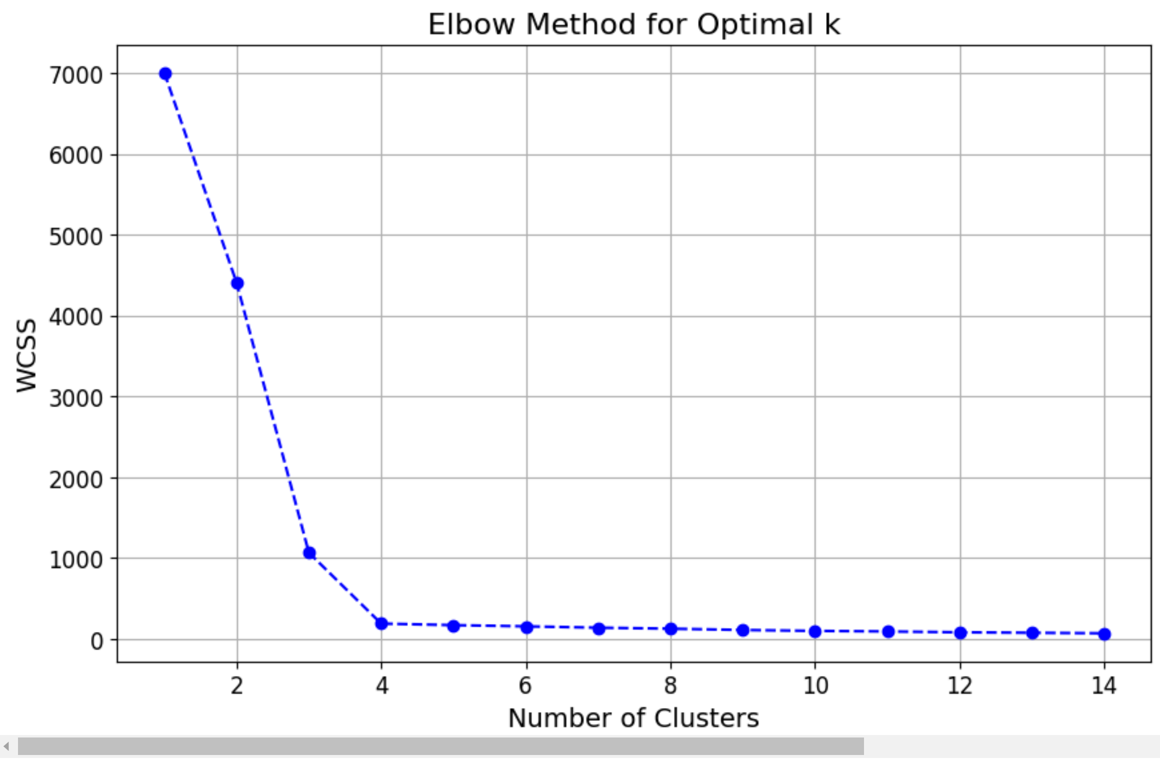
Enhanced Lab04: K-Means

1. Clarifying Concepts

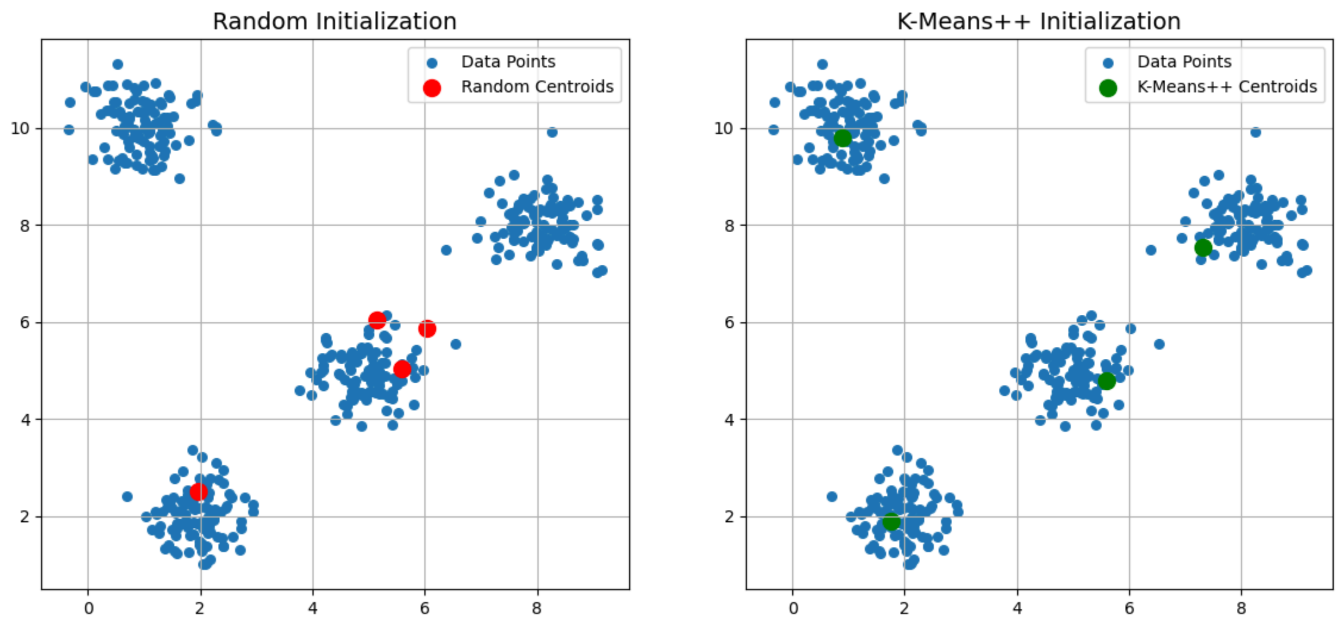
1.1 The Elbow Method and WCSS (Within-Cluster Sum of Squares)

```
import matplotlib.pyplot as plt
import numpy as np
from sklearn.cluster import KMeans

# Generate synthetic data
np.random.seed(42)
data = np.vstack([
    np.random.normal(loc, 0.5, size=(100, 2)) for loc in [(2, 2), (8, 8), (5, 5), (1, 10)]
])


# Calculate WCSS for different k values
wcss = []
for k in range(1, 15):
    kmeans = KMeans(n_clusters=k, init='k-means++', random_state=42)
    kmeans.fit(data)
    wcss.append(kmeans.inertia_)


# Plot the Elbow Method
plt.figure(figsize=(10, 6))
plt.plot(range(1, 15), wcss, marker='o', linestyle='--', color='b')
plt.title('Elbow Method for Optimal k', fontsize=16)
plt.xlabel('Number of Clusters', fontsize=14)
plt.ylabel('WCSS', fontsize=14)
plt.xticks(fontsize=12)
plt.yticks(fontsize=12)
plt.grid(True)
plt.show()
```



1.2 K-Means++ Initialization

```
# Visualizing Random Initialization vs K-Means++
def random_initialization(data, n_clusters):
    np.random.seed(42)
    centroids = data[np.random.choice(data.shape[0], n_clusters, replace=False)]
    return centroids

def kmeans_plus_plus_initialization(data, n_clusters):
    np.random.seed(42)
    centroids = [data[np.random.randint(data.shape[0])]]
    while len(centroids) < n_clusters:
        distances = np.min(
            np.linalg.norm(data[:, np.newaxis] - np.array(centroids), axis=2), axis=1
        )
        probabilities = distances / distances.sum()
        next_centroid = data[np.random.choice(data.shape[0], p=probabilities)]
        centroids.append(next_centroid)
    return np.array(centroids)



# Comparing Initializations
random_centroids = random_initialization(data, 4)
kmeans_pp_centroids = kmeans_plus_plus_initialization(data, 4)

plt.figure(figsize=(14, 6))
plt.subplot(1, 2, 1)
plt.scatter(data[:, 0], data[:, 1], s=30, label='Data Points')
plt.scatter(random_centroids[:, 0], random_centroids[:, 1], color='red', label='Random Centroids', s=100)
plt.title('Random Initialization', fontsize=14)
plt.legend()
plt.grid(True)

plt.subplot(1, 2, 2)
plt.scatter(data[:, 0], data[:, 1], s=30, label='Data Points')
plt.scatter(kmeans_pp_centroids[:, 0], kmeans_pp_centroids[:, 1], color='green', label='K-Means++ Centroids', s=100)
plt.title('K-Means++ Initialization', fontsize=14)
plt.legend()
plt.grid(True)

plt.show()
```



1.3 Theory: K-Means Overview

K-Means Theory

Convergence Criteria:

1. Assign each point to the nearest centroid.
2. Recompute centroids as the mean of assigned points.
3. Repeat until centroid positions stabilize or maximum iterations reached.

Complexity: O(n * k * d * i), where n = samples, k = clusters, d = dimensions, i = iterations.

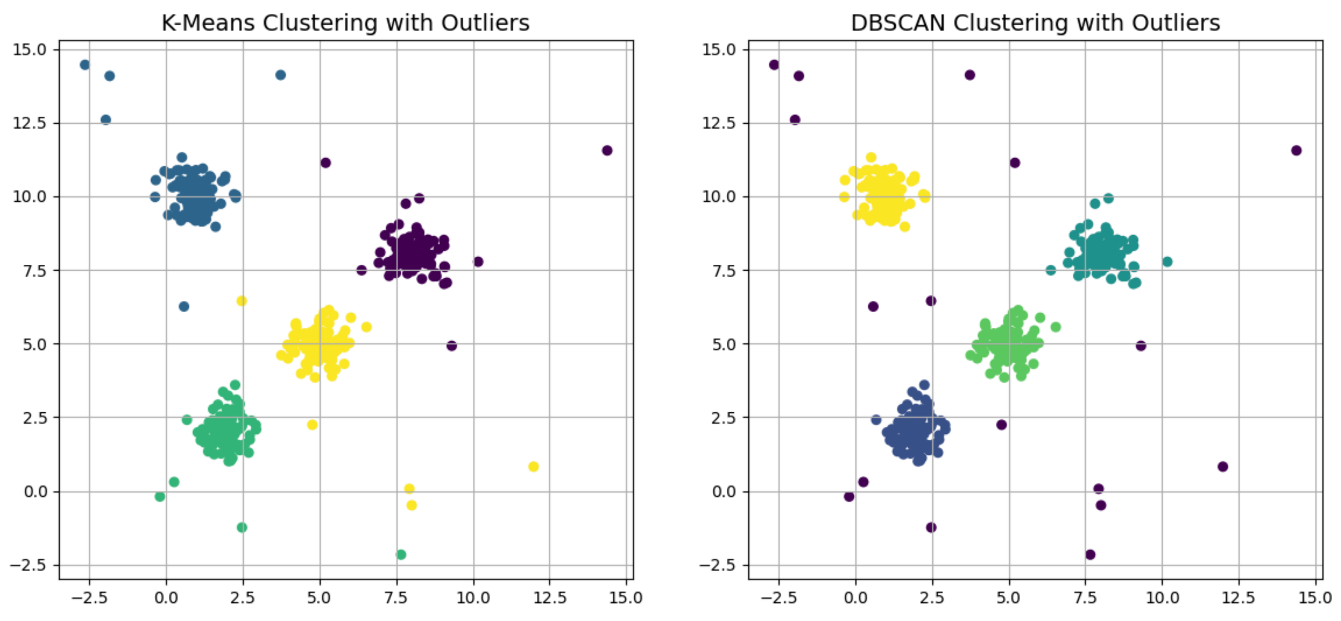
2. Advanced Concepts

2.1 Limitations of K-Means

Limitations of K-Means

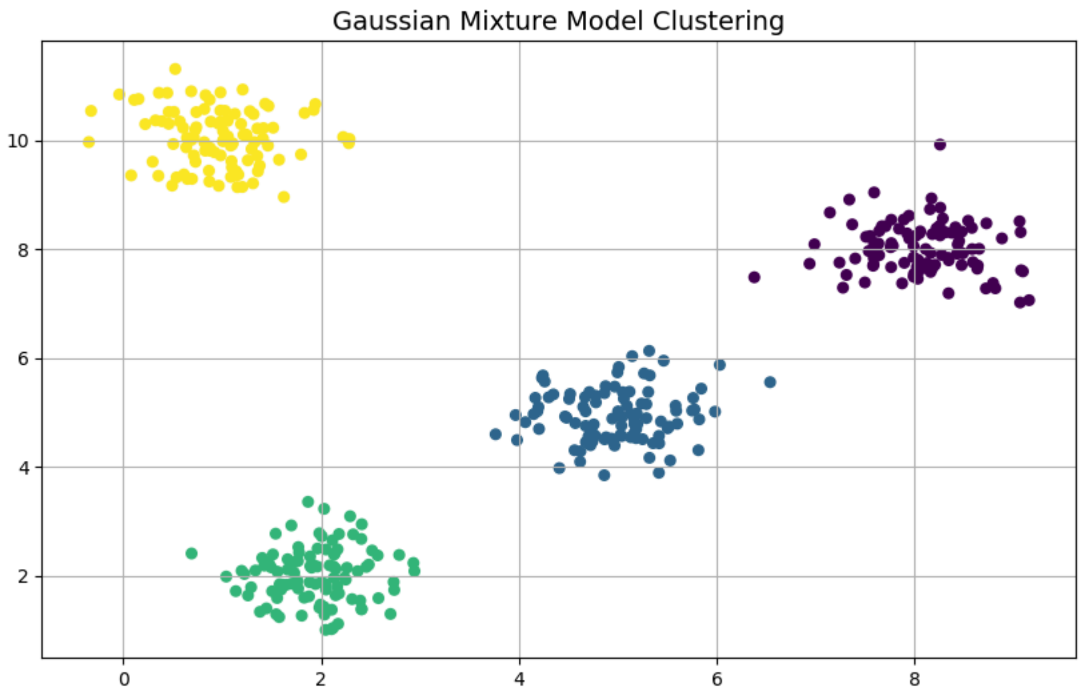
1. Sensitive to initial centroids.
2. Assumes spherical clusters.
3. Poor performance with high-dimensional or categorical data.

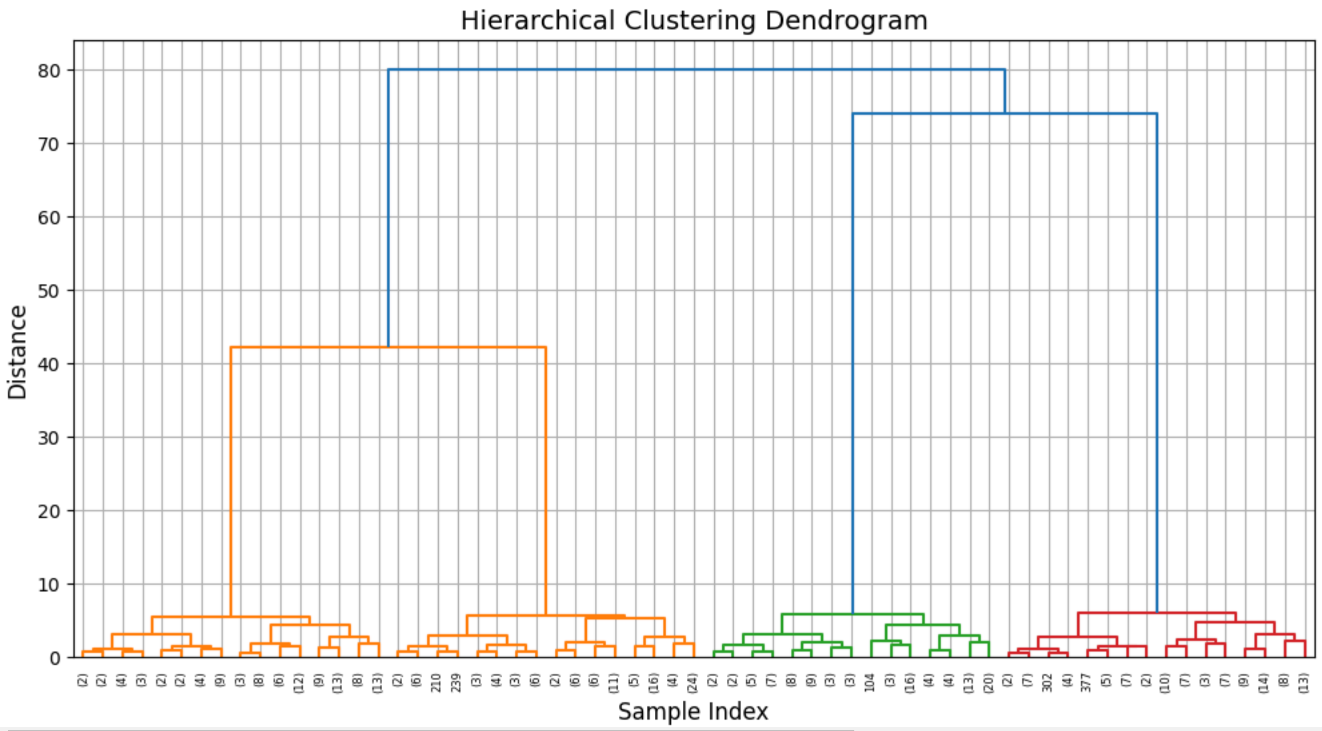
```
# Handling Outliers with Robust K-Means
from sklearn.cluster import DBSCAN

def plot_outliers_effect(data):
    np.random.seed(42)
    noisy_data = np.vstack([
        data,
        np.random.uniform(-3, 15, size=(20, 2))  # Adding outliers
    ])

    kmeans = KMeans(n_clusters=4, random_state=42)
    dbscan = DBSCAN(eps=1.2, min_samples=5)

    kmeans_labels = kmeans.fit_predict(noisy_data)
    dbscan_labels = dbscan.fit_predict(noisy_data)

    plt.figure(figsize=(14, 6))

    plt.subplot(1, 2, 1)
    plt.scatter(noisy_data[:, 0], noisy_data[:, 1], c=kmeans_labels, cmap='viridis', s=30)
    plt.title('K-Means Clustering with Outliers', fontsize=14)
    plt.grid(True)

    plt.subplot(1, 2, 2)
    plt.scatter(noisy_data[:, 0], noisy_data[:, 1], c=dbscan_labels, cmap='viridis', s=30)
    plt.title('DBSCAN Clustering with Outliers', fontsize=14)
    plt.grid(True)

    plt.show()

plot_outliers_effect(data)
```



2.2 Comparison: Gaussian Mixture Models (GMM) and Hierarchical Clustering

```
# Compare with advanced clustering methods
from sklearn.mixture import GaussianMixture
from scipy.cluster.hierarchy import dendrogram, linkage

# GMM Clustering
plt.figure(figsize=(10, 6))
gmm = GaussianMixture(n_components=4, random_state=42).fit(data)
gmm_labels = gmm.predict(data)
plt.scatter(data[:, 0], data[:, 1], c=gmm_labels, cmap='viridis', s=30)
plt.title('Gaussian Mixture Model Clustering', fontsize=14)
plt.grid(True)
plt.show()

# Hierarchical Clustering
linkage_matrix = linkage(data, method='ward')
plt.figure(figsize=(12, 6))
dendrogram(linkage_matrix, truncate_mode='level', p=5)
plt.title('Hierarchical Clustering Dendrogram', fontsize=14)
plt.xlabel('Sample Index', fontsize=12)
plt.ylabel('Distance', fontsize=12)
plt.grid(True)
plt.show()
```





3. Visualizations

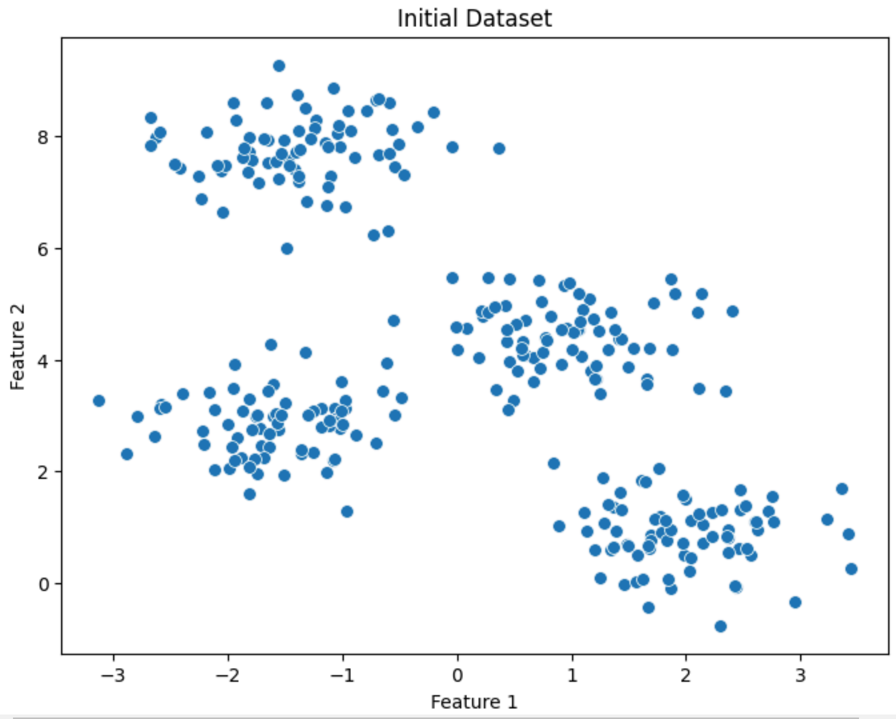
To enhance understanding of K-Means clustering, several visualization techniques are introduced in this section. These visualizations help explain how data points are grouped and how centroids evolve during the clustering process.

3.1 Visualizing the Dataset

Before applying the K-Means algorithm, visualizing the dataset provides insight into its structure and potential clustering.

```
import matplotlib.pyplot as plt
import seaborn as sns
import pandas as pd
from sklearn.datasets import make_blobs

# Generate synthetic dataset for clustering
X, y = make_blobs(n_samples=300, centers=4, cluster_std=0.60, random_state=0)

# Create a DataFrame for better visualization
df = pd.DataFrame(X, columns=['Feature 1', 'Feature 2'])

# Scatter plot of the dataset
plt.figure(figsize=(8, 6))
sns.scatterplot(x='Feature 1', y='Feature 2', data=df, s=50, palette='viridis')
plt.title('Initial Dataset')
plt.show()
```

```
<ipython-input-24-5fccb8aab080>:14: UserWarning: Ignoring `palette` because no `hue` variable has been assigned.
  sns.scatterplot(x='Feature 1', y='Feature 2', data=df, s=50, palette='viridis')
```

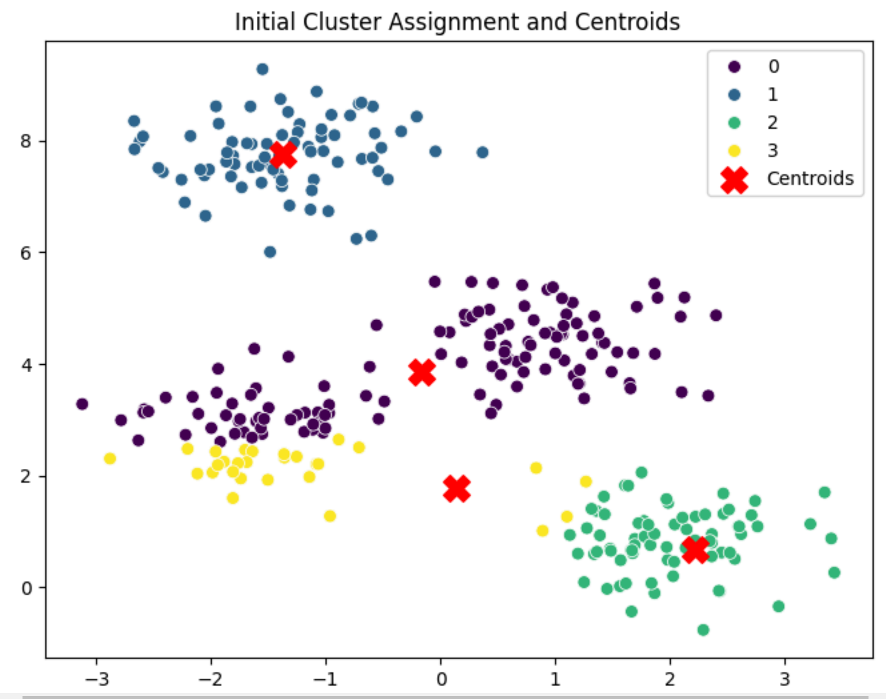


3.2 Visualizing the Clustering Process

Here, we visualize the clustering process, including the assignment of data points to clusters and the movement of centroids over iterations.

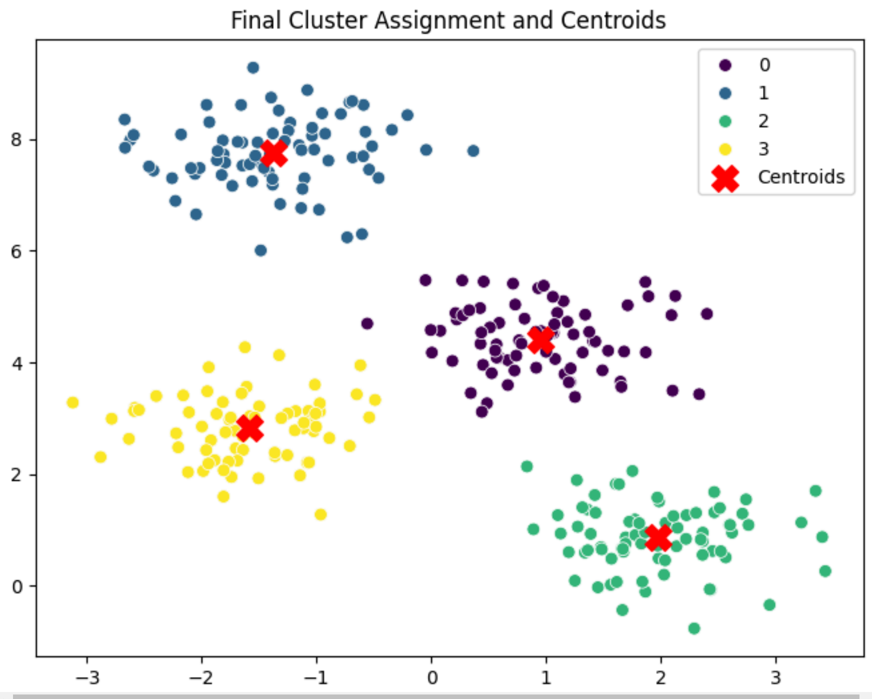
3.2.1 Initial Centroids and Data Assignment

```
from sklearn.cluster import KMeans
import numpy as np

# Initialize KMeans with 4 clusters
kmeans = KMeans(n_clusters=4, init='random', n_init=1, max_iter=1, random_state=0)
kmeans.fit(X)

# Initial cluster assignment and centroids
labels = kmeans.labels_
centroids = kmeans.cluster_centers_

# Plot initial clusters
plt.figure(figsize=(8, 6))
sns.scatterplot(x=X[:, 0], y=X[:, 1], hue=labels, palette='viridis', s=50)
plt.scatter(centroids[:, 0], centroids[:, 1], s=200, c='red', marker='X', label='Centroids')
plt.title('Initial Cluster Assignment and Centroids')
plt.legend()
plt.show()
```



3.2.2 Iterative Updates of Centroids

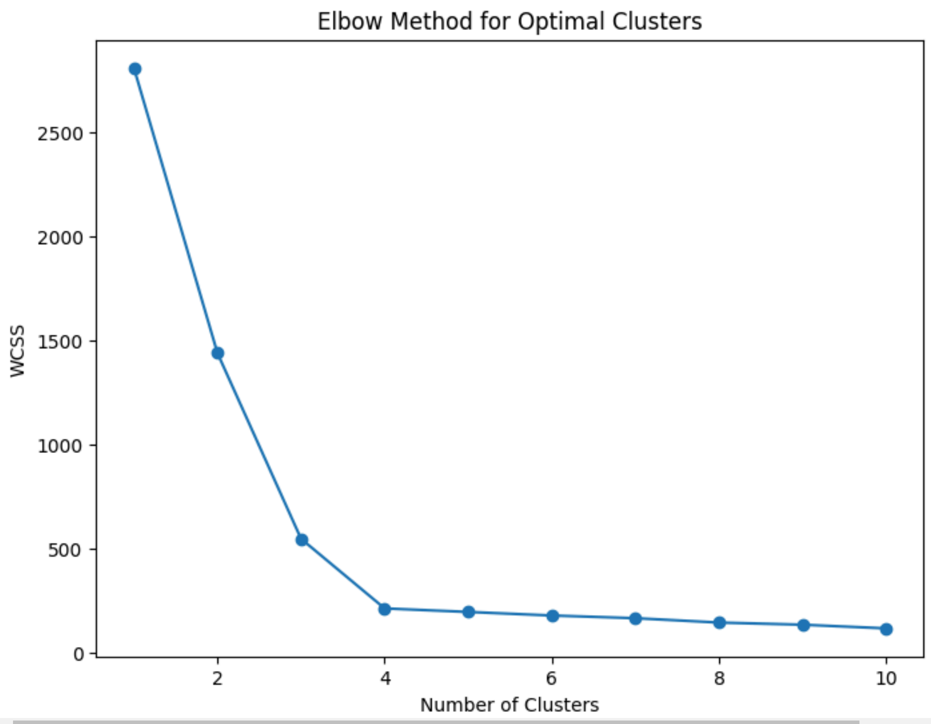
```
# Perform multiple iterations of KMeans
kmeans = KMeans(n_clusters=4, init='random', max_iter=5, random_state=0)
kmeans.fit(X)

# Extract labels and centroids after clustering
labels = kmeans.labels_
centroids = kmeans.cluster_centers_

# Plot final clusters
plt.figure(figsize=(8, 6))
sns.scatterplot(x=X[:, 0], y=X[:, 1], hue=labels, palette='viridis', s=50)
plt.scatter(centroids[:, 0], centroids[:, 1], s=200, c='red', marker='X', label='Centroids')
plt.title('Final Cluster Assignment and Centroids')
plt.legend()
plt.show()
```



3.3 Cluster Quality Assessment

We assess the quality of the clusters using the elbow method, which plots the within-cluster sum of squares (WCSS) for different numbers of clusters.

```
wcss = []
for i in range(1, 11):
    kmeans = KMeans(n_clusters=i, init='k-means++', random_state=0)
    kmeans.fit(X)
    wcss.append(kmeans.inertia_)

# Plot WCSS vs. number of clusters
plt.figure(figsize=(8, 6))
plt.plot(range(1, 11), wcss, marker='o')
plt.title('Elbow Method for Optimal Clusters')
plt.xlabel('Number of Clusters')
plt.ylabel('WCSS')
plt.show()
```

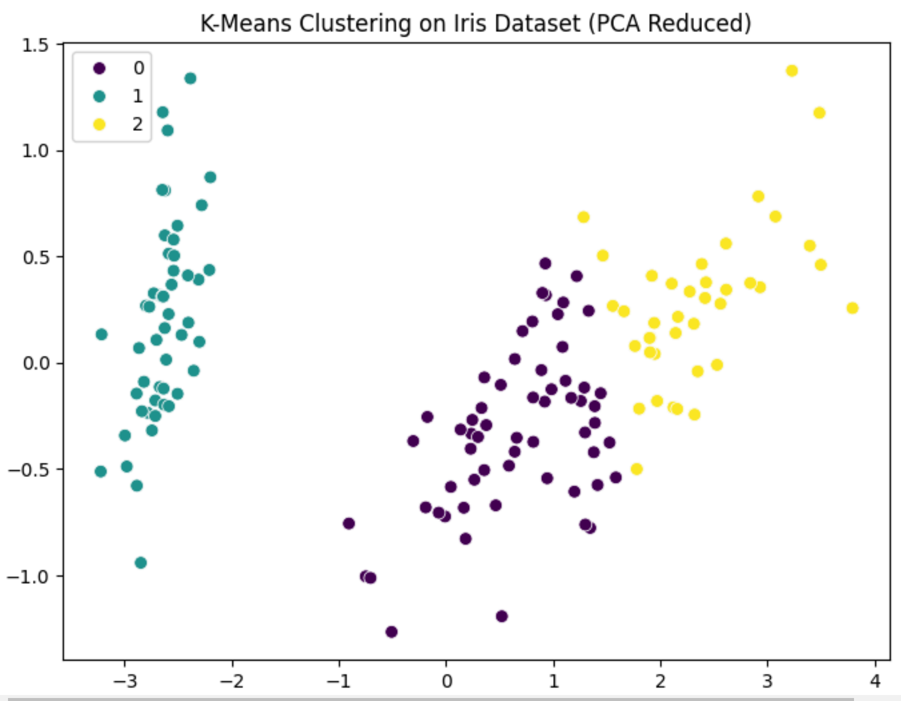


3.4 Visualizing Real-World Applications

3.4.1 Iris Dataset

Using the Iris dataset, we demonstrate clustering and visualize the results in two dimensions.

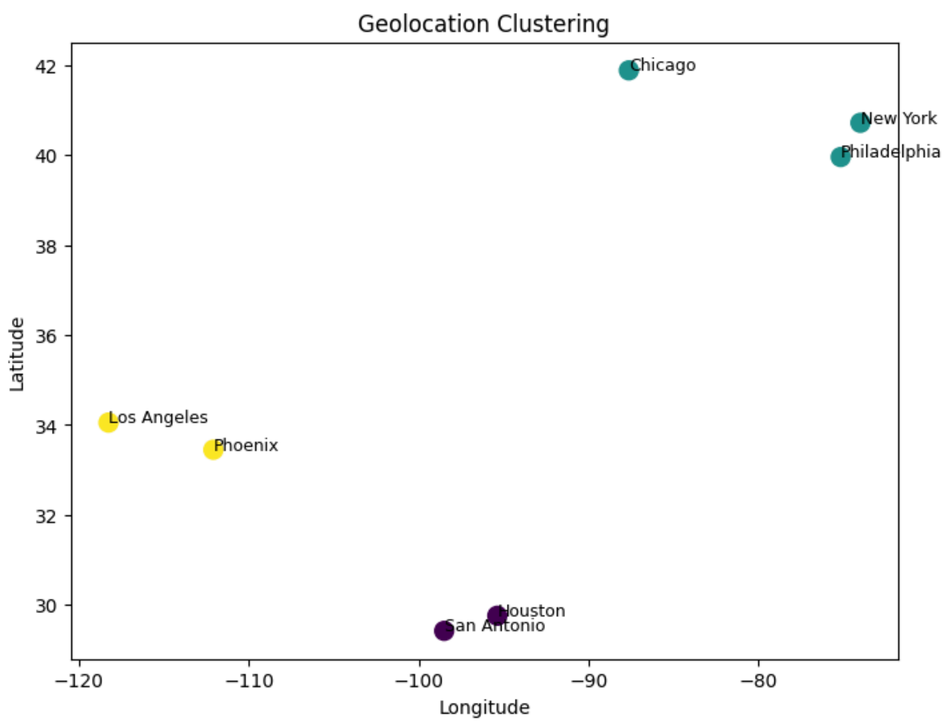
```
from sklearn.datasets import load_iris
from sklearn.decomposition import PCA

iris = load_iris()
X_iris = iris.data
y_iris = iris.target

# Reduce to two dimensions for visualization
pca = PCA(n_components=2)
X_pca = pca.fit_transform(X_iris)

# Apply KMeans
kmeans = KMeans(n_clusters=3, random_state=0)
kmeans.fit(X_pca)
labels = kmeans.labels_

# Plot clusters
plt.figure(figsize=(8, 6))
sns.scatterplot(x=X_pca[:, 0], y=X_pca[:, 1], hue=labels, palette='viridis', s=50)
plt.title('K-Means Clustering on Iris Dataset (PCA Reduced)')
plt.show()
```



3.4.2 Geolocation Data

Clustering geolocations using K-Means.

```
geolocation_data = pd.DataFrame({
    'City': ['New York', 'Los Angeles', 'Chicago', 'Houston', 'Phoenix', 'Philadelphia', 'San Antonio'],
    'Latitude': [40.7128, 34.0522, 41.8781, 29.7604, 33.4484, 39.9526, 29.4241],
    'Longitude': [-74.0060, -118.2437, -87.6298, -95.3698, -112.0740, -75.1652, -98.4936]
})

# Apply KMeans
kmeans = KMeans(n_clusters=3, random_state=0)
labels = kmeans.fit_predict(geolocation_data[['Latitude', 'Longitude']])

# Visualize clusters
plt.figure(figsize=(8, 6))
plt.scatter(geolocation_data['Longitude'], geolocation_data['Latitude'], c=labels, cmap='viridis', s=100)
plt.title('Geolocation Clustering')
for i, city in enumerate(geolocation_data['City']):
    plt.text(geolocation_data['Longitude'][i], geolocation_data['Latitude'][i], city, fontsize=9)
plt.xlabel('Longitude')
plt.ylabel('Latitude')
plt.show()
```


Geolocation Clustering
Chicago
New York
Philadelphia
Los Angeles
Phoenix
Houston
San Antonio
Latitude
Longitude