CS598 PSL — Assignment 1 — Problem 1

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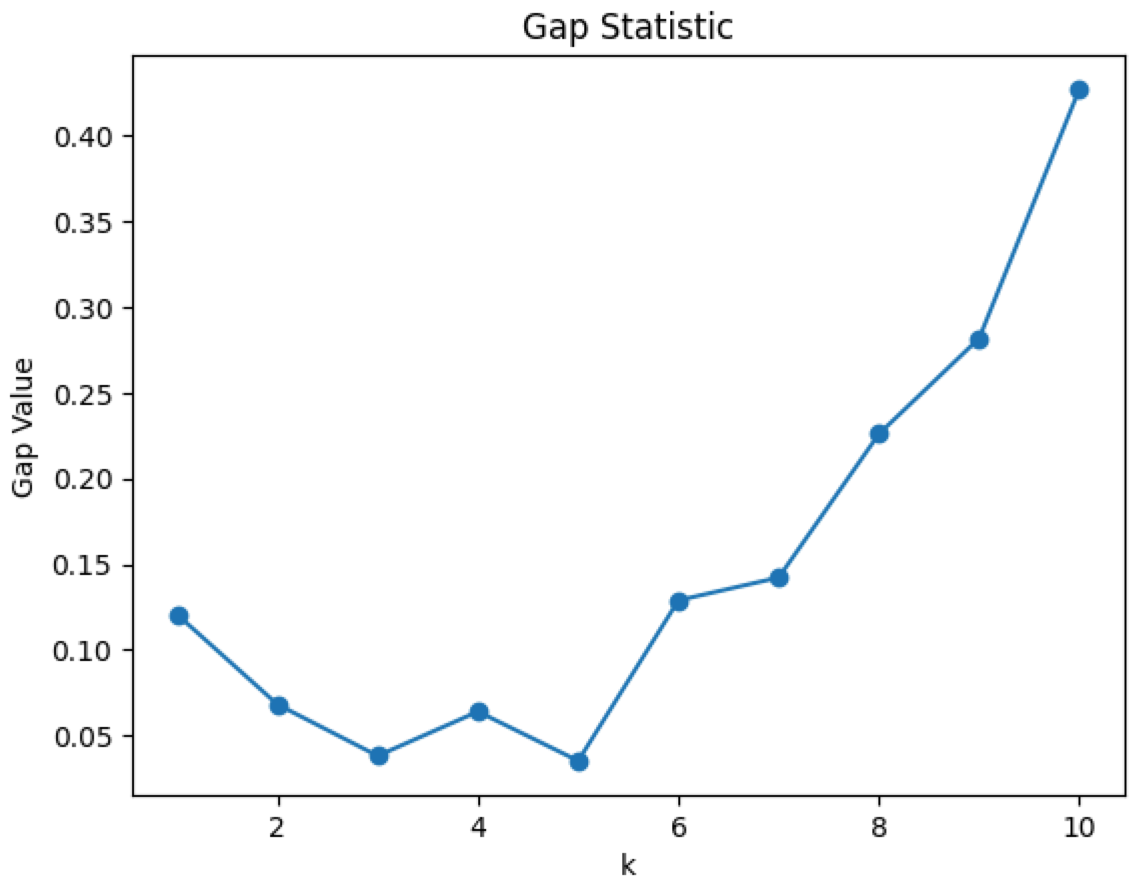
Question 1

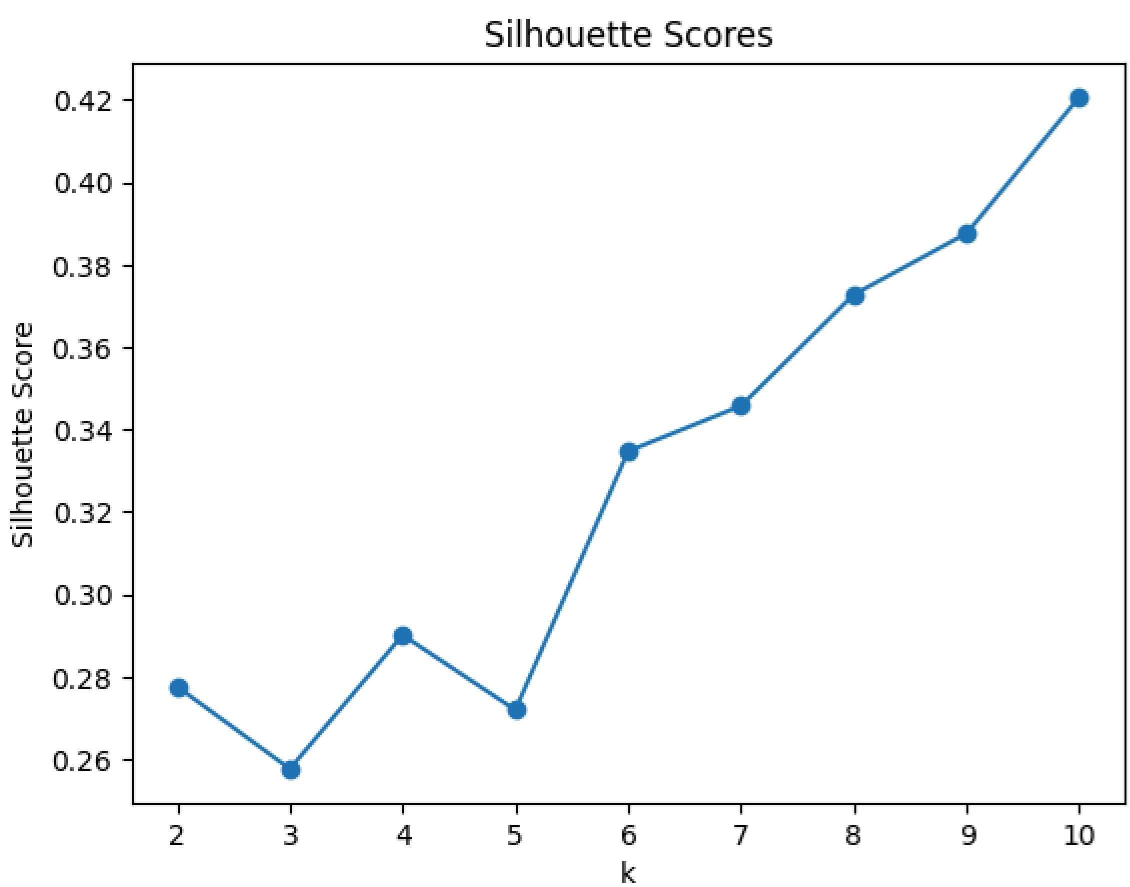
In [1]:
```
#Question 1a
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns

from sklearn.preprocessing import StandardScaler
from sklearn.cluster import KMeans
from sklearn.metrics import silhouette_score

def gap_statistic(X, refs=10, max_clusters=10, random_state=42):
    np.random.seed(random_state)
    shape = X.shape
    tops = X.max(axis=0)
    bottoms = X.min(axis=0)
    dists = np.zeros((refs, shape[0], shape[1]))

    for i in range(refs):
        dists[i] = np.random.uniform(bottoms, tops, size=shape)

    gaps = []
    for k in range(1, max_clusters + 1):
        km = KMeans(n_clusters=k, random_state=random_state).fit(X)
        disp = km.inertia_

        ref_disps = np.zeros(refs)
        for i in range(refs):
            km_ref = KMeans(n_clusters=k, random_state=random_state).fit(dis
            ref_disps[i] = km_ref.inertia_

        gap = np.log(np.mean(ref_disps)) - np.log(disp)
        gaps.append(gap)

    optimal_k = np.argmax(gaps) + 1
    return optimal_k, gaps


df = pd.read_csv("/content/Mall_Customers.csv")

df_encoded = pd.get_dummies(df, columns=["Genre"], drop_first=True)

features = ["Age", "Annual Income (k$)", "Spending Score (1-100)", "Genre_Ma

X = df_encoded[features]
```

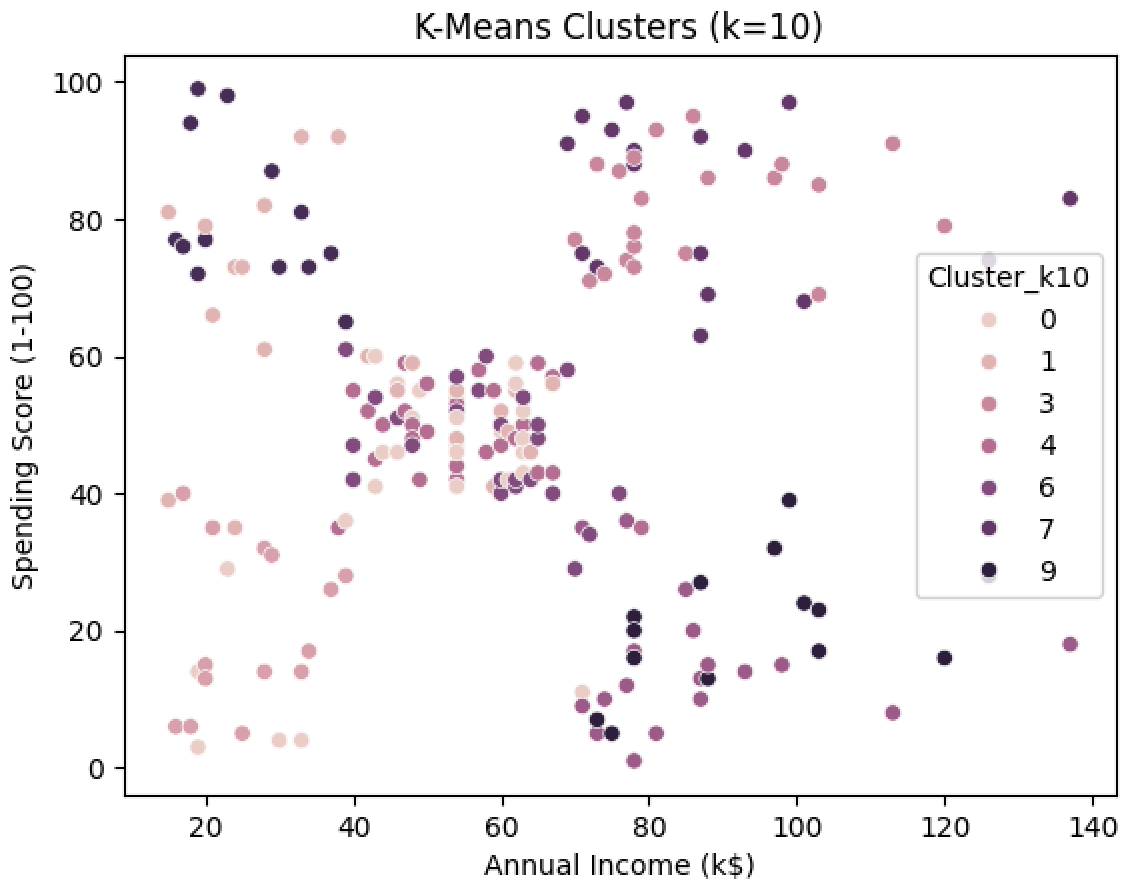
```
scaler = StandardScaler()
X_scaled = scaler.fit_transform(X)



n_clusters_gap, gaps = gap_statistic(X_scaled, refs=10, max_clusters=10)
print("Optimal k (Gap Statistic):", n_clusters_gap)

plt.plot(range(1, 11), gaps, marker='o')
plt.xlabel("k")
plt.ylabel("Gap Value")
plt.title("Gap Statistic")
plt.show()


sil_scores = []
K = range(2, 11)

for k in K:
    km = KMeans(n_clusters=k, random_state=42)
    labels = km.fit_predict(X_scaled)
    sil_scores.append(silhouette_score(X_scaled, labels))

ksil = K[np.argmax(sil_scores)]
print("Optimal k (Silhouette Score):", ksil)

plt.plot(K, sil_scores, marker="o")
plt.xlabel("k")
plt.ylabel("Silhouette Score")
plt.title("Silhouette Scores")
plt.show()

k_values = [n_clusters_gap, ksil]

for k in k_values:
    km = KMeans(n_clusters=k, random_state=42)
    df_encoded[f"Cluster_k{k}"] = km.fit_predict(X_scaled)

for k in k_values:
    sns.scatterplot(
        data=df_encoded,
        x="Annual Income (k$)",
        y="Spending Score (1-100)",
        hue=f"Cluster_k{k}"
    )
    plt.title(f"K-Means Clusters (k={k})")
    plt.show()

for k in k_values:
    print("\n Summary for k =", k, "")
    print(
        df_encoded.groupby(f"Cluster_k{k}")[
            ["Age", "Annual Income (k$)", "Spending Score (1-100)", "Genre_M
        ].mean()
    )
```

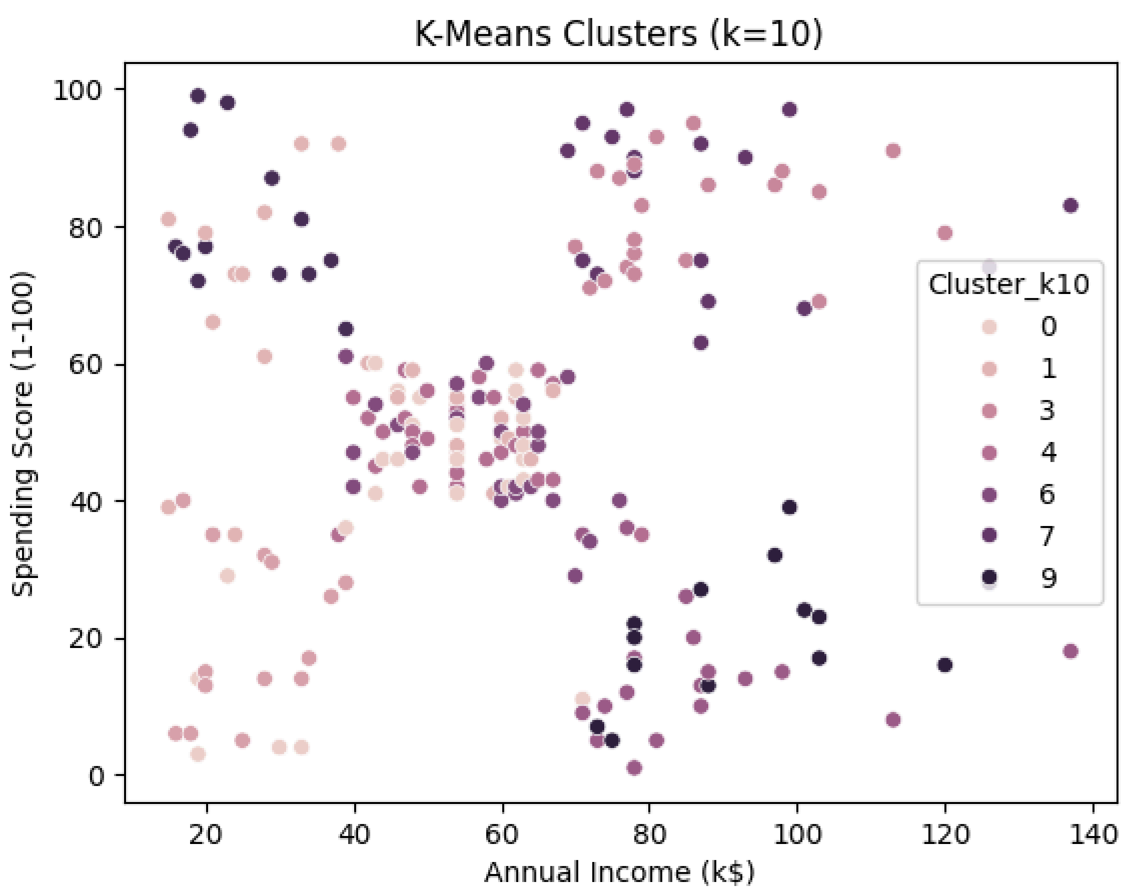
```
Optimal k (Gap Statistic): 10
```




```
Optimal k (Silhouette Score): 10
```




K-Means Clusters (k=10)
Spending Score (1-100)
Annual Income (k$)
Cluster_k10
0
1
3
4
6
7
9
0
20
40
60
80
100
20
40
60
80
100
120
140


K-Means Clusters (k=10)
Spending Score (1-100)
Annual Income (k$)
Cluster_k10
0
1
3
4
6
7
9
0
20
40
60
80
100
20
40
60
80
100
120
140

```
 Summary for k = 10
                   Age  Annual Income (k$)  Spending Score (1-100)  Genre_Ma
le
Cluster_k10
0            58.846154           48.692308               39.846154    1.0000
00
1            25.250000           41.250000               60.916667    1.0000
00
2            41.214286           26.071429               20.142857    0.0714
29
3            32.190476           86.047619               81.666667    0.0000
00
4            54.153846           54.230769               48.961538    0.0000
00
5            38.473684           85.894737               14.210526    1.0000
00
6            27.960000           57.360000               47.120000    0.0000
00
7            33.277778           87.111111               82.666667    1.0000
00
8            25.461538           25.692308               80.538462    0.0000
00
9            43.785714           93.285714               20.642857    0.0000
00
```


```
 Summary for k = 10
                   Age  Annual Income (k$)  Spending Score (1-100)  Genre_Ma
le
Cluster_k10
0            58.846154           48.692308               39.846154    1.0000
00
1            25.250000           41.250000               60.916667    1.0000
00
2            41.214286           26.071429               20.142857    0.0714
29
3            32.190476           86.047619               81.666667    0.0000
00
4            54.153846           54.230769               48.961538    0.0000
00
5            38.473684           85.894737               14.210526    1.0000
00
6            27.960000           57.360000               47.120000    0.0000
00
7            33.277778           87.111111               82.666667    1.0000
00
8            25.461538           25.692308               80.538462    0.0000
00
9            43.785714           93.285714               20.642857    0.0000
00
```


1a.

ii

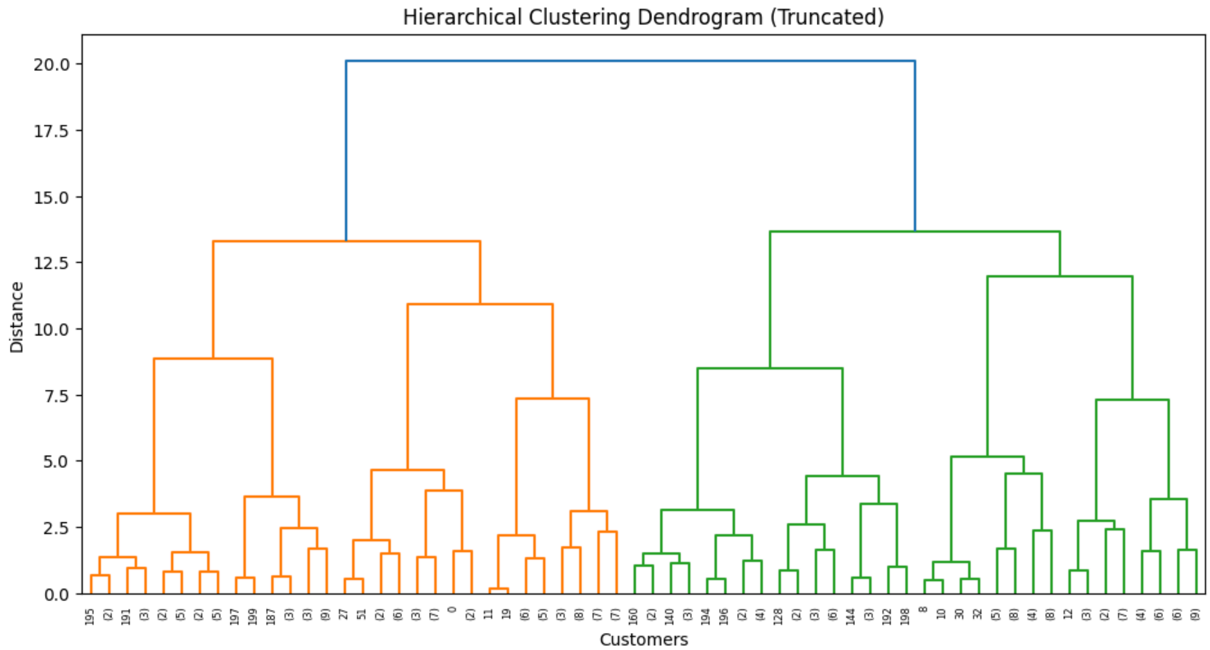
The scatterplots for k = 10 clear regions where spending score and income combine to form customer groups. High-income/high-spending customers cluster cleanly in the upper right region, while low-income/low-spending customers cluster in the lower left. However, as k increases, some clusters become more granular and begin to overlap, sugessting that while k = 10 does separate major behavior patterns, it also creates smaller subclusters that are not perfectly separable in a 2d space. Overall, the clusters show reasonable separability but with some overlap between middle-income, moderate-spending groups.

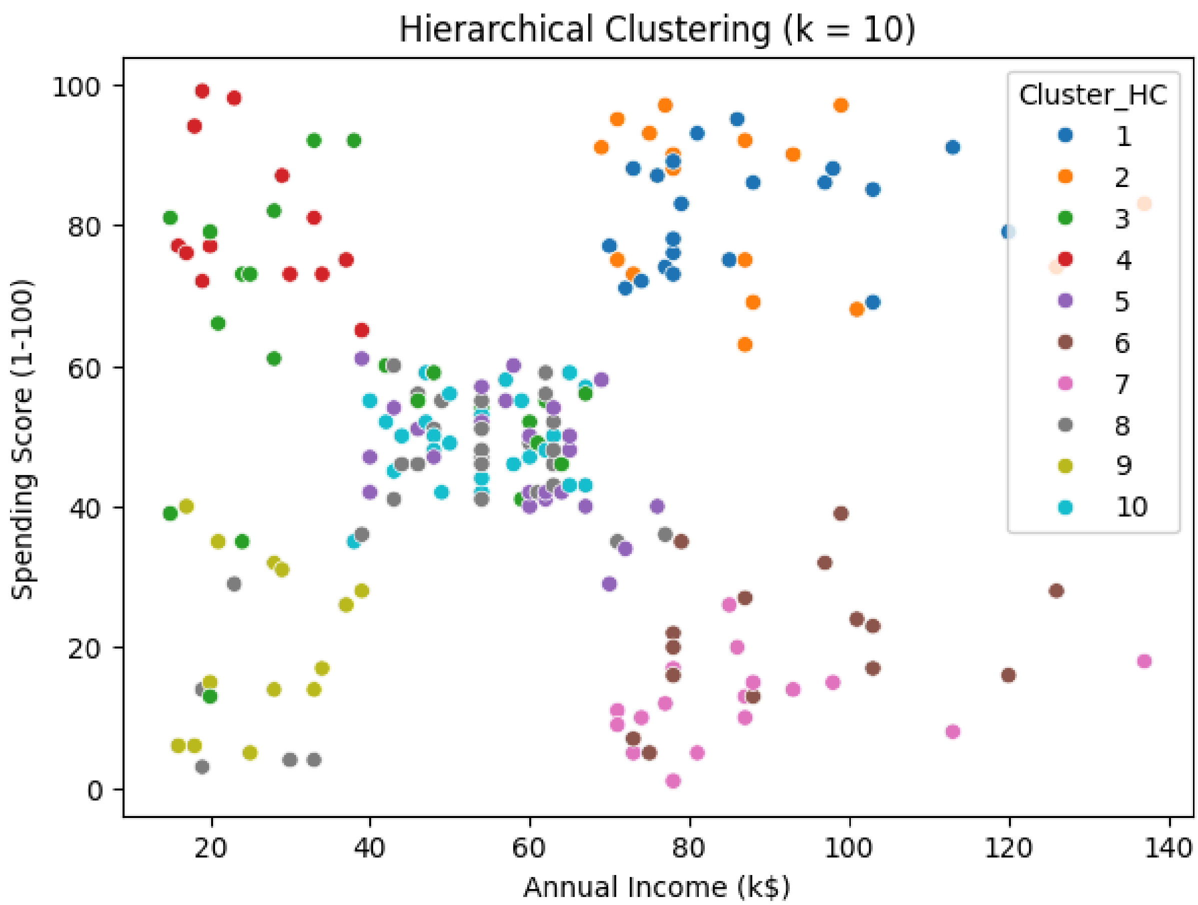
iii

Overall, the k = 10 clustering reveals that customers are primarily differentiated by their income and spending patterns. Younger customers tend to show more impulsive spending behavior, while older customers generally spend less and follow more conservative patterns. There are also noticeable gender differences within some clusters, particularly among the highest and lowest spenders.

In [13]:

```
#Question 1b

from scipy.cluster.hierarchy import dendrogram, linkage, fcluster

Z = linkage(X_scaled, method='ward')

plt.figure(figsize=(12, 6))
dendrogram(Z, truncate_mode='level', p=5)
plt.title("Hierarchical Clustering Dendrogram (Truncated)")
plt.xlabel("Customers")
plt.ylabel("Distance")
plt.show()

k_hier = 10
df_encoded["Cluster_HC"] = fcluster(Z, k_hier, criterion='maxclust')

plt.figure(figsize=(7,5))
sns.scatterplot(
    data=df_encoded,
    x="Annual Income (k$)",
    y="Spending Score (1-100)",
    hue="Cluster_HC",
    palette="tab10"
)
plt.title("Hierarchical Clustering (k = 10)")
plt.show()

print(df_encoded.groupby("Cluster_HC")[
    ["Age", "Annual Income (k$)", "Spending Score (1-100)", "Genre_Male"]
].mean())
```


Hierarchical Clustering Dendrogram (Truncated)
Distance
Customers
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0


Hierarchical Clustering (k = 10)
Spending Score (1-100)
Annual Income (k$)
Cluster_HC
1
2
3
4
5
6
7
8
9
10

```
                  Age  Annual Income (k$)  Spending Score (1-100)  Genre_Mal
e
Cluster_HC
1           32.190476           86.047619               81.666667         0.
0
2           33.277778           87.111111               82.666667         1.
0
3           24.565217           39.217391               59.652174         1.
0
4           25.461538           25.692308               80.538462         0.
0
5           27.960000           57.360000               47.120000         0.
0
6           44.600000           92.333333               21.600000         0.
0
7           38.833333           86.388889               11.666667         1.
0
8           56.551724           50.034483               41.344828         1.
0
9           41.538462           26.538462               20.692308         0.
0
10          54.080000           53.240000               49.520000         0.
0
```

1b.

ii

The hierarchical clustering scatterplot shows similar overall patterns to K-Means, with clear high-income/high-spending and low-income/low-spending groups. However, the hierarchical clusters are less compact and show more overlap because hierarchical clustering does not optimize cluster tightness the way K-Means does. K-Means produces cleaner, more separated clusters, while hierarchical clustering yields more irregular shapes and cluster sizes.

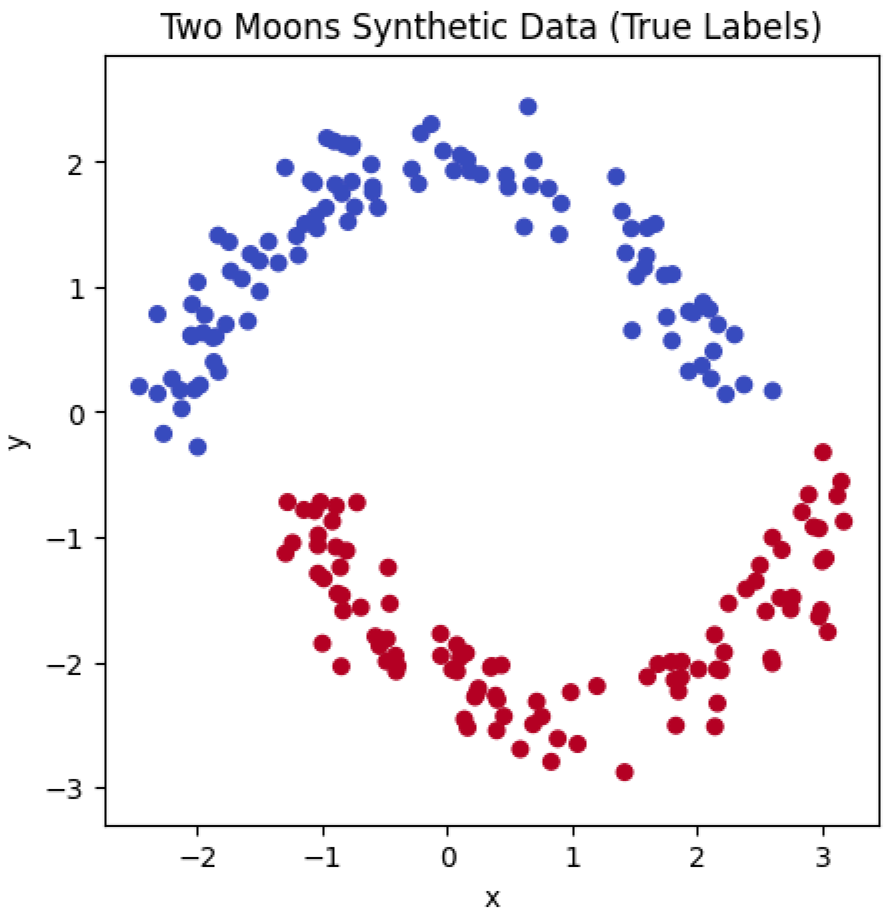
iii

The hierarchical clustering groups mirror the behavioral patterns seen in K-Means. There are high-income/high-spending clusters (Clusters 1–2), low-income/high-spending shoppers (Cluster 4), and high-income but low-spending customers (Clusters 6–7). Middle-income moderate spenders also form several clusters (5, 8, 10). Overall, hierarchical clustering identifies similar customer segments but organizes them slightly differently due to the linkage-based clustering process.

Question 2

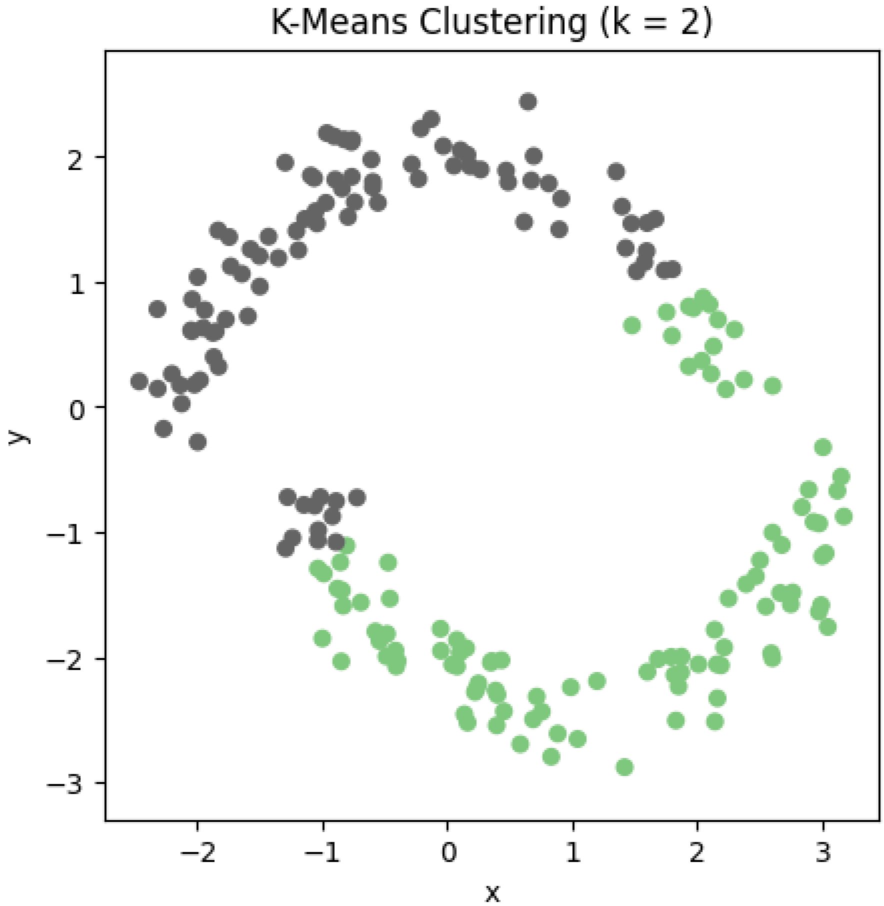
In [14]:
```python
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
```

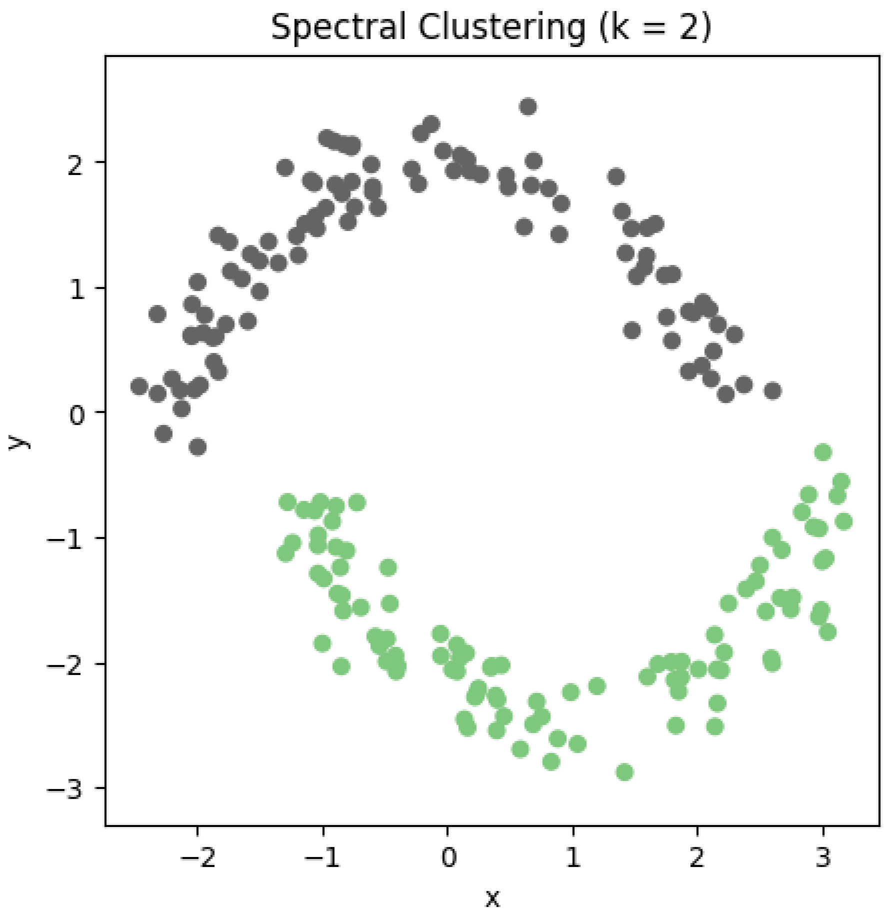
```
from sklearn.cluster import KMeans, SpectralClustering

np.random.seed(598)

n = 200
n_per_moon = n // 2
r = 2
noise_var = 0.05
noise_std = np.sqrt(noise_var)

theta1 = np.random.uniform(0, np.pi, n_per_moon)
x1 = r * np.cos(theta1) + np.random.normal(0, noise_std, n_per_moon)
y1 = r * np.sin(theta1) + np.random.normal(0, noise_std, n_per_moon)
label1 = np.zeros(n_per_moon, dtype=int)

theta2 = np.random.uniform(0, np.pi, n_per_moon)
x2 = 1 - r * np.cos(theta2) + np.random.normal(0, noise_std, n_per_moon)
y2 = -r * np.sin(theta2) - 0.5 + np.random.normal(0, noise_std, n_per_moon)
label2 = np.ones(n_per_moon, dtype=int)

X = np.vstack([np.column_stack([x1, y1]), np.column_stack([x2, y2])])
y = np.concatenate([label1, label2])

df_moons = pd.DataFrame({"x": X[:, 0], "y": X[:, 1], "label": y})

plt.figure(figsize=(5,5))
plt.scatter(df_moons["x"], df_moons["y"], c=df_moons["label"], cmap="coolwar
plt.title("Two Moons Synthetic Data (True Labels)")
plt.xlabel("x")
plt.ylabel("y")
plt.axis("equal")
plt.show()
```



In [15]:
```
# 2a
kmeans = KMeans(n_clusters=2, random_state=42, n_init=10)
df_moons["kmeans_cluster"] = kmeans.fit_predict(X)

plt.figure(figsize=(5,5))
plt.scatter(df_moons["x"], df_moons["y"],
            c=df_moons["kmeans_cluster"], cmap="Accent", s=30)
plt.title("K-Means Clustering (k = 2)")
plt.xlabel("x")
plt.ylabel("y")
plt.axis("equal")
plt.show()

#2b

spec = SpectralClustering(
    n_clusters=2,
    affinity="rbf",
    assign_labels="kmeans",
    random_state=42
)
df_moons["spectral_cluster"] = spec.fit_predict(X)

plt.figure(figsize=(5,5))
plt.scatter(df_moons["x"], df_moons["y"],
            c=df_moons["spectral_cluster"], cmap="Accent", s=30)
plt.title("Spectral Clustering (k = 2)")
```

```
plt.xlabel("x")
plt.ylabel("y")
plt.axis("equal")
plt.show()
```





2a

Using K-Means with k=2 on the two-moons data does not correctly recover the true structure. Because K-Means assumes clusters are roughly spherical, it places a straight decision boundary through the middle of the dataset. As a result, the two curved moon shapes are mixed: some points from the upper moon are grouped with the lower moon and vice versa. The algorithm fails to capture the non-linear geometry of the moons, leading to poor separation between the two true groups.

2b

Spectral clustering with an RBF kernel has two moon shapes. The resulting clusters align almost perfectly with the true labels, cleanly separating the top and bottom moon structures. Compared to part (a), spectral clustering handles the non-linear boundary correctly and produces a more accurate clustering.