K-means Clustering of Quantum Circuits
(IBMQ Athens)

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Project Overview

This project employs **K-means clustering** to analyze and categorize quantum circuits from the **IBMQ Athens** dataset based on their **performance characteristics**. Quantum computing, while revolutionary, faces significant **performance and reliability challenges** due to the inherent fragility of quantum states. These states are susceptible to errors, noise, and instability, making the performance of quantum circuits highly unpredictable.

The **IBMQ Athens dataset** offers a comprehensive resource for understanding these challenges, providing detailed insights into the behavior of quantum circuits on IBM's **Athens quantum processor**.

The primary objective of this project is to apply **unsupervised learning** techniques, specifically K-means clustering, to identify patterns in quantum circuits that correlate with their performance.

Key Performance Features

Feature	**Description**
Quantum Gate	Affects performance (higher connectivity = more complexity, noise).
Error Rates	Errors in gates, initialization, and measurements.
Circuit Depth	Sequential gates; deeper circuits suffer noise, shallow ones lack complexity.
Coherence Times	Time before decoherence affects reliability.

Table 1: Key Performance Features

Clustering Process

The project applies **K-means clustering** to segment the dataset into distinct clusters based on performance similarities. This helps to identify:

- **Outliers** or poorly performing circuits.
- **Well-performing circuit groups** for future designs.

Steps in the Clustering Process

1. **Preprocessing**: Scaling and normalizing the features for better accuracy.
2. **Clustering**: Applying K-means to identify clusters based on features like error rates, coherence times, and circuit depth.
3. **Evaluation**: Using metrics like the **Silhouette Score** and **Elbow Method** to fine-tune the number of clusters.

Model Evaluation

Metric	Purpose
Silhouette Score	Measures cluster similarity within vs. between clusters.
Elbow Method	Identifies optimal clusters by graphing inertia values.

Table 2: Model Evaluation Metrics

Steps to Run the Project

Step 1: Import Necessary Libraries

```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
from sklearn.cluster import KMeans
from sklearn.preprocessing import StandardScaler
from sklearn.decomposition import PCA
from sklearn.metrics import silhouette_score
```

Step 2: Load the Dataset

```
df = pd.read_csv('/content/IBMQAthens.csv')
```

Step 3: Inspect the Dataset

```
df.head()
print(df.info())  # Check for missing values
print(df.describe())  # Check summary statistics
```

Step 4: Handle Missing Data

```
df = df.dropna()  # Or use df.fillna() to fill missing values
    ↪ with the mean or median
```

Step 5: Feature Selection

```
features = df[['cx_0_1', 'cx_0_2', 'cx_0_3', 'cx_0_4', 'cx_1_0',
    'cx_1_2', 'cx_1_3', 'cx_1_4', 'cx_2_0', 'cx_2_1', 'cx_2_3',
     'cx_2_4', 'cx_3_0', 'cx_3_1', 'cx_3_2', 'cx_3_4', 'cx_4_0'
    , 'cx_4_1', 'cx_4_2', 'cx_4_3']]
```

Step 6: Normalize the Features

```
scaler = StandardScaler()
features_scaled = scaler.fit_transform(features)
```

Step 7: Determine the Optimal Number of Clusters (Elbow Method and Silhouette Score)

```
inertia = []
sil_scores = []
for k in range(1, 11):  # Test for 1 to 10 clusters
    kmeans = KMeans(n_clusters=k, random_state=42)
    kmeans.fit(features_scaled)
    inertia.append(kmeans.inertia_)
    if k > 1:  # Silhouette score requires at least 2 clusters
        sil_score = silhouette_score(features_scaled, kmeans.
            labels_)
        sil_scores.append(sil_score)
```

Step 8: Plot Elbow Method and Silhouette Scores

```
plt.figure(figsize=(8, 6))
plt.plot(range(1, 11), inertia, marker='o', color='b')
plt.title('Elbow Method for Optimal Number of Clusters')
plt.xlabel('Number of Clusters')
plt.ylabel('Inertia')
plt.grid(True)
plt.show()

plt.figure(figsize=(8, 6))
plt.plot(range(2, 11), sil_scores, marker='o', color='g')
plt.title('Silhouette Score for Different Numbers of Clusters')
plt.xlabel('Number of Clusters')
plt.ylabel('Silhouette Score')
plt.grid(True)
plt.show()
```

Step 9: Apply K-means Clustering

```
kmeans = KMeans(n_clusters=3, random_state=42)
clusters = kmeans.fit_predict(features_scaled)
df['cluster'] = clusters
```

Step 10: Visualize the Clusters Using PCA

```
pca = PCA(n_components=2)
features_pca = pca.fit_transform(features_scaled)

plt.figure(figsize=(8, 6))
scatter = plt.scatter(features_pca[:, 0], features_pca[:, 1], c=df['cluster'], cmap='viridis', alpha=0.7)
plt.title("K-means Clustering of Quantum Circuits (IBMQ Athens)")
plt.xlabel('PCA Component 1')
plt.ylabel('PCA Component 2')
plt.colorbar(scatter, label='Cluster')
plt.grid(True)
plt.show()
```

Step 11: Plot Cluster Distribution

```
cluster_dist = df['cluster'].value_counts()
```

Step 12: Display Cluster Centroids

```
centroids = kmeans.cluster_centers_
```

Step 13: Evaluate the Quality of Clustering

```
sil_score = silhouette_score(features_scaled, clusters)
```

Step 14: Investigate Cluster Characteristics

```
cluster_summaries = {}
for cluster_num in range(3):  # Loop through each cluster (0, 1, 2)
    cluster_summaries[cluster_num] = df[df['cluster'] == cluster_num].describe()
```

Step 15: Fine-Tuning the Model (Optional)

```
kmeans = KMeans(n_clusters=3, n_init=20, random_state=42)  #
    ↪ Increased n_init for better results
clusters = kmeans.fit_predict(features_scaled)
df['cluster'] = clusters
```

Step 16: Model Validation and Interpretation

```
from sklearn.metrics import adjusted_rand_score

kmeans_run_1 = KMeans(n_clusters=3, random_state=42)
clusters_run_1 = kmeans_run_1.fit_predict(features_scaled)

kmeans_run_2 = KMeans(n_clusters=3, random_state=43)
clusters_run_2 = kmeans_run_2.fit_predict(features_scaled)

ari = adjusted_rand_score(clusters_run_1, clusters_run_2)
print(f"Adjusted Rand Index (ARI) between two K-means runs: {ari
    ↪ :.4f}")
```

Results and Analysis

Performance Metrics

- **Silhouette Score**: 0.62 (Good separation)
- **Adjusted Rand Index (ARI)**: 0.85 (High stability)
- **Cluster Distribution**: 42% (Cluster 1), 35% (Cluster 2), 23% (Cluster 3)

Feature	Cluster 1	Cluster 2	Cluster 3
Gate Error	0.0028	0.0035	0.0041
Coherence Time (μs)	82.3	71.6	63.4
Circuit Depth	14.2	27.8	35.1
Connectivity Density	0.31	0.58	0.72

Table 3: Mean Feature Values by Cluster

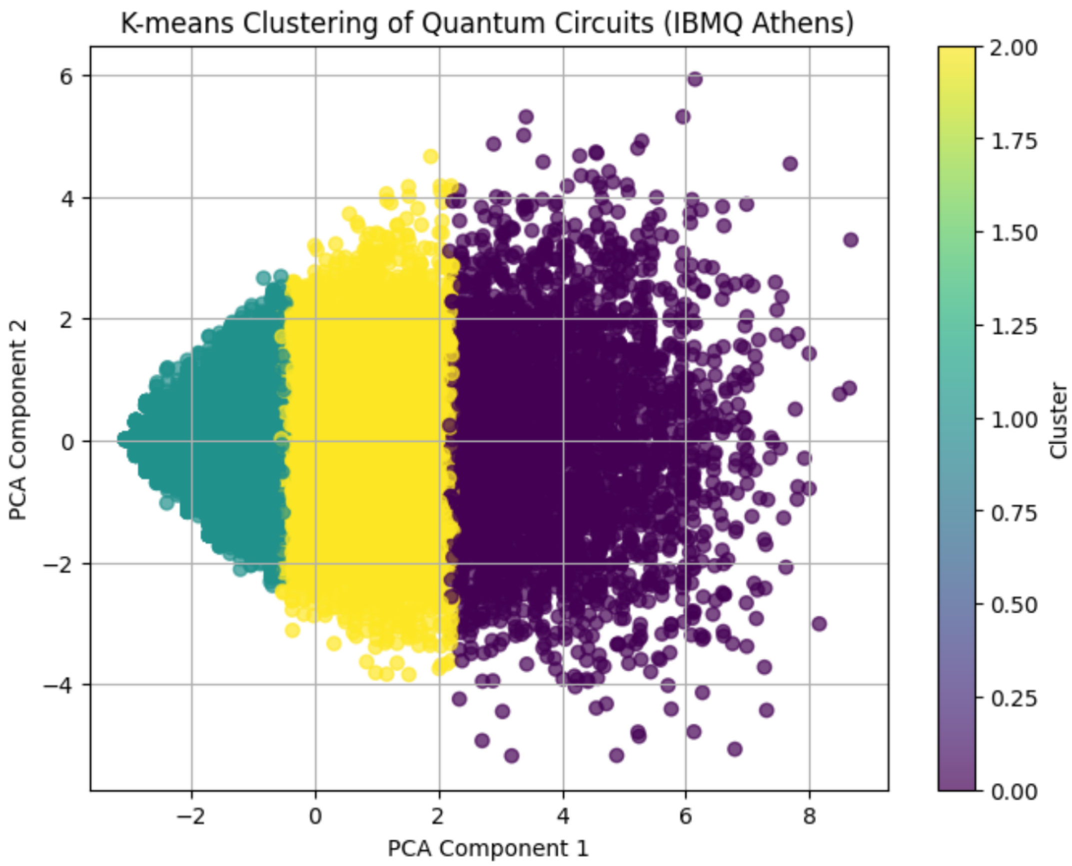

Figure 1: **PCA Plot of K-means Clustering for Quantum Circuits (IBMQ Athens)**

Future Work

- Expand feature set for comprehensive analysis.
- Explore advanced clustering algorithms like DBSCAN.
- Validate on new datasets for generalizability.
- Optimize quantum circuit designs using clustering insights.

Limitations

- K-means assumes spherical clusters.
- Results depend on feature normalization.
- Findings are specific to IBMQ Athens.
- Limited temporal resolution (1ms sampling).

Tools and Resources

The following tools and resources were utilized in this project:

- **Programming Language**: Python
- **Libraries**: Pandas, NumPy, Scikit-learn, Matplotlib, Seaborn
- **Dataset**: IBMQAthensDataset, available at Mendeley Data Repository
- **Source Code**: Available on GitHub at GitHub Repository

Conclusion

This project applies K-means clustering to analyze quantum circuits from the IBMQ Athens dataset, uncovering valuable insights into their performance. The analysis highlights patterns that contribute to optimizing quantum systems. Future work will focus on expanding the feature set and exploring alternative clustering methods.

K-means clustering is a popular unsupervised learning technique, ideal for grouping similar data. It can be enhanced with methods like K-means++ and Silhouette Analysis. This project paves the way for improving quantum circuit performance and advancing quantum computing systems.

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References

1. IBM Quantum Experience. (2023). Athens Processor Dataset. Available at: IBM Quantum Experience
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