances and dimensions in simulation and on hardware. In Section IV we analyze various clustering experiments using synthetic data with two and four dimensions with several datasets. Given the results of the performance analysis in the prior sections, we then apply the findings to a non-trivial clustering problem which is relevant in the energy sector in Section V. In particular, we show that decomposing high-dimensional vectors into 2-dimensional subspace projections, we are able to compute the overall distance in a more parallel fashion which significantly reduces the error induced by existing quantum hardware, simultaneously reducing the total number of circuits.

A. Related Work

Performing clustering and nearest-neighbor type algorithms using quantum computers has been studied in various contexts. Improving the encoding strategy to work better with IBM’s quantum computers was studied by Khan et al. in [10]. In the article, they describe an encoding mechanism for feature vectors and benchmark the approach on IBM’s quantum computer. Feature vectors, after PCA is performed, of dimension two are considered and benchmarked with the MNIST dataset using quantum hardware. Using the IonQ quantum hardware, Johri et al. perform data classification using clustering on their trapped ion quantum computer [11]. In their work, they define an optimized method for encoding 8-dimensional classical data into the quantum computer and use PCA to benchmark against MNIST data for ten different labels and perform their quantum algorithm for nearest-neighbor classification. In these works, an explicit benchmarking of distance estimation accuracy is not demonstrated. Moreover, the only experiments tested on the IBM quantum system were of two dimensions. In a quantum annealing setting, clustering has also been considered. The authors of [12] and [13] map a clustering problem to a quadratic unconstrained binary optimization (QUBO) problem for an adiabatic quantum computer and use hardware to test their approach. Quantum annealing uses a different approach to quantum computing versus the gate based model, indeed no swap-test is involved, and the results from annealing experiments do not paint a clear picture for performance using a universal quantum computing approach.

In [14], Benlamine, et al. review three methods for distance estimation using a quantum approach and benchmark the approaches using nearest-neighbor classification in simulation. Further modified quantum clustering approaches were proposed in [15], [16]. These works did not perform tests on real physical hardware. In [17], Nguyen et al. run experiments to test the accuracy of the swap-test using their trapped ion system in a continuous variable setting, but do not perform any experiments of clustering.

II. PROGRAM SETUP AND CONFIGURATION

In this section, we review the setup and configuration used to perform clustering algorithms. In the first subsection, we review how the synthetic data is generated. Next, we review how the quantum algorithm works as well as the two methods used for classical data embedding in quantum states. Finally, we review the software approach used to execute the algorithms on the quantum cloud hardware.

A. Generating Synthetic Data and Quantum Data Loading

In the experiments conducted, we used synthetic data generated with varying dimension, number of clusters, cluster variance, and minimal distance between the centers. At a high level, the cluster generation algorithm used works by firstly selecting $k$ center points to then generate cluster data around them. Using the center points as the multi-dimensional mean of a multi-variate normal distribution, a set number of cluster points are generated surrounding the center. Input to this algorithm is a cluster-variance parameter which we use to set the variance level of the respective dimension to control the “tightness”—how we measure difficulty of clustering—of the cluster. To avoid the randomly initialized center points being too close to each other, an additional step that resets a center point if it is within some $\epsilon$ distance from the already initialized center points is added. The synthetic data generated can be seen in Figure 1.

To perform the quantum distance estimation algorithm, the generated data points firstly need to be embedded into a multi-qubit quantum state. For this, we use two common types of embeddings, namely amplitude embedding and angle embedding [4], and test them independently. To perform the embeddings, we use the circuit structure shown in Fig. 2 and Fig. 3 respectively. To implement amplitude embedding in code, we use the built-in `initialize` function offered by Qiskit, which is a function that takes as input a real vector and returns the necessary gate set for complex amplitude embedding [18]. For angle embedding, we use two-dimensional rotations to embed two dimensions of a data vector per one qubit. This type of embedding is also referred to as “dense angle embedding” [19], but in this work we will only use the name “angle embedding” to refer to it. The scaling
in terms of circuit depth and number of two-qubit gates varies significantly between the two embeddings. When embedding data using angle embedding, gate depth does not increase with the data dimension, but circuit width grows linearly. On the other hand, embedding classical data using amplitude encoding can scale quite poorly in depth with respect to the data dimension [8]. When using NISQ-era quantum devices, width and depth are some of the properties that should be reduced as far as possible to reduce the effects of noise in any algorithm. We plot the experimental scaling with respect to the data dimension in Fig. 4. The figure shows both the circuit depth and number of non-local gates required for initializing data for a connected quantum computer (i.e. one in which any two qubits can interact without any state-swapping) (solid line), and the 65-qubit IBM Brooklyn topology (dashed line), followed by a swap-test. For the encoding methods, Fig. 5 shows the qubit resource requirement trends against feature vector dimension. The connectivity of the quantum computer topology determines the number of local swaps needed to perform two qubit gates, which results in deeper circuits with more non-local gates.

B. Quantum Circuits for Distance Estimation

To perform clustering, we replace the distance calculation from the classical algorithm with a quantum algorithm for distance estimation. Using amplitude embedding, we use an Euclidean distance approximation based on the one developed in [5] and reiterated in [20]. For angle embedding, we define a simple encoding that scales the data for embedding. The algorithm used for distance estimation firstly embeds the data for two vectors and then performs a swap-test. To approximate the distance, a number of repetitions, or shots, of the circuit are used to aggregate measurement statistics for a single ancilla qubit. The number of repetitions to use will vary problem to problem and hardware to hardware. Theoretically, using a higher number of shots will produce a more precise distance estimates, but each hardware will have a finite precision, and so more shots does not always lead to more accuracy. Moreover, some datasets do not require high-precision distance estimation to cluster accurately if they, for example, have well separated clusters. We explore this further. Once the repetitions are complete, the distance estimation can be calculated via the probabilities of a 0 or 1 measurement outcome of the ancilla qubit

\[
\begin{align*}
\Pr(0) &= \frac{1}{2} + \frac{1}{2} |\langle \psi | \phi \rangle|^2, \\
\Pr(1) &= 1 - \Pr(0) = \frac{1}{2} - \frac{1}{2} |\langle \psi | \phi \rangle|^2,
\end{align*}
\]

Thus, the estimate \(|\langle \psi | \phi \rangle|^2\) provides an approximation to the inner product for our choice of embedding, or at least a measure that scales with the inner-product in the case of angle embedding.

For each of the two embeddings used, the swap-test procedure differs in terms of number of controlled swaps—also known as Fredkin gates [21]—used due to the difference in qubit resources required to perform the data embedding as well as the data representation strategy. For two (not necessarily normalized) data vectors \(a := (a_1, a_2, ..., a_n)\) and \(b := (b_1, b_2, ..., b_n)\)—which in the case for clustering or
We encode the two vectors \( \mathbf{a} \) and \( \mathbf{b} \) given by Eqns. 6 and 7 used to ensure the values are between 0 and \( \pi \). With this embedding, we can encode data using a two-dimensional rotation operation defined by

\[
U(\theta, \gamma) := \begin{pmatrix}
\cos \frac{\theta}{2} & -\sin \frac{\theta}{2} \\
\sin \frac{\theta}{2} & \cos \frac{\theta}{2}
\end{pmatrix}
\]

such that the angle embedded representations are given by \( a' := (a'_1, a'_2, ..., a'_n) \) and \( b' := (b'_1, b'_2, ..., b'_n) \). The mappings given by Eqns. 6 and 7 used to ensure the values are between 0 and \( \pi \). With this embedding, we can encode data using a two-dimensional rotation operation defined by

\[
U(\theta, \gamma) := \begin{pmatrix}
\cos \frac{\theta}{2} & -\sin \frac{\theta}{2} \\
\sin \frac{\theta}{2} & \cos \frac{\theta}{2}
\end{pmatrix}
\]

We encode the two vectors \( a' \) and \( b' \) in \( \lceil n/2 \rceil \) qubits, using 1 qubit per two dimensions of each vector resulting in the final states

\[
\left| \psi \right> := \bigotimes_{i \in \text{odd}(n)} U(a'_i, a'_{i+1}) \left| 0 \right> \quad \text{and} \quad \left| \phi \right> := \bigotimes_{i \in \text{odd}(n)} U(b'_i, b'_{i+1}) \left| 0 \right>,
\]

where \( \text{odd}(n) \) is the set of odd numbers from 1 to \( n \). To recover the distance estimation, an ancilla qubit is introduced to the system. A Hadamard gate is applied to the ancilla followed by a series of \( n/2 \) controlled-swap gates using the ancilla as the control and one qubit from \( \left| \psi \right> \) and one from \( \left| \phi \right> \). A final Hadamard gate is applied to the ancilla qubit and then is measured. The overall circuit is depicted in Fig. 3. The goal in this case is to produce an estimate for \( \text{Pr}(1) \), which is a valid distance metric. Because we are using arbitrary data which is not normalized in advance, we accommodate for this in the distance metric. For this, we set \( Z := |a|^2 + |b|^2 \) such that \( a \) and \( b \) are normalized as \( a = a/\sqrt{Z} \) and \( b = b/\sqrt{Z} \). The final distance metric is therefore given by

\[
d(a, b) = \sqrt{Z \cdot P(1)},
\]

where \( P(1) \) is given in Eqn. 2.

C. Running Clustering on the Quantum Cloud

To implement the circuit preparation and execution of the quantum circuits in software, we use IBM’s Qiskit Python Software Development Kit (SDK) [22].

A property of the \( k \)-means clustering algorithm is that it is highly parallelizable, and we use this property to execute the
clustering algorithm more time-efficiently. In each iteration of $k$-means clustering, a distance is calculated between the current set of centroids and each point in the dataset. These distance calculations are independent of each other and can be computed in parallel using multi-processing or in a batch job. In the quantum case, to parallelize, we take two approaches. Firstly, we prepare one circuit per distance estimation and then send the collection of circuits as a batch job to the cloud service. The response is the measurement results of the circuits which can then be post-processed according the embedding. The second way we parallelize the algorithm is to embed multiple swap-tests into one circuit and execute them on the same quantum computer at once. This allows for multiple distance estimations to be done on a single quantum computer.

We developed the first parallel approach in two ways, one using our own approach and later, when it became available, using a Qiskit native approach. For the first approach, we use many computational thread processes (locally) to send requests simultaneously to the server to reduce computation time. In simulation, the approach improved performance, but when there is only one quantum computer, this makes no difference. The advantage from parallel execution is achieved with multiple quantum computers working together to compute distance estimations as described in [23].

The second approach was sending batches of circuit jobs via a recently added feature called Qiskit Runtime. This feature allows the user to submit many circuit jobs at once such that there is only one job to queue. The performance improvement between parallel execution via multi-processing and batch-circuit execution that we observed was significant. The complete algorithms for the two applied $k$-means clustering approaches are described by Algorithms 1 and 2 respectively.

III. BENCHMARKING DISTANCE ESTIMATION

To develop a clear understanding of how well clustering and nearest-neighbor classification can be performed using current quantum hardware, it is helpful to test how accurately distance estimation can be performed on quantum devices. In this section, we benchmark a variety of cases for performing distance estimation and compare the estimations using simulation and real quantum hardware. Simulation in this case is done using the noisless quantum computing simulation platform offered via the Qiskit framework using the OpenQASM backend. Software for the simulation is prepared in exactly the same way in which the quantum circuit logic is sent to the quantum cloud services, we can simply switch the target backend from the simulated backend to the hardware. To perform the analysis, we test three difference cases. We firstly test how varying the number of circuit shots affects the estimation in both two and four dimensions. Next, we vary the distance of the data points also in two and four dimensions. Lastly, we test how varying the data dimensions affects the estimation up to 32 dimensions using amplitude embedding and up to 26 dimensions using angle embedding.

### Algorithm 1 Clustering on the Quantum Cloud with Multi-processing

**Input:**
- $k$: The number of clusters
- data: The data to cluster
- embedding: The choice of data embedding
- $\epsilon$: The minimum distance between two cluster centers
- maxIterations: The maximum number of iterations to make
- processes: A list of running processes

**Output:** An ordered list of labels for the data points

```
1: centroids ← initialize the centroids using $\epsilon$ min distance
2: convergence ← false, $i$ ← 0
3: while not convergence do
4:    circuits ← generate all circuits with the data, centroids, and embedding choice
5:    dists ← initialize empty shared storage
6:   while not all circuits have been processed do
7:       if a process is idle then
8:          job ← send single circuit to server and await response
9:          dist ← process job results according to the embedding
10:        add dist with circuit number to shared storage
11:       else
12:           wait
13:    Sort dists according to circuit number
14:    dists ← using the returned, ordered measurement results from the server, complete the distance estimation procedure
15:    labels ← using the distances to the centroids, label the data points
16:    centroids ← with the updated labels, recompute the centroids as an average position of the labeled data. Delete centroids for empty clusters.
17:    Check for centroid convergence, update convergence
18:    $i$ ← $i$ + 1
19:    Check if $i = maxIterations$ and break accordingly
20: return labels
```

In all tests, for each resulting data point, we use 100 repetitions, plotting the average output and the standard deviation. In each case, we use the measurement error mitigation feature when running the experiments on the physical hardware. To execute the 100 instances, we make 100 copies of the circuits and use the circuit-runner service to execute the circuits in a batched job.

The results of varying the number of circuit shots are plotted in Fig. 6. In this experiment, we created a circuit for the vectors $(1, 0)$ and $(1, 1)$. Comparing simulation to the physical device results, in simulation we see a convergence in the number of shots to the true answer, and moreover the average is close to the true distance as desired. With the real hardware, we see no convergence trends behind the dotted line, and using more shots than around 2,000 does not generally perform better than using the maximum number of shots 8,192. In some cases, a lower number of shots performed better, having a lower variance in the standard deviation than with more shots. On the other hand, when we switched to a quantum computer that supported a higher number of shots, much better and more consistent results are seen. For 4D, the points $(1, 0, 0, 0)$ and $(1, 1, 1, 1)$ are used, and the same effects are more or less seen. Convergence is not reached using real hardware, but a relatively rapid convergence is seen in simulation, where with a high number of shots, the results improve significantly. We
Algorithm 2 Clustering on the Quantum Cloud with Batched Circuits

**Input:**
- $k$: The number of clusters
- data: The data to cluster
- embedding: The choice of data embedding
- $\epsilon$: The minimum distance between two cluster centers
- maxIterations: The maximum number of iterations to make

**Output:** An ordered list of labels for the data points

1: centroids $\leftarrow$ initialize the centroids using $\epsilon$ min distance
2: convergence $\leftarrow$ false, $i \leftarrow 0$
3: while not convergence do
4: circuits $\leftarrow$ generate all circuits with the data, centroids, and embedding choice
5: job $\leftarrow$ send the collection of circuits to the cloud server for processing and await response
6: dists $\leftarrow$ using the returned, ordered measurement results from the server, complete the distance estimation procedure
7: labels $\leftarrow$ using the distances to the centroids, label the data points
8: centroids $\leftarrow$ with the updated labels, recompute the centroids as an average position of the labeled data.
9: Check for centroid convergence, update convergence
10: $i \leftarrow i + 1$
11: Check if $i = \text{maxIterations}$ and break accordingly
12: return labels

reiterate that in some cases, depending on the dataset, high-precision distance estimation is not necessary for clustering.

An important point of note is that for angle embedding, the difference of output between the simulation and the hardware is much starker than with amplitude embedding. The reason behind this is due to the fact that on the IBM quantum devices, the accuracy of qubit rotations is less precise with the available gate basis of $\{\text{CX, ID, RZ, SX, X}\}$ and therefore significant differences between the simulation, where such rotations are highly precise, are observed [24]. Another noteworthy aspect is that in some instances, the variance in the standard deviation can become very small for the 100 samples, with no recognizable trend. See for example Fig. 6 the 7,000 shots point in the upper-left plot and the 6,000 shot point in the lower-left plot. We suspect this may come from a periodic hardware calibration that is performed by IBM that was executed on the quantum devices between experimental runs.

For the next set of experiments, we vary the distance between two points in 2D and 4D (see Fig. 7). The vectors we chose have the form $(1, \ldots, 1)$ and $(x, \ldots, x)$ where we vary $x$ to modify the distance between the points. The results of the 2D experiments show that simulation and the physical device have similar outputs for $x \leq 5$, but for $x > 5$, the outputs from simulation and real device start to diverge. In 4D, the effects of encoding show a stark difference between amplitude and angle embeddings. Interestingly, the simulation results for 4D amplitude embedding match very closely to the hardware execution for all tested values of $x$, more so even than in 2D. On the other hand, angle embedding performs far worse in 4D than in 2D, where already for $x = 5$, the difference between simulation and real hardware is significant. This extra noise is again likely due the fact that for more dimensions, the limited precision of the angle embedding is now applied for another two dimensions and that an additional controlled-swap is introduced.

In the last set of experiments, we vary the dimension of the data to observe the limits to the number of features we can use and with what level of accuracy. We test up to 32 dimensions for amplitude embedding and up to 26 dimensions for angle embedding, using the 27 qubit device IBMQ Sydney to its capacity in the angle embedding case. We compare vectors with shape $(1, \ldots, 1)$, to vectors $(2, \ldots, 2)$, $(3, \ldots, 3)$, and $(4, \ldots, 4)$. In Tables 1 and 2, we show the percent-difference between the simulation outputs and the results from the quantum computer for amplitude and angle embedding respectively, where Fig. 8 displays the corresponding results. We observe that at further distances, simulation and hardware results tend to agree more closely in both embedding types. These results motivate data scaling techniques, where mapping the data into a space where the data is more separated could result in more accuracy, a hypothesis we intend to explore in future work.

| Dim. | $x = 2$ | $x = 3$ | $x = 4$ |
|------|---------|---------|---------|
| 2    | 66.44%  | 9.56%   | 13.69%  |
| 4    | 97.95%  | 30.29%  | 9.21%   |
| 8    | 128.25% | 61.44%  | 8.42%   |
| 16   | 133.22% | 54.98%  | 34.08%  |
| 32   | 110.86% | 47.40%  | 24.72%  |

Table 1. Amplitude Embedding: Percent difference comparison between simulation and real data for the distance between data points of varying dimension and distance on IBMQ Sydney.

| Dim. | $x = 2$ | $x = 3$ | $x = 4$ |
|------|---------|---------|---------|
| 2    | 85.87%  | 61.87%  | 61.26%  |
| 4    | 144.24% | 117.87% | 98.77%  |
| 8    | 161.70% | 131.13% | 115.94% |
| 16   | 156.84% | 128.40% | 113.8%  |
| 26   | 158.58% | 129.59% | 111.42% |

Table 2. Angle Embedding: Percent difference comparison between simulation and real data for the distance between data points of varying dimension and distance on IBMQ Sydney.

IV. **Benchmarking Quantum Clustering**

In this section we benchmark the quantum $k$-means clustering algorithm using various dimensions and number of clusters using synthetic data. To determine the accuracy of clustering using the quantum approaches, we generated three types of synthetic data using two and four dimensions. The first two types of data that we generate are an easy dataset, a hard dataset both with four clusters and 15 data points in each cluster, as seen in Fig. 1(a) and (b). This totals 60 data points. The third dataset we use has a variance between the easy and hard sets, but with eight clusters and 14 points per cluster, seen in Fig. 1(c). The number of data points and clusters was selected to most easily work with the Circuit
Fig. 6. The distance estimation for amplitude encoding (upper) and angle embedding (lower) of $(1, 0)$ and $(1, 1)$ in 2D (left) and $(1, 0, 0, 0)$ $(1, 1, 1, 1)$ in 4D (right). The circuit for measuring the distance between these the two points is generated and ran a varying number of shots. Displayed is the average output of 100 trials with the standard deviation shaded around the average. The black dotted line indicates where the quantum hardware used switches from IBMQ Bogota on the left of the line to IBMQ Casablanca on the right.

Fig. 7. Plots for varying the distance between points. The plots on the left are for amplitude (top) and angle (bottom) embedding in two dimensions. The right plots are for amplitude (top) and angle (bottom) embedding in four dimensions. We run the experiments for a vector of shape $(1, ... , 1)$ for the base points and, $(x, ..., x)$ for the varying point. We repeat the experiments 100 times with 2,048 shots plotting the average with the standard deviation.
Fig. 8. Results for varying data dimension using the vector \((1, ..., 1)\), estimating distance to vectors \((2, ..., 2), (3, ..., 3), (4, ..., 4)\). The plots are ordered respectively from top to bottom. We run the experiment 100 times with 2,048 circuit shots and plot the average output and standard deviation of simulation after running on the IBMQ Sydney device for up to 32 dimensions with amplitude embedding (left) and 26 dimensions with angle embedding (right).

Runner service, reaching the limits to how many circuits can be sent at once.

In the case of the four cluster easy and hard datasets, we analyze the quantum clustering approach using the same execution parameters for both datasets. We use both amplitude and angle embedding with a maximum of five iterations, or until convergence of the centroid locations is reached. We use the outputs of the classical algorithm implementation as the base truth, 8,192 shots for each experiment, and use the option for measurement error mitigation in all cases. For these sets of experiments, we submit jobs to quantum devices which have a quantum volume of 32. The results of the experiments for 2D are seen in Figs. [2] The results displayed are, on the left side, left column, the confusion matrices comparing the classical baseline to the quantum outputs using amplitude embedding, and the equivalent for angle embedding in the right column. We observe that in the simulation setting the classical outputs are matched perfectly, however, for real hardware, the results show a relatively low accuracy in the labeling for both embeddings. The results are similar for the hard dataset as seen on the right side of Figs. [9]

For the 8-cluster data, we perform the same simulation steps, but for a maximum of three iterations with 8,192 shots. In simulation, convergence is reached with two iterations with perfect labeling results. We test both 2D and 4D datasets. The 2D results are shown in Fig. [10] For 4D data the results had very low accuracy, with essentially a random labeling and we neglect showing the results here.

Overall, these experiments motivate that using one instance of executing the distance estimation circuit with low shot counts produce a distance estimation that is not accurate enough to cluster data. To mitigate noise, we predict that we can instead average multiple distance estimations to improve estimation consistency while simultaneously increasing the circuit shots. We test this hypothesis in the next section.
V. APPLICATIONS FOR ENERGY SUBGRID CLUSTERING

The motivation for performing a detailed analysis on how well real quantum hardware performs on various distance related metrics for high dimensional data is because, typically, many real-world datasets are non-trivial, high dimensional, and not well clusterable. In classical computing solutions involving unsupervised clustering, the problem of aggregating and grouping sets of objects usually involves some dimension reduction techniques and some type of domain knowledge to tune any machine learning algorithm used. Indeed, a standard k-means approach—in the classical sense—when used in practice involves a fine balance of mitigation and optimization techniques depending on the data. Selecting the optimal clusters, choosing the initial centroid locations, choosing an optimal subset size of the dataset for large datasets, dealing with outliers, and dimension reduction are all points to consider when applying k-means to an unlabelled dataset. Celebi et al. analyze the effects of these points in [25].

Here, we focus more on the quantum aspect of k-means clustering. After using standard techniques for pre-processing the data and selecting initial centroids we direct our efforts to improving the distance estimation accuracy. Since quantum machine learning and variations of clustering are touted as being a possible avenue for quantum advantage, we aim to employ the findings in the previous sections to a real use-case which provides business value. In doing so, we propose an alternative implementation of the distance estimation circuit to overcome some of the deficiencies revealed in the previous section, namely, the inability of the vanilla quantum k-means algorithm to be able to handle classical input vector dimensions more than four.

A. German Electricity Grid Data

Predictive maintenance is a major area of applied research in the energy operations sector [26], [27]. The ability to determine areas of the electrical grid which are susceptible to failing in some pre-determined timespan has many obvious benefits for customers downstream from any grid infrastructure which may fail. One possible approach to this problem is using data-driven analysis of different partitions of the full dataset. Celebi et al. analyze the effects of these points in [25].

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Here, we focus more on the quantum aspect of k-means clustering. After using standard techniques for pre-processing the data and selecting initial centroids we direct our efforts to improving the distance estimation accuracy. Since quantum machine learning and variations of clustering are touted as being a possible avenue for quantum advantage, we aim to employ the findings in the previous sections to a real use-case which provides business value. In doing so, we propose an alternative implementation of the distance estimation circuit to overcome some of the deficiencies revealed in the previous section, namely, the inability of the vanilla quantum k-means algorithm to be able to handle classical input vector dimensions more than four.

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network grid to group and find similar types of subgrid assets. This can be done by taking into account data features such as 1) the amount of renewable and non-renewable electricity flowing through the grid subsection; 2) the number of power lines within a subsection; and 3) descriptive statistics about the ages of the assets contained in the subsection. Given such a collection of asset properties for electrical grid assets, we aim to employ unsupervised $k$-means clustering to classify various subgrids of part of the German Electrical Grid [28].

The dataset consists of 81,350 low voltage power lines from a Distribution System Operator (DSO) grid in Germany. Each power line has seven numerical features as described in Table 3. Low voltage subgrid networks are connected to high voltage entry and exit points in the grid. For a given high voltage transformer in the grid network, we collect the low voltage lines which are part of its respective subnetwork and compute numerical features describing the entire subset of low power lines. Specifically, for each subgrid we compute: the number of non-powerline assets, the total number of connected assets, and the minimum, maximum and sum of each of the features listed in Table 3. There are 1,037 subgrids and therefore we have a final dataset of 1,037 feature vectors, each of dimension 26.

| Name                                      | Unit |
|-------------------------------------------|------|
| Conductor cross-section                   | cm²  |
| Operating Voltage                         | kV   |
| Average Renewable Energy In-feed Load     | MWh  |
| Average Non-Renewable Energy In-feed Load | MWh  |
| Number of Exits of Next Major Substation  | #    |
| Line Length                                | m    |
| Sum MVA at closest HV exist               | MVA  |

Table 3. Description of the features for each powerline in the dataset.

B. Results

To cluster the data, we firstly perform a preprocessing step to reduce the total feature vector dimension to eight using Principal Component Analysis (PCA) which results in a 97.7% explained variance. We also produced a dataset with six dimensions using PCA which accounted for 91.4% of the variance. This second dataset was used for the angle embedding approach to fit in a 7-qubit quantum computer, the quantum computer topology we had most access to in this work.

With an initial classical analysis using the elbow-method [29], the optimal number of clusters for this dataset was determined to be $k = 5$. From this dimension-reduced dataset of 1,087 points, we randomly selected 180 points to cluster, where 180 points allows us to send 900 circuits ($180 \times 5 = 900$) to IBM’s cloud service in one job (an upper limit for some hardware). Important to any unsupervised clustering algorithm is the choice of initial centroid points. In order to ensure a quick convergence, and to reduce the number of quantum iterations, we ran the classical algorithm with a variety of random seeds such that convergence was reached within three iterations. The classical clustering results are depicted in Fig. 11(a), using t-Distributed Stochastic Neighbor Embedding (t-SNE) [30] on the high-dimensional data to generate a 2D projection. Using the initial centroids that achieved this, we then ran the quantum clustering experiment.

To validate the quantum approaches we used, we firstly compare the labeling output from noiseless simulation to the labels output using the classical approach, and then repeat the comparison running on real quantum devices. Because the classical approach converged in three iterations, we allow the quantum versions to run with a maximum of five iterations.

In simulation, the balanced accuracy of the experiments were 100% with amplitude encoding and 97.8% for angle encoding. Given that simulation produces high-accuracy, we performed a series of tests on the quantum hardware.

1) Clustering using amplitude encoding: The first test we perform is to simply run the same logic as in the simulation. We use 12,000 shots per distance estimate and run the full
clustering algorithm for five iterations. The clustering result using amplitude encoding are given in Fig. 11(b). The grid data is of relative high-dimension and the circuits to prepare the data are roughly 120 gate-depth with approximately 70 non-local gates for amplitude embedding. For angle embedding, the gate depth is expectantly shallower at approximately 86 but with roughly 103 non-local gates, depending on the randomization of circuit transpilation step. With the level of noise occurring, five iterations does not improve the results, and indeed we speculate further iterations would not have led to improved results either. Here, our observation is that the labeling is essentially random due to the noise in the distance estimation circuits, never leading to a converging state.

2) Classification using amplitude encoding: As a second test, we implemented a pure nearest-neighbor classification application. We being by training the model offline classically to determine optimal centroid locations, then, at runtime, we compute only the prediction step quantumly to determine which cluster test set data points belong to. Fig. 12(a) shows the accuracy results of the outcome, where we used 30,000 shots to estimate the distances using amplitude embedding in 8D. We see the majority of points were assigned to one class, similarly to how the five iterations of clustering performed.

3) Distance estimation with vector subspace parallelization: So far, our approach to distance estimation has been to use the approach as stated in [5], however, the accuracy in practice using this approach has thus far been relatively low. From the benchmarking section, the highest accuracy was seen in the two-dimensional data experiments. Using this as motivation, we propose a new technique of parallelizing the distance calculation for high dimensional vectors by using distances between two-dimensional subspaces of the full feature vectors.

Given input data vectors \( a := (a_1, a_2, \ldots, a_n) \) and \( b := (b_1, b_2, \ldots, b_n) \), the distance between them can be decomposed as

\[
d(a, b) = d(a_{1,2}, b_{1,2}) + d(a_{3,4}, b_{3,4}) + \cdots + d(a_{n-1,n}, b_{n-1,n}),
\]

where \( a_{i,j} = P_{i,j}(a) \) and \( b_{i,j} = P_{i,j}(b) \) are projections of the respective vectors to the \((i,j)\)-th vector subspace. The circuit for this parallel distance estimate using angle embedding is depicted in Fig. 13.

This approach has various benefits in terms of mitigating noise. Firstly, it uses only low-dimensional projections. In this case, we use two-dimensional projections, aligned with our benchmarking results, but as hardware improves, we can extend this to larger dimensions to reduce the number of total independent measurements until we can eventually use the entire vector. Next, these low-dimensional circuits will be in general shallower and thinner, which will improve the accuracy and moreover reduce the computation time, allowing for more shots within the same execution timespan. Because in some cases we observed a large standard deviation, with shorter execution time, one can also execute the circuit many times to produce an average distance estimate the same timespan, mitigating Gaussian noise in the system.

Because the distance estimation circuits are indeed thinner, we can load multiple circuits into one QPU proportional to the number of qubits. For example, because the swap-test with angle embedding in 2D uses three qubits per swap-test, we can load two distance calculations at a time in a seven qubit quantum computer, reducing the number of total circuits to execute by 50%. This approach could be generalized to contain as many swap-tests as there are (the floor of) one third the number of qubits, which could in turn result in again using one circuit for distance estimation, simply with a modified pre- and post-processing step. These benefits make this much more NISQ compatible than performing the distance estimation with all dimensions considered at once.
After verifying this approach produced accurate results in simulation, to tested how well it mitigates the effects of noise in the classification task, we ran the circuit implementing \( \langle a'_1, a'_2 \rangle \) using two approaches. For the first approach we used amplitude encoding and executed each distance estimation circuit independently five times, averaging the results and using the average as the distance estimate. We used 15,000 shots per execution and since the circuit uses four qubits, we could fit just one circuit at a time on the 7-qubit device. The confusion matrix of the results is in Fig. 12(b), showing a vast improvement.

For the second approach, we perform classification again, now using angle embedding, but in this case, since just three qubits per swap-test are required, we could load two distance estimates in parallel into the 7-qubit device. Using 15,000 shots with, in this case, two repetitions per circuit, we again use the average for the estimate. The results of the classification are shown in Fig. 12(c). Again, we see a strong improvement for the classification problem over the amplitude encoding approach, with a balanced classification accuracy of 73.3% and raw accuracy of 83.3%.

4) Clustering with vector subspace parallelization: Given the promising results from the classification task using the vector subspace parallelization, we again perform the full clustering algorithm using the angle embedding approach. We use the distance estimation \( \langle a'_{n-2}, a'_{n-3} \rangle \) with 12,000 shots and one repetition on the IBM Perth machine with a total of five iterations for the clustering algorithm. The clustering results are shown in Fig. 11(c). Although the labels were reduced to three classes, two fewer than in the classical algorithm, we see a much clearer separation of the classes in comparison to using amplitude encoding for all eight dimensions.

VI. CONCLUSION AND OUTLOOK

In this work, we thoroughly investigated the potential of using quantum \( k \)-means clustering in a practical manner on current NISQ quantum hardware. In terms of distance estimation comparison between classical and quantum distance calculations, we clearly observed a high level of difference between simulation and running on physical devices—especially comparing the distance estimation results using angle embeddings. The results which used batched job submission via Qiskit Runtime showed to vastly improve performance, allowing for more circuit executions, improving reliability, as well as drastic speed improvements when dealing with large datasets due to the reduction in job-queuing time.

The best \( k \)-means clustering results observed were from clustering datasets of 2-dimensional data points. When we increased the number of clusters from four to a more complex scenario of eight clusters, and changed the input vector dimension from two to four, the results worsened. We experimented with an industrial unsupervised learning problem, labeling high-dimensional energy grid data using \( k \)-means clustering. Using the state-of-the-art approach, the clustering and classification results proved inaccurate when executed over real hardware. When we changed the distance metric and used our vector subspace parallelization approach, we saw a significant improvement in both our classification and clustering experiments. For amplitude embeddings, the balanced accuracy of the classification went from 17% using the standard approach to 84.8% with this novel distance estimation method. With angle embedding, loading two swap-tests into one circuit to execute in parallel, albeit an overall wider circuit, proved to also have a large performance improvement over the amplitude encoding approach, with a balanced classification accuracy of 73.3% and raw accuracy of 83.3%.

This work provides a first step into quantum clustering for practical, industrial use-cases, but still there are questions to be answered. Future work will be to consider other clustering algorithms such as \( k \)-medoids which uses alternative distance metrics, considering other quantum approaches for distance estimation as in [12], [31] or those better suited for NISQ hardware as proposed in [32]. Indeed, many algorithms require a distance calculation step, and so benchmarking their quantum performance leaves many possibilities for future work.

Although it is well known that quantum computing is in its early stages of development, it is important to investigate what boundaries exist in relation to non-trivial problems that move beyond fundamental algorithm proof-of-concepts. Clustering, and particularly distance estimation, are widely used in various industry applications. With this work, we have tested a large set of experiments that can be performed on the quantum cloud using only the core features of the platform. Quantum technology is continuously and rapidly improving and we expect that as NISQ-era quantum computers mature, these types of analysis and industry-driven use-case studies will continue to be necessary to provide valuable insight into how they will be used for real-life applications.

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