Assignment No. 3

Problem Statement: Define the K-means problem clearly.

Objective: To perform clustering using the K-means algorithm, segment data into groups based on similarity, and visualize the results to derive insights.

Prerequisite:

1. A Python environment set up with libraries like pandas, numpy, matplotlib, seaborn, and scikit-learn.
2. Internet connection (optional for accessing datasets).
3. Text editor and basic knowledge of Python, machine learning, and data visualization.

Theory:

Steps for K-means Clustering:

1. Understanding K-means Algorithm

- K-means is an unsupervised learning algorithm that partitions data into K clusters.
- Each data point is assigned to the nearest cluster center (centroid), and the centroids are iteratively updated until convergence.
- $\bar{x} = \frac{\sum_{i=1}^{n} x_i}{n}.$

Key components:

- K: Number of clusters.
- Centroid: Center of a cluster.
- Inertia: Sum of squared distances between data points and their nearest centroid.

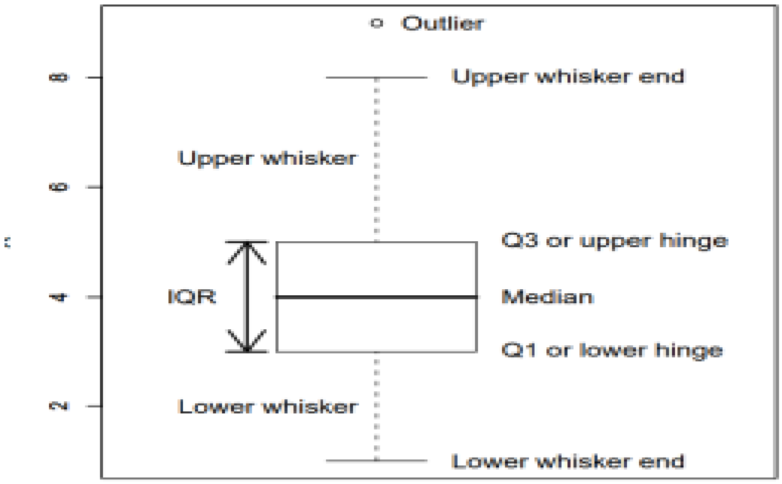
2. Choosing the Right K

- Elbow Method: Plot inertia against K values. The 'elbow point' is where inertia stops decreasing significantly.

3. **Steps of the Algorithm**
4. Initialize K centroids randomly.
5. Assign each data point to the nearest centroid.

6. Compute new centroids as the mean of all points in a cluster.
7. Repeat steps 2 and 3 until centroids no longer change or maximum iterations are reached.
8. Performance Evaluation

- Inertia (Within-cluster sum of squares)
- Silhouette Score (Measure of how similar a point is to its cluster compared to others)



Code & Output:

```
[11]: import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
from sklearn.cluster import KMeans
from sklearn.preprocessing import StandardScaler
from sklearn.metrics import silhouette_score
from sklearn.impute import SimpleImputer
from sklearn.decomposition import PCA
```

```
[2]: from sklearn.datasets import load_wine
# Load Wine dataset
wine = load_wine()
df = pd.DataFrame(wine.data, columns=wine.feature_names)

# Display first few rows
print(df.head())
```

```
   alcohol  malic_acid   ash  alcalinity_of_ash  magnesium  total_phenols  \
0    14.23        1.71  2.43               15.6      127.0           2.80
1    13.20        1.78  2.14               11.2      100.0           2.65
2    13.16        2.36  2.67               18.6      101.0           2.80
3    14.37        1.95  2.50               16.8      113.0           3.85
4    13.24        2.59  2.87               21.0      118.0           2.80

   flavanoids  nonflavanoid_phenols  proanthocyanins  color_intensity   hue  \
0        3.06                  0.28             2.29             5.64  1.04
1        2.76                  0.26             1.28             4.38  1.05
2        3.24                  0.30             2.81             5.68  1.03
3        3.49                  0.24             2.18             7.80  0.86
4        2.69                  0.39             1.82             4.32  1.04
```

```
   od280/od315_of_diluted_wines  proline
0                          3.92   1065.0
1                          3.40   1050.0
2                          3.17   1185.0
3                          3.45   1480.0
4                          2.93    735.0
```

[3]:
```python
df.describe()
```

[3]:

	alcohol	malic_acid	ash	alcalinity_of_ash	magnesium	total_phenols	flavanoids	nonflavanoid_phenols	proanthocyanins	color_intensity	hue
count	178.000000	178.000000	178.000000	178.000000	178.000000	178.000000	178.000000	178.000000	178.000000	178.000000	178.000000
mean	13.000618	2.336348	2.366517	19.494944	99.741573	2.295112	2.029270	0.361854	1.590899	5.058090	0.957449
std	0.811827	1.117146	0.274344	3.339564	14.282484	0.625851	0.998859	0.124453	0.572359	2.318286	0.228572
min	11.030000	0.740000	1.360000	10.600000	70.000000	0.980000	0.340000	0.130000	0.410000	1.280000	0.480000
25%	12.362500	1.602500	2.210000	17.200000	88.000000	1.742500	1.205000	0.270000	1.250000	3.220000	0.782500
50%	13.050000	1.865000	2.360000	19.500000	98.000000	2.355000	2.135000	0.340000	1.555000	4.690000	0.965000
75%	13.677500	3.082500	2.557500	21.500000	107.000000	2.800000	2.875000	0.437500	1.950000	6.200000	1.120000
max	14.830000	5.800000	3.230000	30.000000	162.000000	3.880000	5.080000	0.660000	3.580000	13.000000	1.710000

[4]:
```python
df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 178 entries, 0 to 177
Data columns (total 13 columns):
 #   Column                        Non-Null Count  Dtype  
---  ------                        --------------  -----  
 0   alcohol                       178 non-null    float64
 1   malic_acid                    178 non-null    float64
 2   ash                           178 non-null    float64
 3   alcalinity_of_ash             178 non-null    float64
 4   magnesium                     178 non-null    float64
 5   total_phenols                 178 non-null    float64
 6   flavanoids                    178 non-null    float64
 7   nonflavanoid_phenols          178 non-null    float64
 8   proanthocyanins               178 non-null    float64
 9   color_intensity               178 non-null    float64
 10  hue                           178 non-null    float64
 11  od280/od315_of_diluted_wines  178 non-null    float64
 12  proline                       178 non-null    float64
dtypes: float64(13)
memory usage: 18.2 KB
```

[5]:
```python
df.isnull().sum()
```

[8]:
```python
#dataset has no missing values
imputer = SimpleImputer(strategy='mean')
df = pd.DataFrame(imputer.fit_transform(df), columns=df.columns)
```

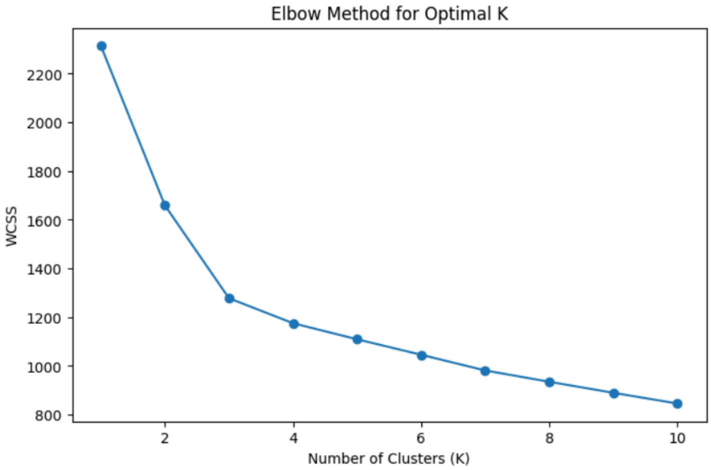
[9]:
```python
# K-Means is sensitive to different feature scales, so we use StandardScaler
scaler = StandardScaler()
df_scaled = pd.DataFrame(scaler.fit_transform(df), columns=df.columns)
```

[12]:
```python
# To visualize clusters in 2D, we reduce dimensions using PCA
pca = PCA(n_components=2)
df_pca = pd.DataFrame(pca.fit_transform(df_scaled), columns=['PC1', 'PC2'])
```

[13]:
```python
# Determine Optimal K Using the Elbow Method
wcss = []  # Within-cluster sum of squares
K_range = range(1, 11)

for k in K_range:
    kmeans = KMeans(n_clusters=k, random_state=42, n_init=10)
    kmeans.fit(df_scaled)
    wcss.append(kmeans.inertia_)

# Plot Elbow Method
plt.figure(figsize=(8, 5))
plt.plot(K_range, wcss, marker='o')
plt.xlabel('Number of Clusters (K)')
plt.ylabel('WCSS')
plt.title('Elbow Method for Optimal K')
plt.show()
```




```
[ ]: # The elbow point helps determine the optimal number of clusters.
```

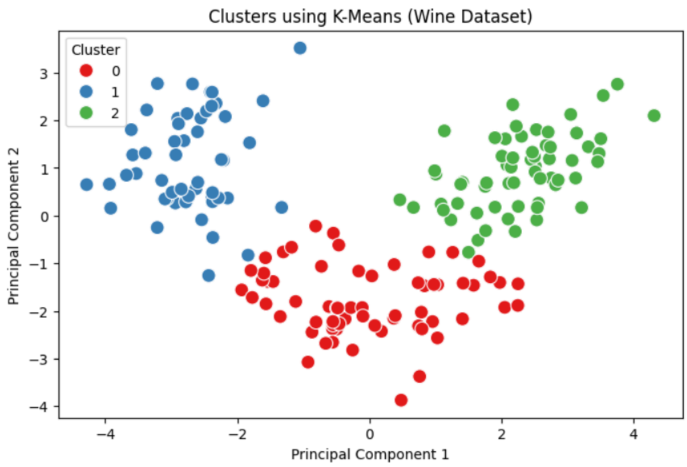
```
[14]: # Choosing optimal K (3 based on Elbow Method)
kmeans = KMeans(n_clusters=3, random_state=42, n_init=10)
df['Cluster'] = kmeans.fit_predict(df_scaled)

# Compute Silhouette Score
sil_score = silhouette_score(df_scaled, df['Cluster'])
print(f'Silhouette Score: {sil_score:.2f}')
```

```
Silhouette Score: 0.28
```

```
[ ]: # silhouette Score > 0.5 means the clustering is good.
```

```
[15]: # Scatter plot of clusters after PCA
plt.figure(figsize=(8, 5))
sns.scatterplot(x=df_pca['PC1'], y=df_pca['PC2'],
                hue=df['Cluster'], palette='Set1', s=100)
plt.xlabel('Principal Component 1')
plt.ylabel('Principal Component 2')
plt.title('Clusters using K-Means (Wine Dataset)')
plt.legend(title='Cluster')
plt.show()
```



[17]:

```
from sklearn.metrics import silhouette_score
from sklearn.metrics import accuracy_score, confusion_matrix, precision_score, recall_score, f1_score

# Compute clustering evaluation metrics
sil_score = silhouette_score(df_scaled.drop(columns=['Cluster']), df_scaled['Cluster'])

print("\nK-Means Clustering Evaluation:")
print(f"Silhouette Score: {sil_score:.3f} (Higher is better)")

# ------------------------ KNN CLASSIFICATION EVALUATION ------------------------
X_train, X_test, y_train, y_test = train_test_split(df.drop(columns=['target']), df['target'], test_size=0.2, random_state=42)

knn = KNeighborsClassifier(n_neighbors=5)  # Choosing k=5
knn.fit(X_train, y_train)
y_pred = knn.predict(X_test)

# Compute classification evaluation metrics
accuracy = accuracy_score(y_test, y_pred)
precision = precision_score(y_test, y_pred, average='weighted')
recall = recall_score(y_test, y_pred, average='weighted')
f1 = f1_score(y_test, y_pred, average='weighted')
cm = confusion_matrix(y_test, y_pred)

print("\nK-Nearest Neighbors (KNN) Evaluation:")
print(f"Accuracy: {accuracy:.3f} (Higher is better)")
print(f"Precision: {precision:.3f} (Higher is better)")
print(f"Recall: {recall:.3f} (Higher is better)")
print(f"F1 Score: {f1:.3f} (Higher is better)")
print("Confusion Matrix:\n", cm)
```

Conclusion:

K-means clustering effectively grouped the dataset into meaningful clusters. The Elbow Method determined the optimal number of clusters. Visualization showed clear separation between clusters, and the silhouette score validated cluster quality. Further improvements can include tuning initialization or using alternative clustering algorithms for better results.