report_notebook

November 11, 2025

1 CMPT 459 Assignment 2 Report Notebook

1.1 1. Implement KMeans

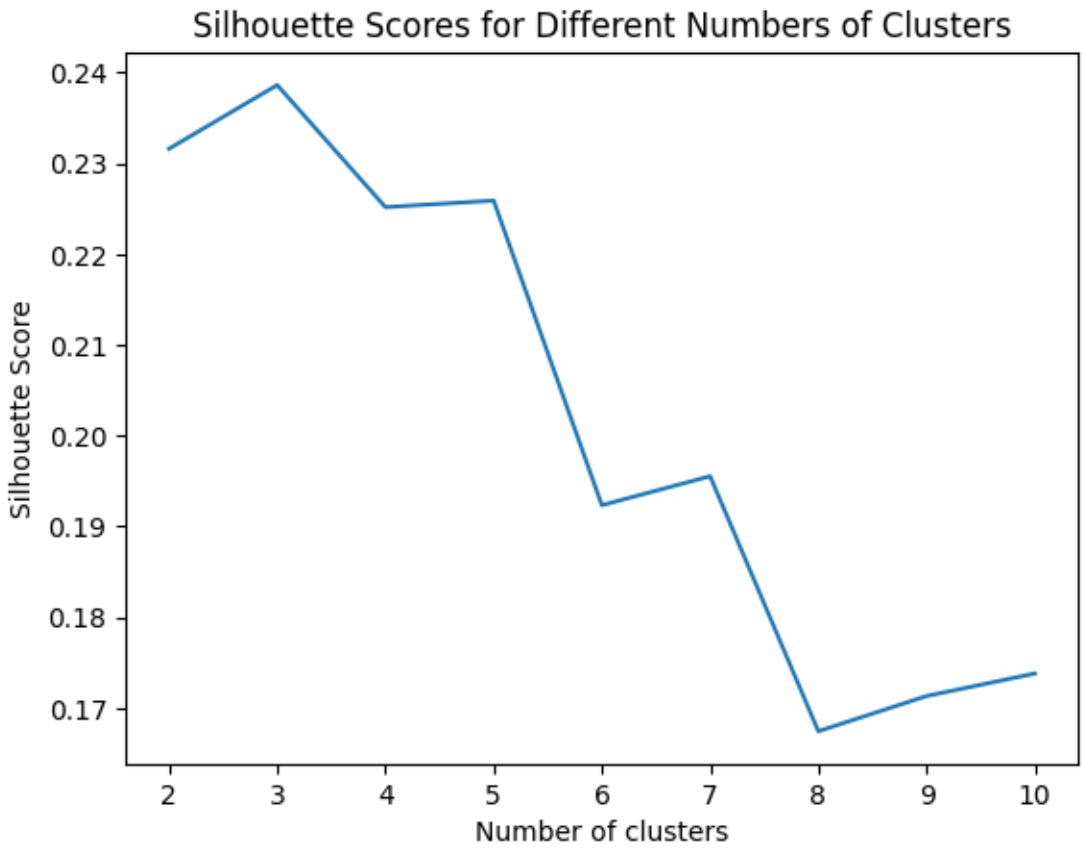
1.2 2. Plot silhouette coefficient for all clustering with random initialization

[6]:
```
import numpy as np
import matplotlib.pyplot as plt
from kmeans import KMeans
from main import read_data, preprocess_data, PCA, visualize_cluster
```

[2]:
```
heart = read_data('scRNAseq_human_pancreas.csv')
heart = preprocess_data(heart)
X = PCA(heart.X, 100)
np.shape(X)
```

[2]:
```
(4359, 100)
```

[3]:
```
silhouette_scores = []
best_clustering_with_random_init = None
best_score_with_random_init = -1
for i in range(2, 11):
    kmeans = KMeans(n_clusters=i, init='random', max_iter=300)
    clustering = kmeans.fit(X)
    score = kmeans.silhouette(clustering, X)
    silhouette_scores.append(score)
    if score > best_score_with_random_init:
        best_score_with_random_init = score
        best_clustering_with_random_init = clustering
plt.plot(range(2, 11), silhouette_scores)
plt.xlabel('Number of clusters')
plt.ylabel('Silhouette Score')
plt.title('Silhouette Scores for Different Numbers of Clusters')
plt.show()
```

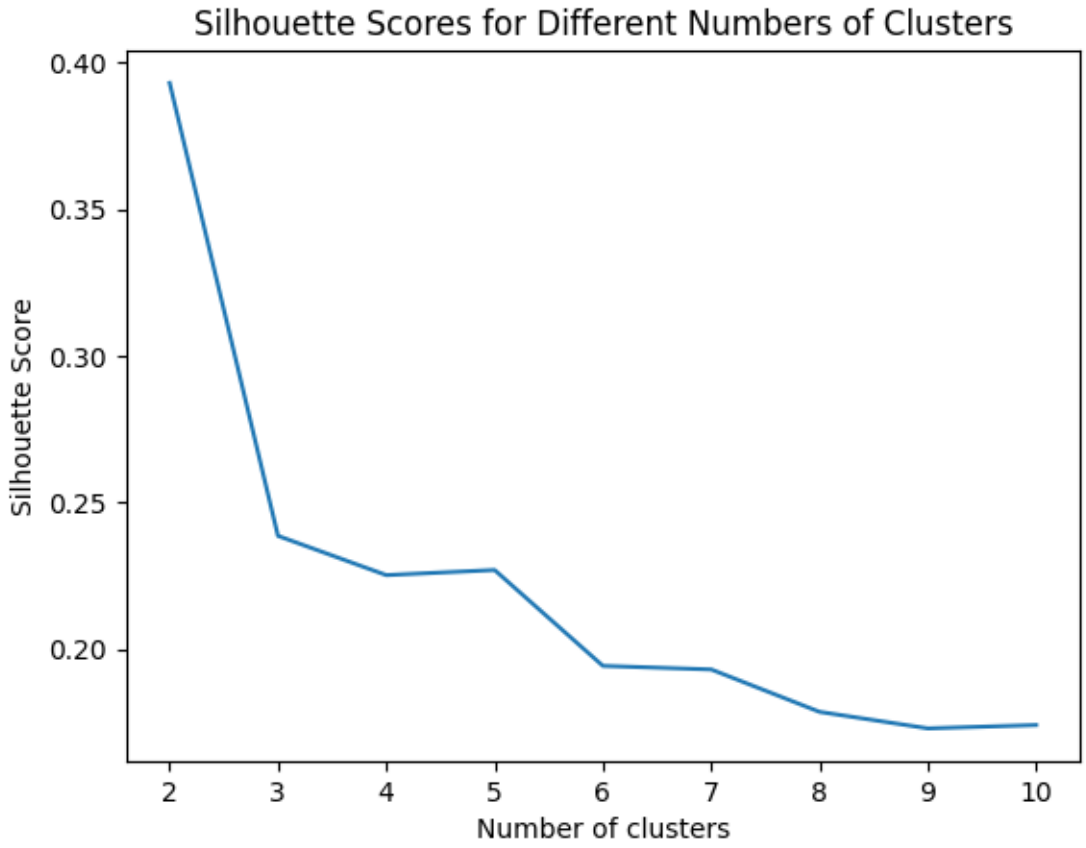


What is the best k? - k = 3 gives the highest silhouette coefficient (global optimum). - k = 2 or k = 5 also gives a high silhouette coefficient, but not as high as k = 3. (local optimum) - We will use k = 3 for the scatter plot visualization.

1.3 3. Plot silhouette coefficient for all clustering with random initialization

[4]:
```
silhouette_scores = []
best_clustering_with_kmeans_init = None
best_score_with_kmeans_init = -1
for i in range(2, 11):
    kmeans = KMeans(n_clusters=i, init='kmeans++', max_iter=300)
    clustering = kmeans.fit(X)
    score = kmeans.silhouette(clustering, X)
    silhouette_scores.append(score)
    if score > best_score_with_kmeans_init:
        best_score_with_kmeans_init = score
        best_clustering_with_kmeans_init = clustering
plt.plot(range(2, 11), silhouette_scores)
plt.xlabel('Number of clusters')
plt.ylabel('Silhouette Score')
```

```
plt.title('Silhouette Scores for Different Numbers of Clusters')
plt.show()
```



What is the best k? - Depend on our goal - If we want to maximize silhouette coefficient, k = 2 is the best choice. - Depends on the domain context, k = 3 or k = 5 might provide more meaningful and interpretable clusters

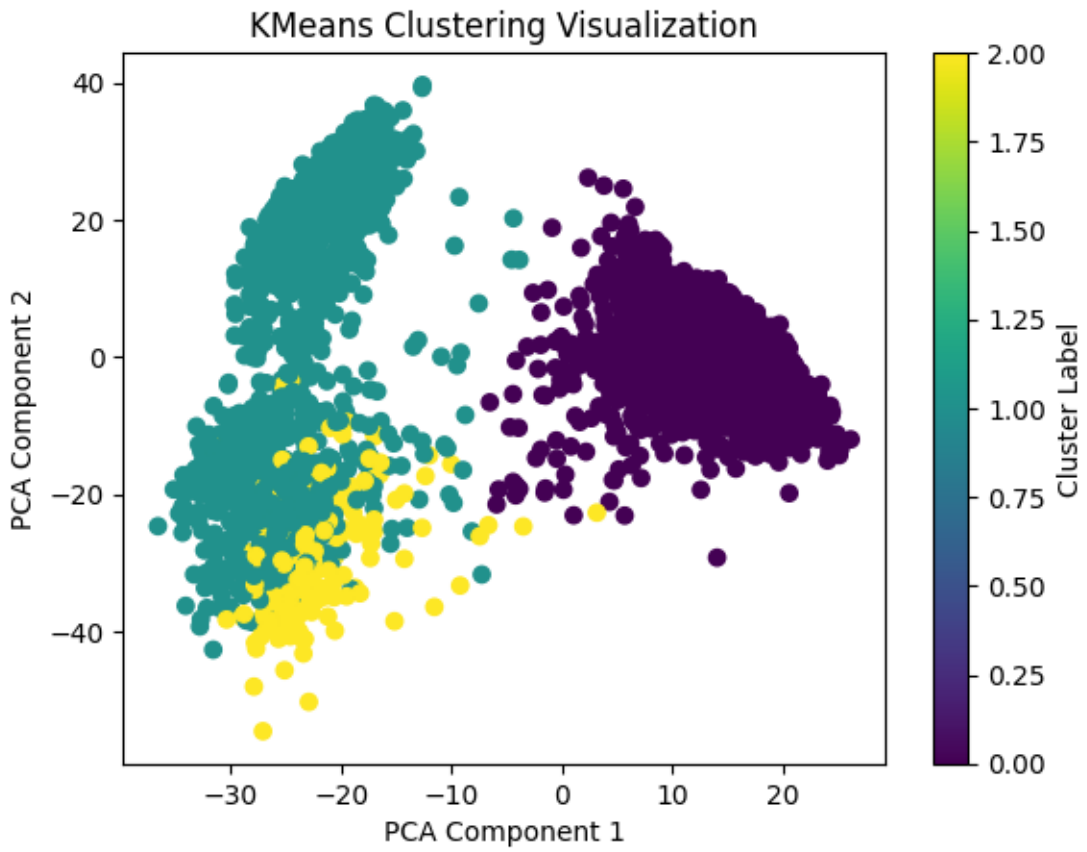
In conclusion, while the silhouette coefficient suggests k = 2 is the mathematically optimal choice for cluster seperation, the local peak at k = 3 or k = 5, combined with the context of the data and objectives of the analysis, might make those values more suitable for practical applications. (We will use k = 2 for the scatter plot visualization below.)

1.4 4. Cluster Scatter Plots

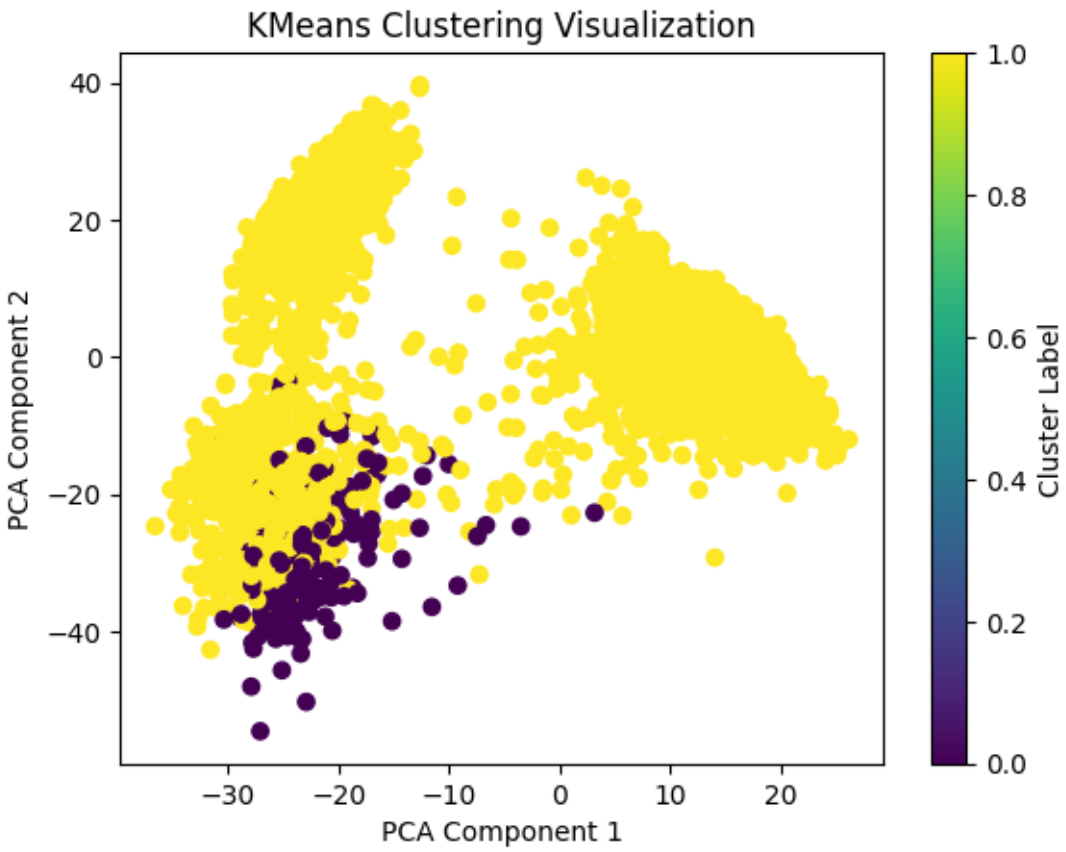
Cluster Scatter Plot with Random Initialization (k=3)

[ ]:
```
X = PCA(X, 2)
```

[17]:
```
visualize_cluster(X[:, 0], X[:, 1], best_clustering_with_random_init)
```



[18]:
```
visualize_cluster(X[:, 0], X[:, 1], best_clustering_with_kmeans_init)
```


KMeans Clustering Visualization
PCA Component 2
PCA Component 1
Cluster Label
40
20
0
−20
−40
−30
−20
−10
0
10
20
1.0
0.8
0.6
0.4
0.2
0.0

[ ]: