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SUBJECT : ML LAB
GITHUB:

[https://github.com/DhananjoyShaw/ML_LAB](https://github.com/DhananjoyShaw/ML_LAB/tree/main/Assignment%204)
[/tree/main/Assignment%204](https://github.com/DhananjoyShaw/ML_LAB/tree/main/Assignment%204)

GOOGLE COLAB



```
In [1]: !pip install numpy==1.26.4
!pip install scikit-learn-extra
```

```
Requirement already satisfied: numpy==1.26.4 in /usr/local/lib/python3.12/dist-packages (1.26.4)
Collecting scikit-learn-extra
  Using cached scikit-learn-extra-0.3.0.tar.gz (818 kB)
  Installing build dependencies ... done
  Getting requirements to build wheel ... done
  Preparing metadata (pyproject.toml) ... done
Requirement already satisfied: numpy>=1.13.3 in /usr/local/lib/python3.12/dist-packages (from scikit-learn-extra) (1.26.4)
Requirement already satisfied: scipy>=0.19.1 in /usr/local/lib/python3.12/dist-packages (from scikit-learn-extra) (1.16.3)
Requirement already satisfied: scikit-learn>=0.23.0 in /usr/local/lib/python3.12/dist-packages (from scikit-learn-extra) (1.6.1)
Requirement already satisfied: joblib>=1.2.0 in /usr/local/lib/python3.12/dist-packages (from scikit-learn>=0.23.0->scikit-learn-extra) (1.5.2)
Requirement already satisfied: threadpoolctl>=3.1.0 in /usr/local/lib/python3.12/dist-packages (from scikit-learn>=0.23.0->scikit-learn-extra) (3.6.0)
Building wheels for collected packages: scikit-learn-extra
  Building wheel for scikit-learn-extra (pyproject.toml) ... done
  Created wheel for scikit-learn-extra: filename=scikit_learn_extra-0.3.0-cp312-cp312-linux_x86_64.whl size=2178130 sha256=f0fd711516bce7259a606e4af9a617c3e13c9c28c04438b8ce4d6b30c92ealdd
  Stored in directory: /root/.cache/pip/wheels/17/4d/c3/c6d5d563c1bf8146d059d63be3678abc2f2801fba0aaf5f0b8
Successfully built scikit-learn-extra
Installing collected packages: scikit-learn-extra
Successfully installed scikit-learn-extra-0.3.0
```

```
In [2]: import pandas as pd
import matplotlib.pyplot as plt
import numpy as np
from sklearn.metrics import silhouette_score, calinski_harabasz_score, davies_bouldin_score
```

Clustering in Iris Dataset

```
In [3]: from sklearn.datasets import load_iris
import pandas as pd
import matplotlib.pyplot as plt

# Load iris dataset
iris = load_iris()
df_iris = pd.DataFrame(iris.data, columns=iris.feature_names)
df_iris['species'] = [iris.target_names[i] for i in iris.target]

# Rename columns to match your plotting code
df_iris.columns = ['sepal_length', 'sepal_width', 'petal_length', 'petal_width']

# Prepare data
X = df_iris.drop('species', axis=1)
```

```

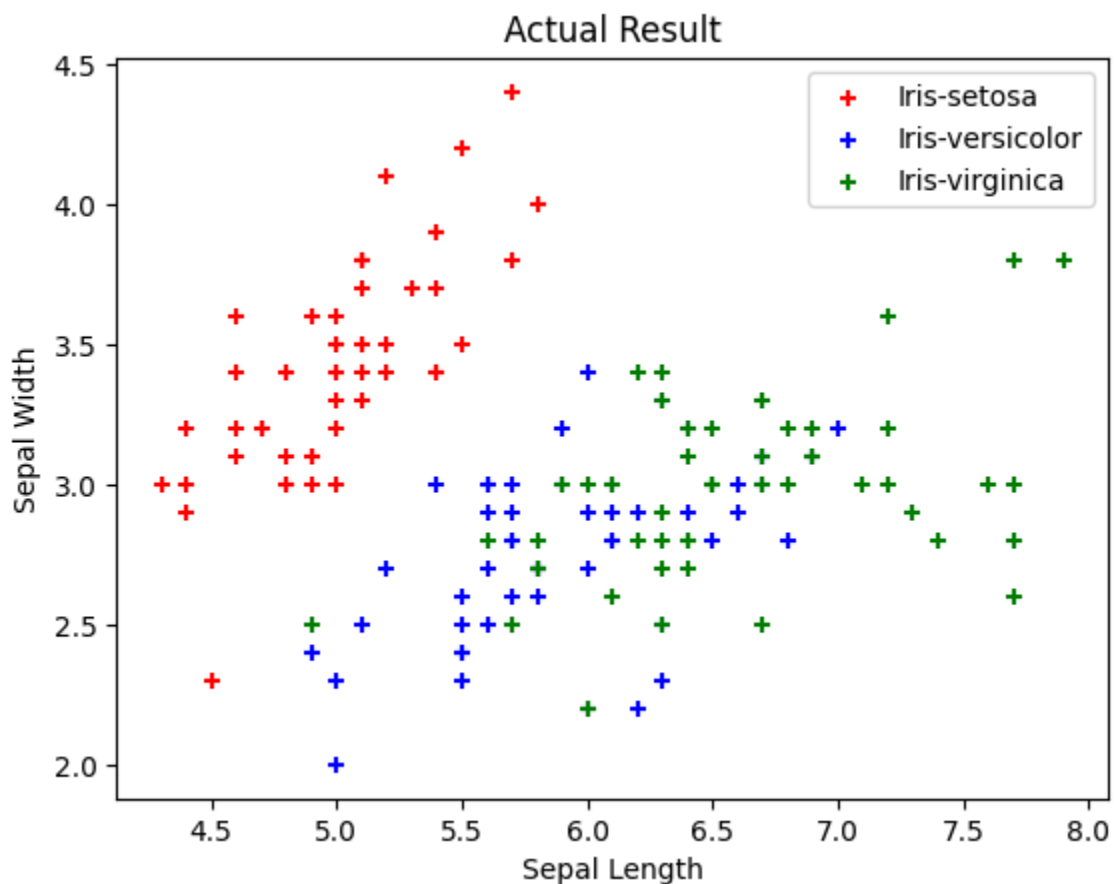
y = df_iris.species

# Actual Clustering Result
newDf0 = df_iris[df_iris.species == "setosa"]
newDf1 = df_iris[df_iris.species == "versicolor"]
newDf2 = df_iris[df_iris.species == "virginica"]

# Plot
plt.title("Actual Result")
plt.xlabel("Sepal Length")
plt.ylabel("Sepal Width")
plt.scatter(newDf0.sepal_length, newDf0.sepal_width, color="red", marker="+",
plt.scatter(newDf1.sepal_length, newDf1.sepal_width, color="blue", marker="+",
plt.scatter(newDf2.sepal_length, newDf2.sepal_width, color="green", marker="+",
plt.legend()

# 📢 This line displays the plot
plt.show()

```



Partition Based: K-means Clustering in Iris Dataset

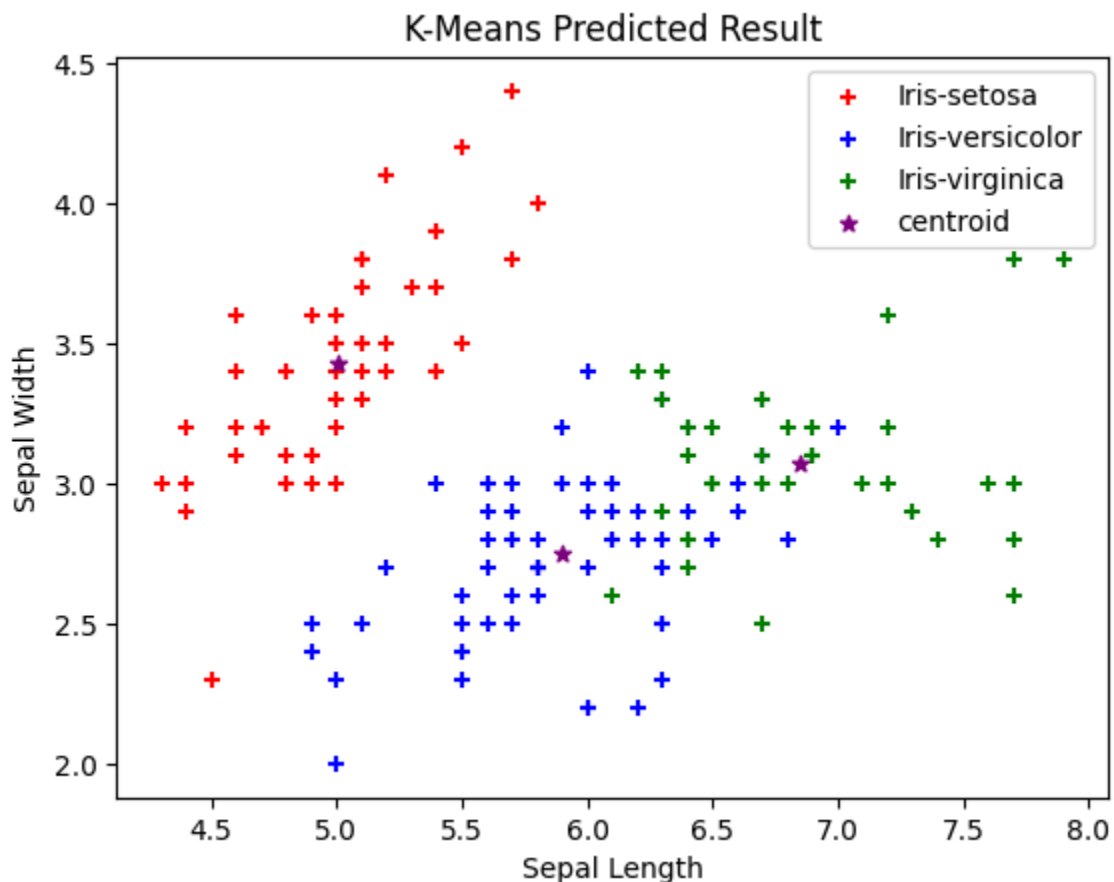
```
In [4]: from sklearn.cluster import KMeans
```

```

km = KMeans(n_clusters=3, n_init=10)
y_predicted = km.fit_predict(X)
newDf = df_iris
newDf["cluster"] = y_predicted
newDf0 = newDf[newDf.cluster==0]
newDf1 = newDf[newDf.cluster==1]
newDf2 = newDf[newDf.cluster==2]
plt.title("K-Means Predicted Result")
plt.xlabel("Sepal Length")
plt.ylabel("Sepal Width")
plt.scatter(newDf0.sepal_length, newDf0.sepal_width, color="red",
marker="+", label="Iris-setosa")
plt.scatter(newDf1.sepal_length, newDf1.sepal_width, color="blue",
marker="+", label="Iris-versicolor")
plt.scatter(newDf2.sepal_length, newDf2.sepal_width, color="green",
marker="+", label="Iris-virginica")
plt.scatter(km.cluster_centers_[0], km.cluster_centers_[1], color="purple")
plt.legend()

```

Out[4]: <matplotlib.legend.Legend at 0x78c2275f87a0>



```

In [5]: from sklearn.metrics import rand_score, adjusted_rand_score
from sklearn.metrics import mutual_info_score, adjusted_mutual_info_score, nor

# True labels
y_true = df_iris['species']

```

```

# Predicted cluster labels
y_pred = newDf['cluster']

# Rand Index
ri = rand_score(y_true, y_pred)
ari = adjusted_rand_score(y_true, y_pred)

# Mutual Information scores
mi = mutual_info_score(y_true, y_pred)
ami = adjusted_mutual_info_score(y_true, y_pred)
nmi = normalized_mutual_info_score(y_true, y_pred)

# Print results
print(f"Rand Index: {ri:.4f}")
print(f"Adjusted Rand Index: {ari:.4f}")
print(f"Mutual Information: {mi:.4f}")
print(f"Adjusted Mutual Information: {ami:.4f}")
print(f"Normalized Mutual Information: {nmi:.4f}")

```

```

Rand Index: 0.8797
Adjusted Rand Index: 0.7302
Mutual Information: 0.8256
Adjusted Mutual Information: 0.7551
Normalized Mutual Information: 0.7582

```

```

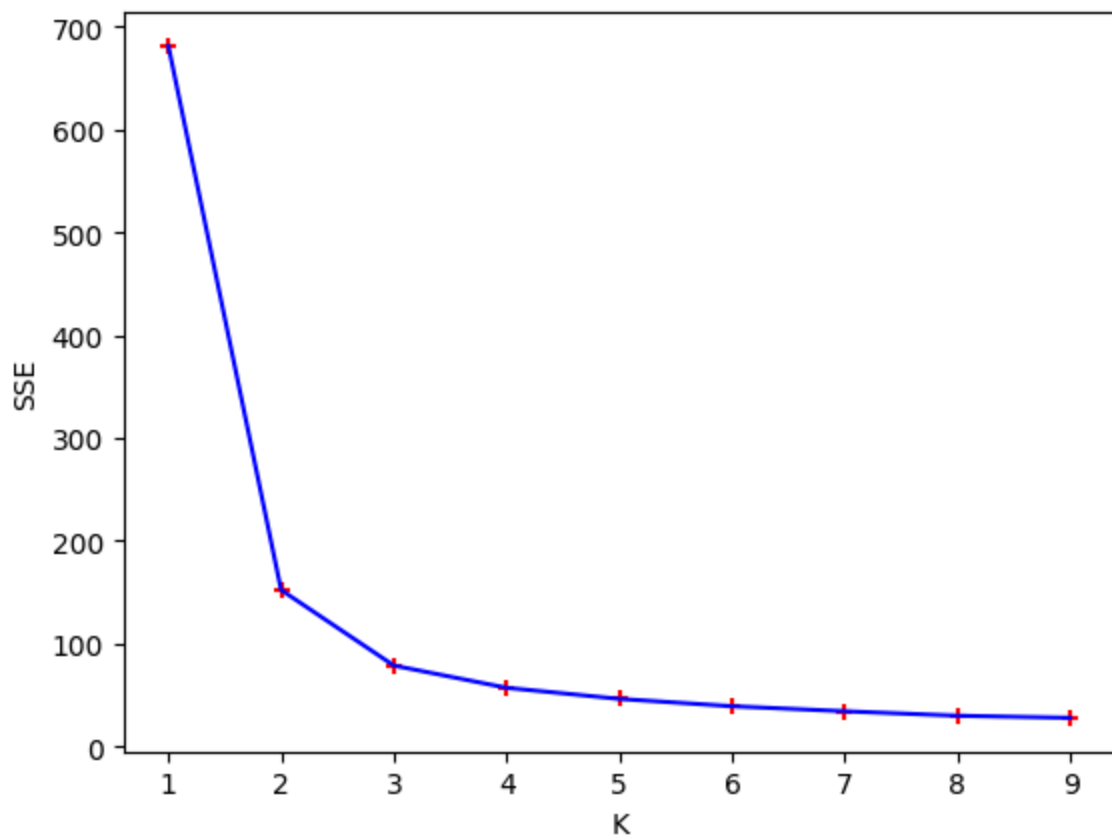
In [6]: sse = []
        k_range = range(1, 10)
        for k in k_range:
            km = KMeans(n_clusters=k, n_init=10)
            km.fit_predict(X)
            sse.append(km.inertia_)
        plt.xlabel("K")
        plt.ylabel("SSE")
        plt.scatter(k_range, sse, color="red", marker="+")
        plt.plot(k_range, sse, color="blue")

```

```

Out[6]: [matplotlib.lines.Line2D at 0x78c225007380>]

```



```
In [7]: # Evaluating Metrics
silhouette_result = silhouette_score(X, km.labels_)
print("Silhouette Score: ", silhouette_result)
calinski_result = calinski_harabasz_score(X, km.labels_)
print("Calinski Harabasz Score: ", calinski_result)
davies_result = davies_bouldin_score(X, km.labels_)
print("Davies Bouldin Score: ", davies_result)
# Evaluating Cohesion & Separation
labels = km.labels_
centroids = km.cluster_centers_
SSE = np.sum((X - centroids[labels])**2)
overall_centroid = np.mean(X, axis=0)
SSB = np.sum([np.sum((X[labels == i] - centroids[i])**2) for i in
range(3)])
N = X.shape[0]
cohesion_scores = SSE/N
cohesion = np.mean(cohesion_scores)
separation = SSB/N
print(f"\nCohesion Score: {cohesion_scores}")
print(f"Separation Score: {separation}")
```

Silhouette Score: 0.3263554408272626
Calinski Harabasz Score: 411.0450636495753
Davies Bouldin Score: 0.9822734189189105

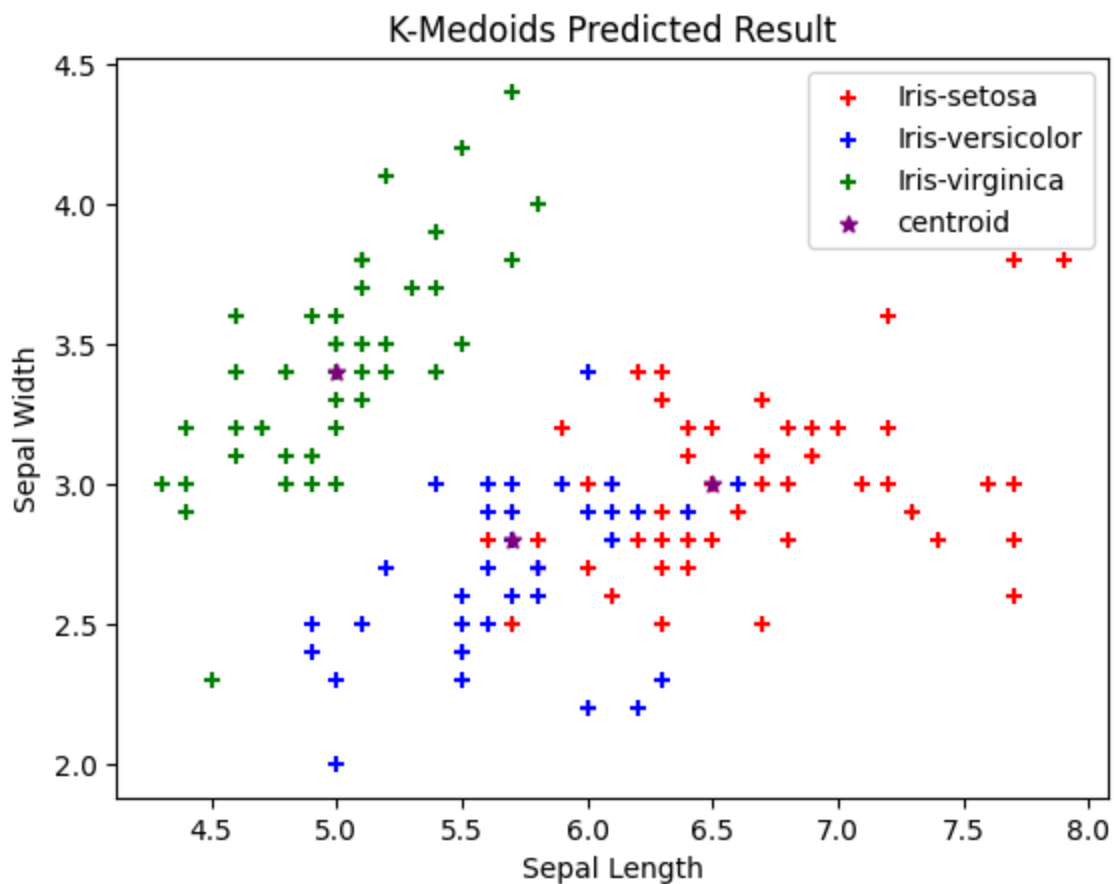
Cohesion Score: sepal_length 0.053063
sepal_width 0.057558
petal_length 0.048022
petal_width 0.028123
dtype: float64
Separation Score: 0.07853547008547009

/usr/local/lib/python3.12/dist-packages/numpy/core/fromnumeric.py:86: FutureWarning: The behavior of DataFrame.sum with axis=None is deprecated, in a future version this will reduce over both axes and return a scalar. To retain the old behavior, pass axis=0 (or do not pass axis)
return reduction(axis=axis, out=out, **passkwargs)

Partition Based: K-medoids Clustering in Iris Dataset

```
In [8]: # Clustering using K-medoids algorithm
from sklearn_extra.cluster import KMedoids
km = KMedoids(n_clusters=3)
y_predicted = km.fit_predict(X)
newDf = df_iris
newDf["cluster"] = y_predicted
newDf0 = newDf[newDf.cluster==0]
newDf1 = newDf[newDf.cluster==1]
newDf2 = newDf[newDf.cluster==2]
plt.title("K-Medoids Predicted Result")
plt.xlabel("Sepal Length")
plt.ylabel("Sepal Width")
plt.scatter(newDf0.sepal_length, newDf0.sepal_width, color="red",
marker="+", label="Iris-setosa")
plt.scatter(newDf1.sepal_length, newDf1.sepal_width, color="blue",
marker="+", label="Iris-versicolor")
plt.scatter(newDf2.sepal_length, newDf2.sepal_width, color="green",
marker="+", label="Iris-virginica")
plt.scatter(km.cluster_centers_[0], km.cluster_centers_[1],
color="purple", marker="*", label="centroid")
plt.legend()
```

Out[8]: <matplotlib.legend.Legend at 0x78c222110cb0>



```
In [9]: from sklearn.metrics import rand_score, adjusted_rand_score
from sklearn.metrics import mutual_info_score, adjusted_mutual_info_score, normalized_mutual_info_score

# True labels
y_true = df_iris['species']

# Predicted cluster labels
y_pred = newDf['cluster']

# Rand Index
ri = rand_score(y_true, y_pred)
ari = adjusted_rand_score(y_true, y_pred)

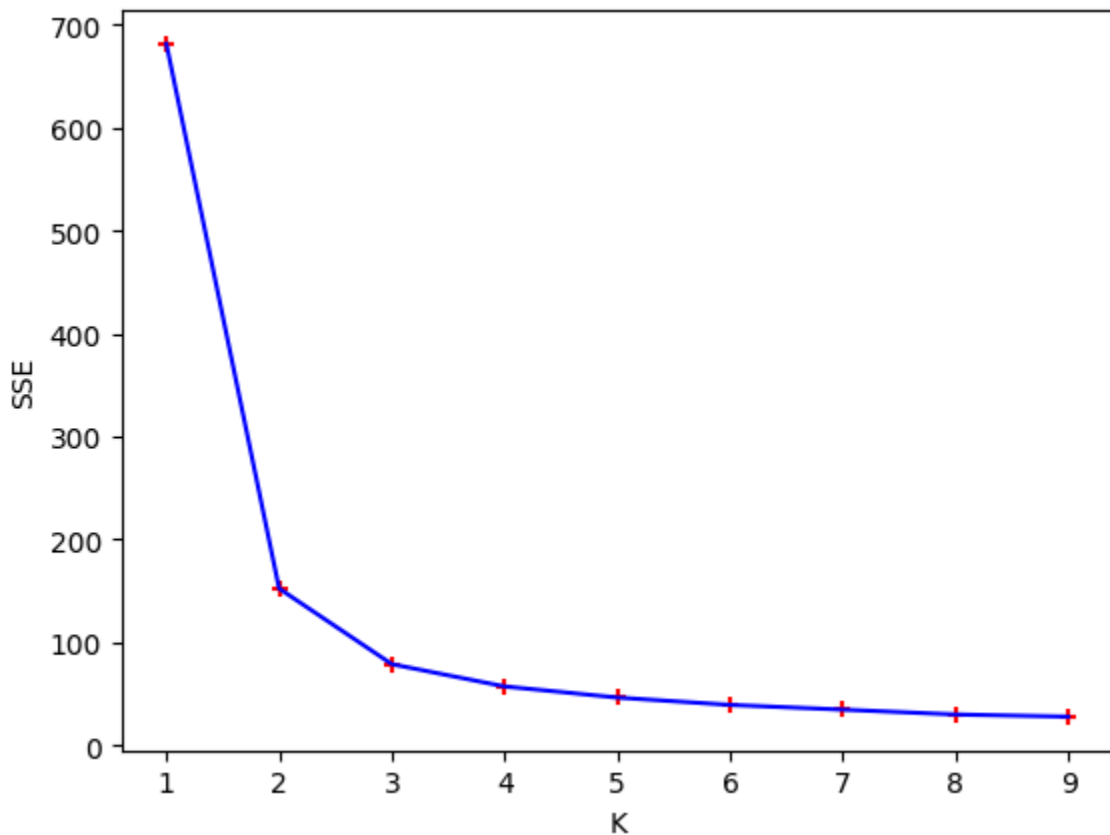
# Mutual Information scores
mi = mutual_info_score(y_true, y_pred)
ami = adjusted_mutual_info_score(y_true, y_pred)
nmi = normalized_mutual_info_score(y_true, y_pred)

# Print results
print(f"Rand Index: {ri:.4f}")
print(f"Adjusted Rand Index: {ari:.4f}")
print(f"Mutual Information: {mi:.4f}")
print(f"Adjusted Mutual Information: {ami:.4f}")
print(f"Normalized Mutual Information: {nmi:.4f}")
```


Rand Index: 0.8923
Adjusted Rand Index: 0.7583
Mutual Information: 0.8555
Adjusted Mutual Information: 0.7830
Normalized Mutual Information: 0.7857

```
In [10]: sse = []
k_range = range(1, 10)
for k in k_range:
    km = KMeans(n_clusters=k, n_init=10)
    km.fit_predict(X)
    sse.append(km.inertia_)
plt.xlabel("K")
plt.ylabel("SSE")
plt.scatter(k_range, sse, color="red", marker="+")
plt.plot(k_range, sse, color="blue")
```

Out[10]: [



```
In [11]: # Evaluating Metrics
silhouette_result = silhouette_score(X, km.labels_)
print("Silhouette Score: ", silhouette_result)
calinski_result = calinski_harabasz_score(X, km.labels_)
print("Calinski Harabasz Score: ", calinski_result)
davies_result = davies_bouldin_score(X, km.labels_)
print("Davies Bouldin Score: ", davies_result)
# Evaluating Cohesion & Separation
labels = km.labels_
```

```

centroids = km.cluster_centers_
SSE = np.sum((X - centroids[labels])**2)
overall_centroid = np.mean(X, axis=0)
SSB = np.sum([np.sum((X[labels == i] - centroids[i])**2) for i in
range(3)])
N = X.shape[0]
cohesion_scores = SSE/N
cohesion = np.mean(cohesion_scores)
separation = SSB/N
print(f"\nCohesion Score: {cohesion}")
print(f"Separation Score: {separation}")

```

Silhouette Score: 0.34595488596099394
 Calinski Harabasz Score: 413.40662034398076
 Davies Bouldin Score: 0.9323507432928486

Cohesion Score: 0.046435714760385785
 Separation Score: 0.07709897660818713

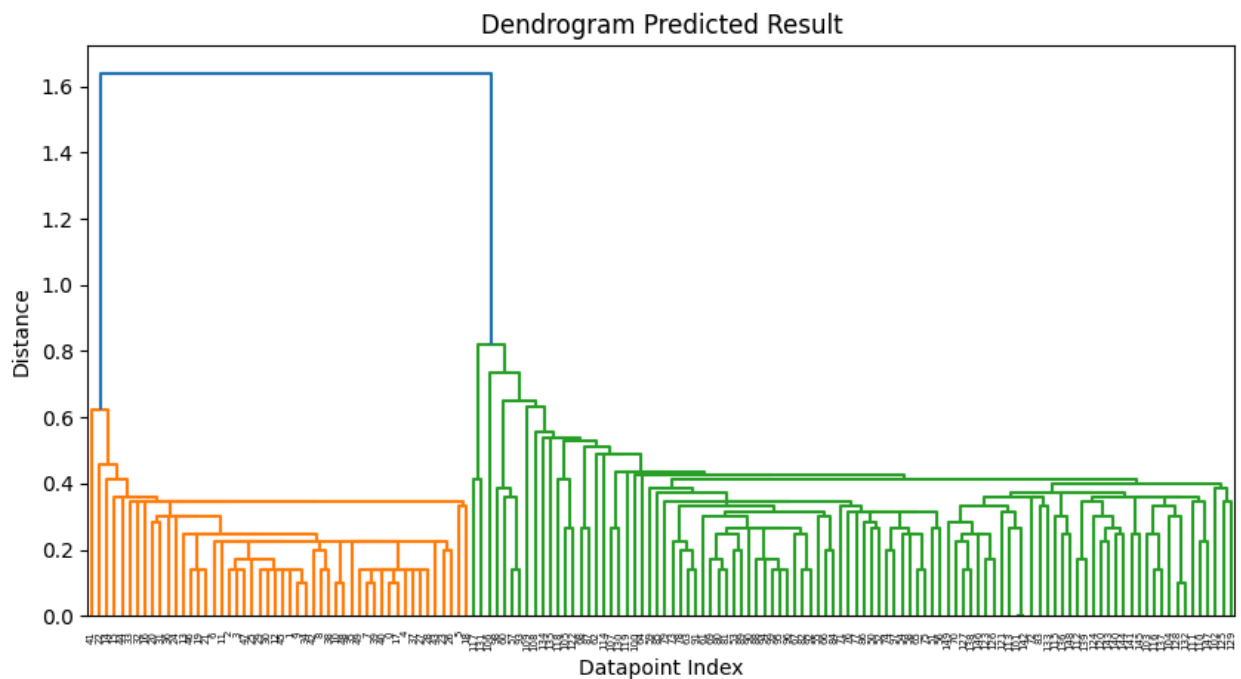
/usr/local/lib/python3.12/dist-packages/numpy/core/fromnumeric.py:86: FutureWarning: The behavior of DataFrame.sum with axis=None is deprecated, in a future version this will reduce over both axes and return a scalar. To retain the old behavior, pass axis=0 (or do not pass axis)
 return reduction(axis=axis, out=out, **passkwargs)

Hierarchical: Dendrogram Clustering in Iris Dataset

```

In [12]: # Clustering using Dendrogram Clustering algorithm
from scipy.cluster.hierarchy import dendrogram, linkage, fcluster
Z = linkage(X, method='single')
# Create and plot the dendrogram
plt.figure(figsize=(10, 5))
dn = dendrogram(Z)
plt.title('Dendrogram Predicted Result')
plt.xlabel('Datapoint Index')
plt.ylabel('Distance')
plt.show()

```



```
In [13]: from scipy.cluster.hierarchy import fcluster
from sklearn.metrics import rand_score, adjusted_rand_score
from sklearn.metrics import mutual_info_score, adjusted_mutual_info_score, normalized_mutual_info_score

# True labels (numeric)
y_true = df_iris['species']

# Cut the dendrogram to form 3 clusters
y_pred = fcluster(Z, t=3, criterion='maxclust')

# Rand Index
ri = rand_score(y_true, y_pred)
ari = adjusted_rand_score(y_true, y_pred)

# Mutual Information scores
mi = mutual_info_score(y_true, y_pred)
ami = adjusted_mutual_info_score(y_true, y_pred)
nmi = normalized_mutual_info_score(y_true, y_pred)

# Print results
print(f"Rand Index: {ri:.4f}")
print(f"Adjusted Rand Index: {ari:.4f}")
print(f"Mutual Information: {mi:.4f}")
print(f"Adjusted Mutual Information: {ami:.4f}")
print(f"Normalized Mutual Information: {nmi:.4f}")
```

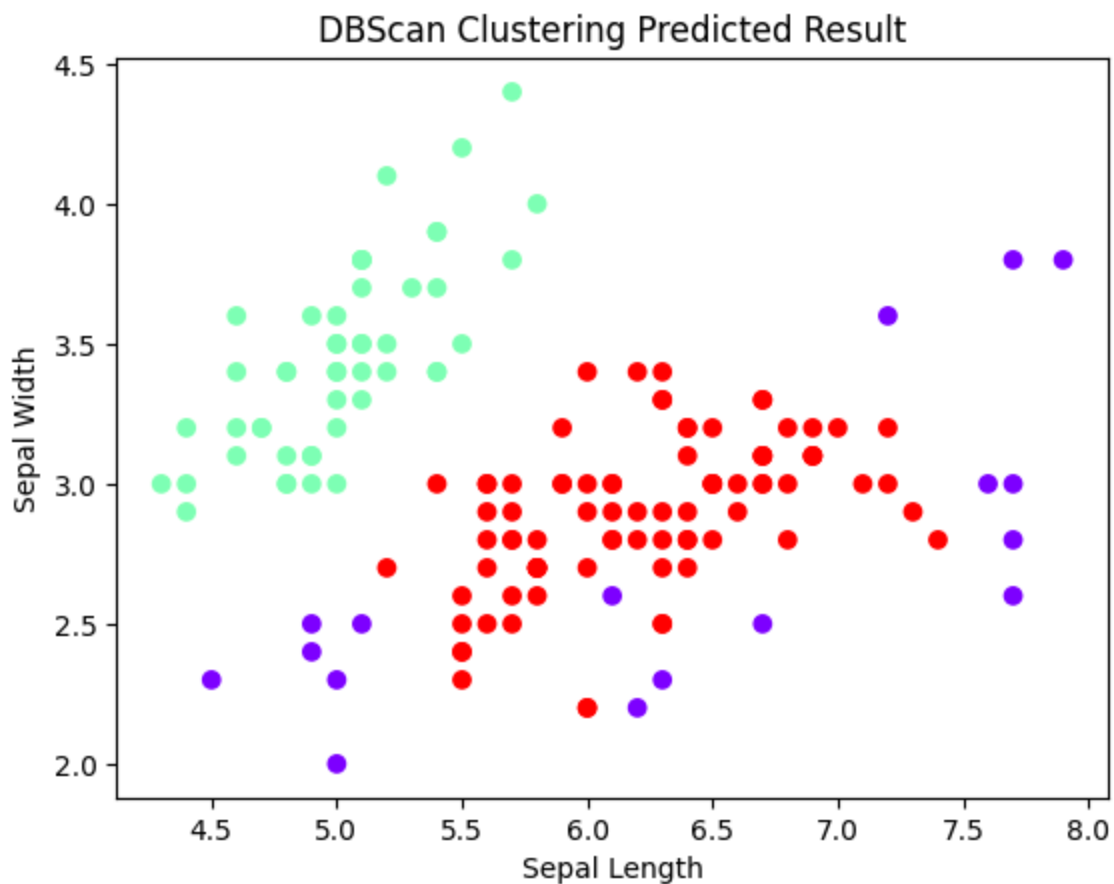
```
Rand Index: 0.7766
Adjusted Rand Index: 0.5638
Mutual Information: 0.6459
Adjusted Mutual Information: 0.7126
Normalized Mutual Information: 0.7175
```

```
In [14]: labels = fcluster(Z, 3, criterion='maxclust')
silhouette_result = silhouette_score(X, labels)
print("Silhouette Score: ", silhouette_result)
calinski_result = calinski_harabasz_score(X, labels)
print("Calinski Harabasz Score: ", calinski_result)
davies_result = davies_bouldin_score(X, labels)
print("Davies Bouldin Score: ", davies_result)
```

Silhouette Score: 0.5121107753649307
Calinski Harabasz Score: 277.99467626461944
Davies Bouldin Score: 0.4471537628542408

Density Based: DBSCAN Clustering in Iris Dataset

```
In [15]: # Clustering using DBSCAN Clustering algorithm
from sklearn.cluster import DBSCAN
dbscan = DBSCAN(eps=0.5, algorithm='auto', metric='euclidean')
y = dbscan.fit_predict(X)
plt.scatter(df_iris.sepal_length, df_iris.sepal_width,
c=dbscan.labels_, cmap='rainbow')
plt.xlabel('Sepal Length')
plt.ylabel('Sepal Width')
plt.title('DBScan Clustering Predicted Result')
plt.show()
```



```
In [16]: from sklearn.metrics import rand_score, adjusted_rand_score
from sklearn.metrics import mutual_info_score, adjusted_mutual_info_score, normalized_mutual_info_score

# True labels
y_true = df_iris['species']

# Predicted cluster labels from DBSCAN
y_pred = dbscan.labels_

# If you want to ignore noise points (-1), you can filter them:
# mask = y_pred != -1
# y_true_filtered = y_true[mask]
# y_pred_filtered = y_pred[mask]

# Compute Rand Index
ri = rand_score(y_true, y_pred)
ari = adjusted_rand_score(y_true, y_pred)

# Compute Mutual Information scores
mi = mutual_info_score(y_true, y_pred)
ami = adjusted_mutual_info_score(y_true, y_pred)
nmi = normalized_mutual_info_score(y_true, y_pred)

# Print results
print(f"Rand Index: {ri:.4f}")
print(f"Adjusted Rand Index: {ari:.4f}")
```

```

print(f"Mutual Information: {mi:.4f}")
print(f"Adjusted Mutual Information: {ami:.4f}")
print(f"Normalized Mutual Information: {nmi:.4f}")

```

```

Rand Index: 0.7719
Adjusted Rand Index: 0.5206
Mutual Information: 0.6152
Adjusted Mutual Information: 0.5990
Normalized Mutual Information: 0.6044

```

In [17]: `y_pred`

```

Out[17]: array([[ 0,  0,  0,  0,  0,  0,  0,  0,  0,  0,  0,  0,  0,  0,  0,  0,  0,  0,
                  0,  0,  0,  0,  0,  0,  0,  0,  0,  0,  0,  0,  0,  0,  0,  0,  0,  0,
                  0,  0,  0,  0,  0,  0,  0, -1,  0,  0,  0,  0,  0,  0,  0,  0,  0,  0,  1,
                  1,  1,  1,  1,  1,  1, -1,  1,  1, -1,  1,  1,  1,  1,  1,  1,  1,  1,  1,
                 -1,  1,  1,  1,  1,  1,  1,  1,  1,  1,  1,  1,  1,  1,  1,  1,  1,  1,  1,
                  1,  1, -1,  1,  1,  1,  1,  1, -1,  1,  1,  1,  1, -1,  1,  1,  1,  1,
                  1,  1,  1, -1, -1,  1, -1, -1,  1,  1,  1,  1,  1,  1,  1,  1, -1, -1,
                  1,  1,  1, -1,  1,  1,  1,  1,  1,  1,  1,  1, -1,  1,  1, -1, -1,
                  1,  1,  1,  1,  1,  1,  1,  1,  1,  1,  1,  1,  1,  1,  1,  1,  1,  1])

```

```

In [18]: # Evaluating Metrics
silhouette_result = silhouette_score(X, dbscan.labels_)
print("Silhouette Score: ", silhouette_result)
calinski_result = calinski_harabasz_score(X, dbscan.labels_)
print("Calinski Harabasz Score: ", calinski_result)
davies_result = davies_bouldin_score(X, dbscan.labels_)
print("Davies Bouldin Score: ", davies_result)

```

```

Silhouette Score: 0.48603419703456857
Calinski Harabasz Score: 220.29751498443005
Davies Bouldin Score: 7.222448016359581

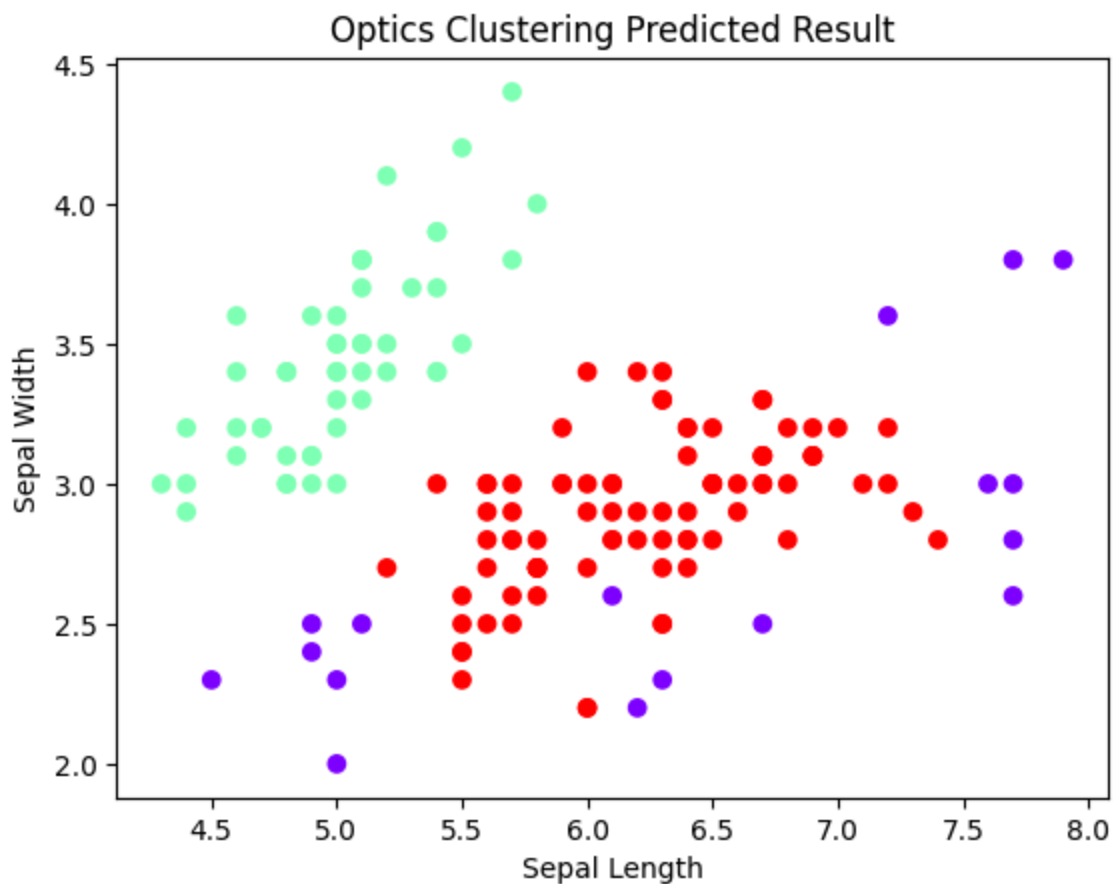
```

Density Based: Optics Clustering in Iris Dataset

```

In [19]: # Clustering using Optics Clustering algorithm
from sklearn.cluster import OPTICS
optics_cluster = OPTICS(min_samples=5, xi=0.05,
                        cluster_method='dbscan')
optics_cluster.fit(X)
plt.scatter(df_iris.sepal_length, df_iris.sepal_width,
            c=dbscan.labels_, cmap='rainbow')
plt.xlabel('Sepal Length')
plt.ylabel('Sepal Width')
plt.title('Optics Clustering Predicted Result')
plt.show()

```



```
In [20]: from sklearn.cluster import OPTICS
from sklearn.metrics import rand_score, adjusted_rand_score
from sklearn.metrics import mutual_info_score, adjusted_mutual_info_score, normalized_mutual_info_score
import matplotlib.pyplot as plt

# Run OPTICS
optics_cluster = OPTICS(min_samples=5, xi=0.05, cluster_method='dbscan')
y_pred = optics_cluster.fit_predict(X) # predicted cluster labels

# Plot clusters
plt.scatter(df_iris.sepal_length, df_iris.sepal_width, c=y_pred, cmap='rainbow')
plt.xlabel('Sepal Length')
plt.ylabel('Sepal Width')
plt.title('OPTICS Clustering Predicted Result')
plt.show()

# True labels
y_true = df_iris['species']

# Compute Rand Index
ri = rand_score(y_true, y_pred)
ari = adjusted_rand_score(y_true, y_pred)

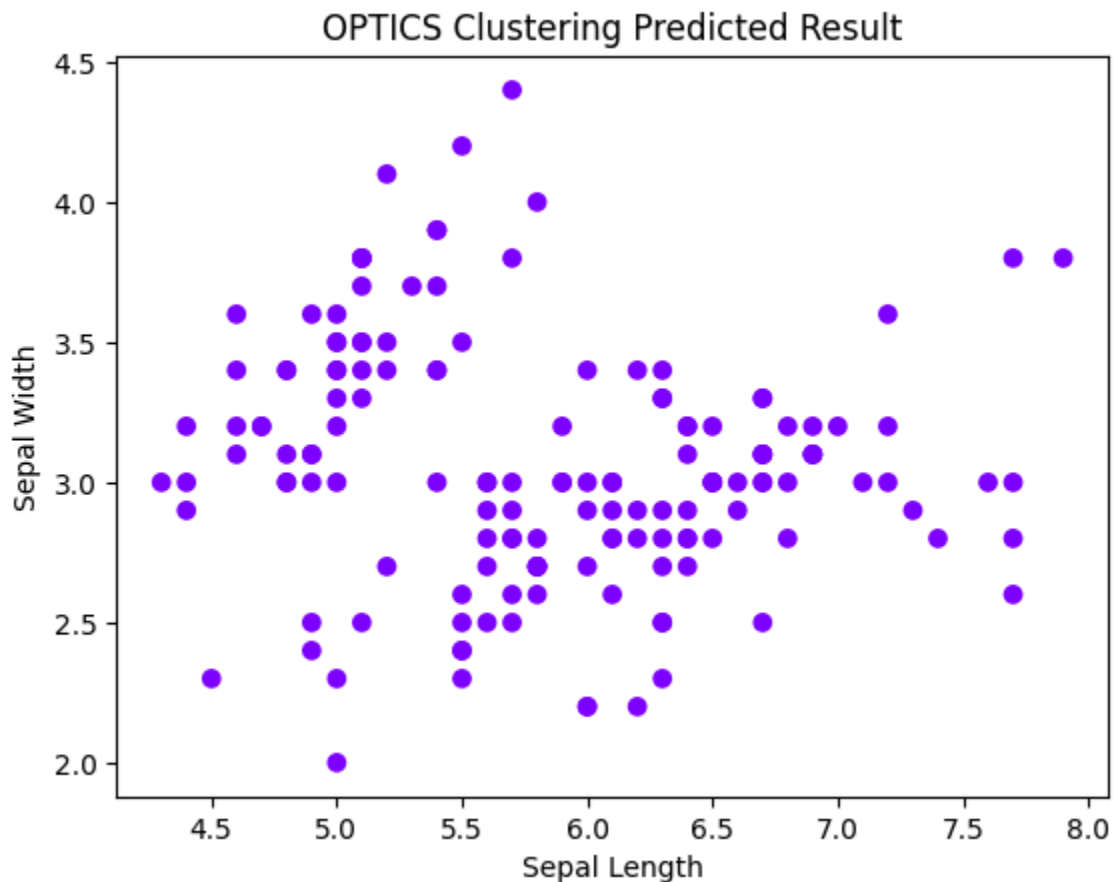
# Compute Mutual Information scores
mi = mutual_info_score(y_true, y_pred)
ami = adjusted_mutual_info_score(y_true, y_pred)
```

```

nmi = normalized_mutual_info_score(y_true, y_pred)

# Print results
print(f"Rand Index: {ri:.4f}")
print(f"Adjusted Rand Index: {ari:.4f}")
print(f"Mutual Information: {mi:.4f}")
print(f"Adjusted Mutual Information: {ami:.4f}")
print(f"Normalized Mutual Information: {nmi:.4f}")

```



```

Rand Index: 0.3289
Adjusted Rand Index: 0.0000
Mutual Information: 0.0000
Adjusted Mutual Information: 0.0000
Normalized Mutual Information: 0.0000

```

K-means++ Clustering in Iris Dataset

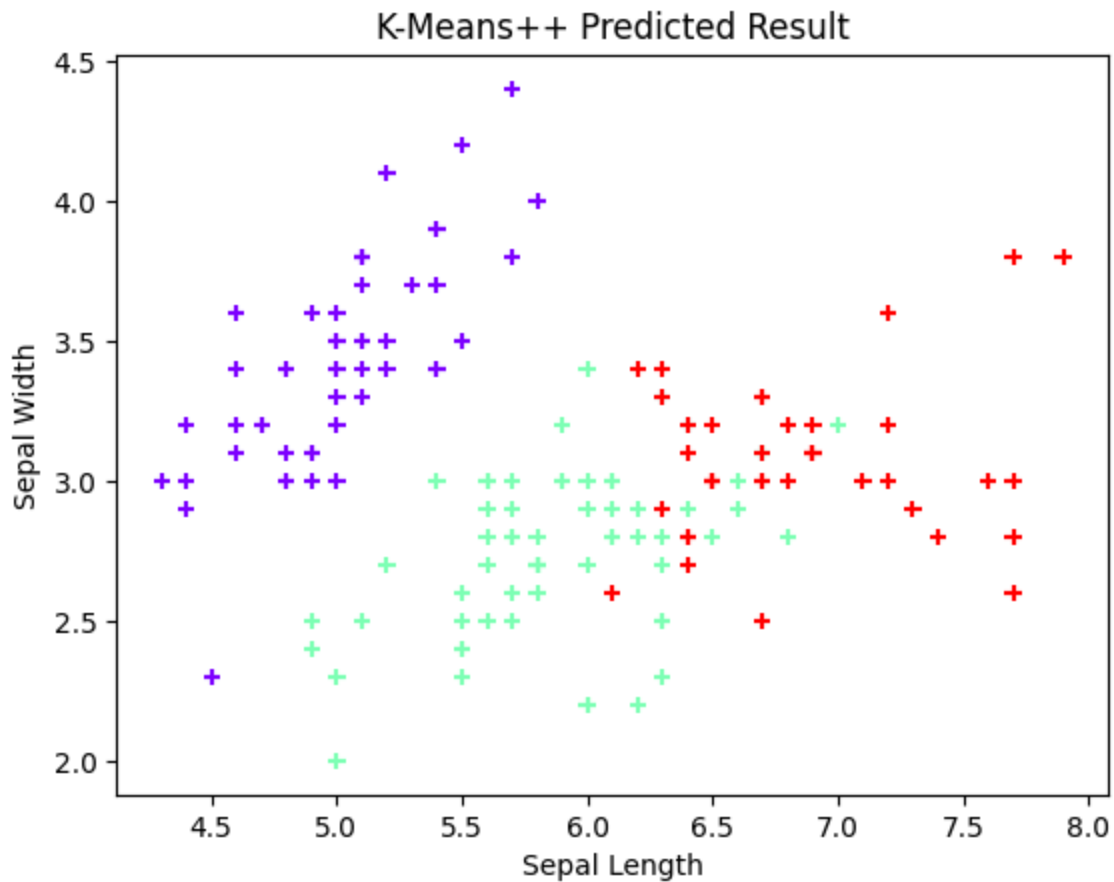
```

In [21]: # Clustering using K-means++ algorithm
from sklearn.cluster import KMeans
km = KMeans(init='k-means++', n_clusters=3, n_init=10, max_iter=300,
            random_state=42)
km = KMeans(n_clusters=3, n_init=10)
y_predicted = km.fit_predict(X)
plt.title("K-Means++ Predicted Result")
plt.xlabel("Sepal Length")

```



```
plt.ylabel("Sepal Width")
plt.scatter(df_iris.sepal_length, df_iris.sepal_width, c=km.labels_,
            cmap='rainbow', marker="+")
plt.show()
```



```
In [22]: from sklearn.metrics import rand_score, adjusted_rand_score
from sklearn.metrics import mutual_info_score, adjusted_mutual_info_score, normalized_mutual_info_score

# True labels
y_true = df_iris['species']

# Predicted cluster labels from K-Means++
y_pred = km.labels_ # or y_predicted

# Compute Rand Index
ri = rand_score(y_true, y_pred)
ari = adjusted_rand_score(y_true, y_pred)

# Compute Mutual Information scores
mi = mutual_info_score(y_true, y_pred)
ami = adjusted_mutual_info_score(y_true, y_pred)
nmi = normalized_mutual_info_score(y_true, y_pred)

# Print results
print(f"Rand Index: {ri:.4f}")
print(f"Adjusted Rand Index: {ari:.4f}")
```

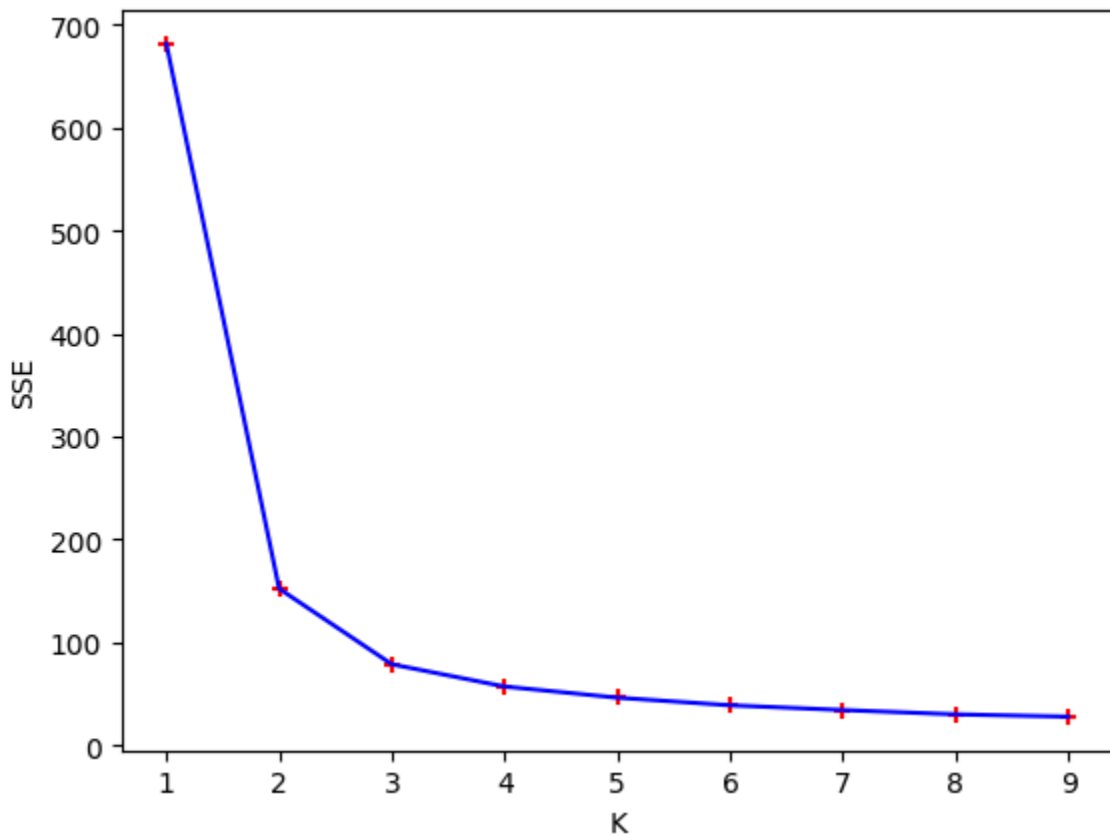
```
print(f"Mutual Information: {mi:.4f}")
print(f"Adjusted Mutual Information: {ami:.4f}")
print(f"Normalized Mutual Information: {nmi:.4f}")
```

Rand Index: 0.8797
Adjusted Rand Index: 0.7302
Mutual Information: 0.8256
Adjusted Mutual Information: 0.7551
Normalized Mutual Information: 0.7582

In [23]: *# Visualisation of SSE (Sum of Squared Errors) & Elbow Graph:*

```
sse = []
k_range = range(1, 10)
for k in k_range:
    km = KMeans(n_clusters=k, n_init=10)
    km.fit_predict(X)
    sse.append(km.inertia_)
plt.xlabel("K")
plt.ylabel("SSE")
plt.scatter(k_range, sse, color="red", marker="+")
plt.plot(k_range, sse, color="blue")
# We can see here, our elbow is at K=3
```

Out[23]: [



In [24]: *# Evaluating Metrics*

```
silhouette_result = silhouette_score(X, km.labels_)
print("Silhouette Score: ", silhouette_result)
```

```

calinski_result = calinski_harabasz_score(X, km.labels_)
print("Calinski Harabasz Score: ", calinski_result)
davies_result = davies_bouldin_score(X, km.labels_)
print("Davies Bouldin Score: ", davies_result)
# Evaluating Cohesion & Separation
labels = km.labels_
centroids = km.cluster_centers_
SSE = np.sum((X - centroids[labels])**2)
overall_centroid = np.mean(X, axis=0)
SSB = np.sum([np.sum((X[labels == i] - centroids[i])**2) for i in
range(3)])
N = X.shape[0]
cohesion_scores = SSE/N
cohesion = np.mean(cohesion_scores)
separation = SSB/N
print(f"\nCohesion Score: {cohesion}")
print(f"Separation Score: {separation}")

```

Silhouette Score: 0.34022340175905735
 Calinski Harabasz Score: 411.54596312475513
 Davies Bouldin Score: 0.9373777898644661

Cohesion Score: 0.046637035341978134
 Separation Score: 0.07776974955504704

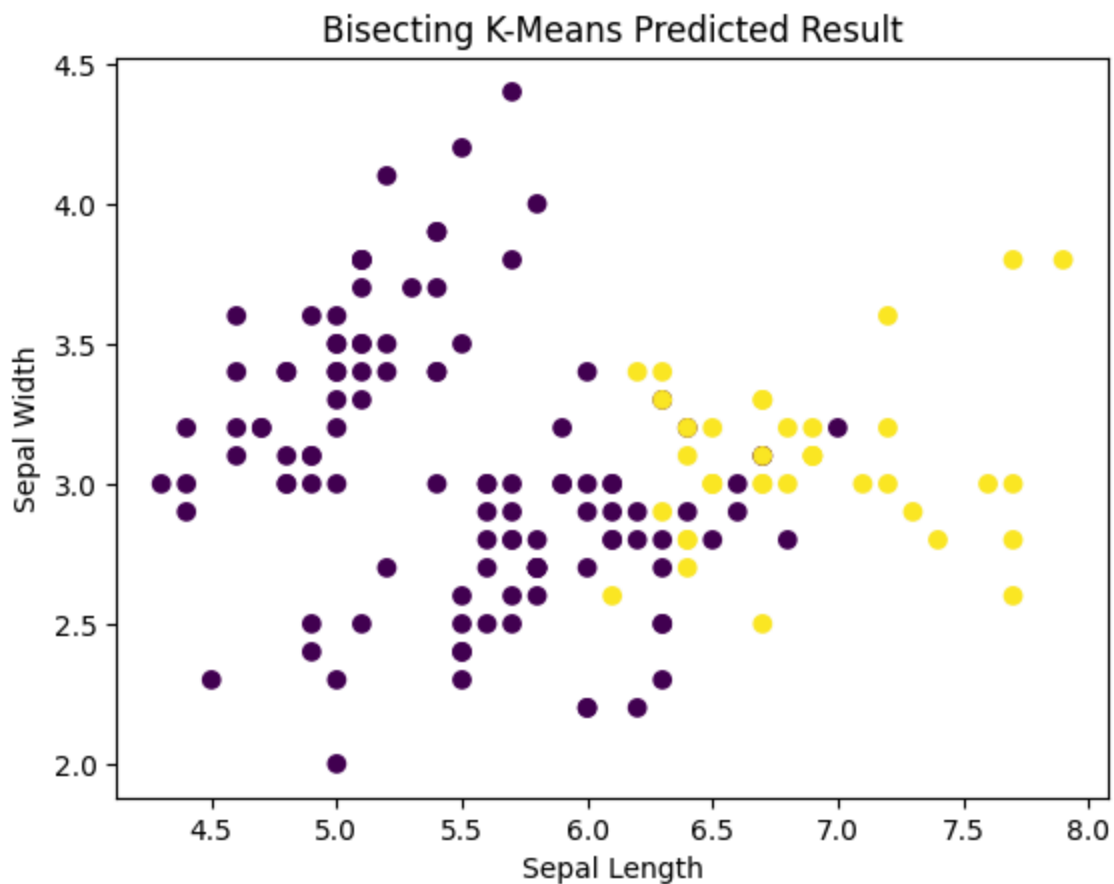
/usr/local/lib/python3.12/dist-packages/numpy/core/fromnumeric.py:86: FutureWarning: The behavior of DataFrame.sum with axis=None is deprecated, in a future version this will reduce over both axes and return a scalar. To retain the old behavior, pass axis=0 (or do not pass axis)
 return reduction(axis=axis, out=out, **passkwargs)

Bisecting K-means Clustering in Iris Dataset

```

In [25]: # Clustering using Bisecting K-means algorithm
from sklearn.cluster import KMeans
km = KMeans(n_clusters=1, n_init=10, random_state=0).fit(X)
K=3
for i in range(K-1):
    largest_cluster = np.argmax(np.bincount(km.labels_))
    largest_cluster_mask = (km.labels_ == largest_cluster)
    X_split = X[largest_cluster_mask]
    km.labels_[largest_cluster_mask] = KMeans(n_clusters=2, n_init=10,
random_state=0).fit(X_split).labels_
plt.title("Bisecting K-Means Predicted Result")
plt.xlabel("Sepal Length")
plt.ylabel("Sepal Width")
plt.scatter(df_iris.sepal_length, df_iris.sepal_width, c=km.labels_,
cmap='viridis')
plt.show()

```



```
In [26]: from sklearn.metrics import rand_score, adjusted_rand_score
from sklearn.metrics import mutual_info_score, adjusted_mutual_info_score, normalized_mutual_info_score

# True labels
y_true = df_iris['species']

# Predicted cluster labels from Bisecting K-Means
y_pred = km.labels_

# Compute Rand Index
ri = rand_score(y_true, y_pred)
ari = adjusted_rand_score(y_true, y_pred)

# Compute Mutual Information scores
mi = mutual_info_score(y_true, y_pred)
ami = adjusted_mutual_info_score(y_true, y_pred)
nmi = normalized_mutual_info_score(y_true, y_pred)

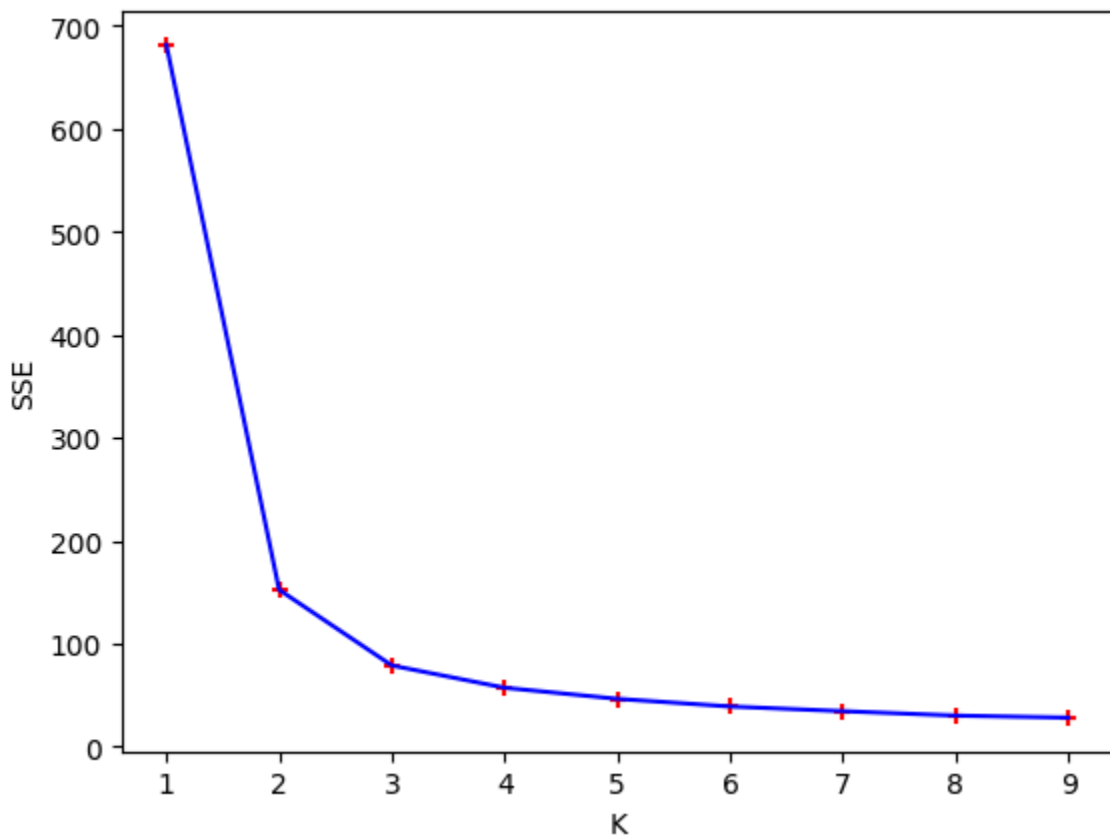
# Print results
print(f"Rand Index: {ri:.4f}")
print(f"Adjusted Rand Index: {ari:.4f}")
print(f"Mutual Information: {mi:.4f}")
print(f"Adjusted Mutual Information: {ami:.4f}")
print(f"Normalized Mutual Information: {nmi:.4f}")
```

Rand Index: 0.6023
Adjusted Rand Index: 0.2646
Mutual Information: 0.3123
Adjusted Mutual Information: 0.3701
Normalized Mutual Information: 0.3753

In [27]: *# Visualisation of SSE (Sum of Squared Errors) & Elbow Graph:*

```
sse = []  
k_range = range(1, 10)  
for k in k_range:  
    km = KMeans(n_clusters=k, n_init=10)  
    km.fit_predict(X)  
    sse.append(km.inertia_)  
plt.xlabel("K")  
plt.ylabel("SSE")  
plt.scatter(k_range, sse, color="red", marker="+")  
plt.plot(k_range, sse, color="blue")  
# We can see here, our elbow is at K=3
```

Out[27]: [matplotlib.lines.Line2D at 0x78c22197aff0>]



In [28]: *# Evaluating Metrics*

```
silhouette_result = silhouette_score(X, km.labels_)  
print("Silhouette Score: ", silhouette_result)  
calinski_result = calinski_harabasz_score(X, km.labels_)  
print("Calinski Harabasz Score: ", calinski_result)  
davies_result = davies_bouldin_score(X, km.labels_)  
print("Davies Bouldin Score: ", davies_result)
```

```
# Evaluating Cohesion & Separation
labels = km.labels_
centroids = km.cluster_centers_
SSE = np.sum((X - centroids[labels])**2)
overall_centroid = np.mean(X, axis=0)
SSB = np.sum([np.sum((X[labels == i] - centroids[i])**2) for i in
range(3)])
N = X.shape[0]
cohesion_scores = SSE/N
cohesion = np.mean(cohesion_scores)
separation = SSB/N
print(f"\nCohesion Score: {cohesion}")
print(f"Separation Score: {separation}")
```

Silhouette Score: 0.3449089481871134
 Calinski Harabasz Score: 408.7039167054135
 Davies Bouldin Score: 0.9971811693416696

Cohesion Score: 0.04694793290043289
 Separation Score: 0.06160779220779222

/usr/local/lib/python3.12/dist-packages/numpy/core/fromnumeric.py:86: FutureWarning: The behavior of DataFrame.sum with axis=None is deprecated, in a future version this will reduce over both axes and return a scalar. To retain the old behavior, pass axis=0 (or do not pass axis)
 return reduction(axis=axis, out=out, **passkwargs)

WINE DATASET

In [29]: `pip install ucimlrepo`

```
Collecting ucimlrepo
  Downloading ucimlrepo-0.0.7-py3-none-any.whl.metadata (5.5 kB)
Requirement already satisfied: pandas>=1.0.0 in /usr/local/lib/python3.12/dist-packages (from ucimlrepo) (2.2.2)
Requirement already satisfied: certifi>=2020.12.5 in /usr/local/lib/python3.12/dist-packages (from ucimlrepo) (2025.10.5)
Requirement already satisfied: numpy>=1.26.0 in /usr/local/lib/python3.12/dist-packages (from pandas>=1.0.0->ucimlrepo) (1.26.4)
Requirement already satisfied: python-dateutil>=2.8.2 in /usr/local/lib/python3.12/dist-packages (from pandas>=1.0.0->ucimlrepo) (2.9.0.post0)
Requirement already satisfied: pytz>=2020.1 in /usr/local/lib/python3.12/dist-packages (from pandas>=1.0.0->ucimlrepo) (2025.2)
Requirement already satisfied: tzdata>=2022.7 in /usr/local/lib/python3.12/dist-packages (from pandas>=1.0.0->ucimlrepo) (2025.2)
Requirement already satisfied: six>=1.5 in /usr/local/lib/python3.12/dist-packages (from python-dateutil>=2.8.2->pandas>=1.0.0->ucimlrepo) (1.17.0)
Downloading ucimlrepo-0.0.7-py3-none-any.whl (8.0 kB)
Installing collected packages: ucimlrepo
Successfully installed ucimlrepo-0.0.7
```

In [30]: `from ucimlrepo import fetch_ucirepo`

```
# fetch dataset
wine = fetch_ucirepo(id=109)

# data (as pandas dataframes)
X = wine.data.features
y = wine.data.targets

# metadata
print(wine.metadata)

# variable information
print(wine.variables)
df = X.copy()
df['class'] = y # add target column
print(df.head())
```

```
{'uci_id': 109, 'name': 'Wine', 'repository_url': 'https://archive.ics.uci.edu/
dataset/109/wine', 'data_url': 'https://archive.ics.uci.edu/static/public/109/d
ata.csv', 'abstract': 'Using chemical analysis to determine the origin of wine
s', 'area': 'Physics and Chemistry', 'tasks': ['Classification'], 'characterist
ics': ['Tabular'], 'num_instances': 178, 'num_features': 13, 'feature_types':
['Integer', 'Real'], 'demographics': [], 'target_col': ['class'], 'index_col':
None, 'has_missing_values': 'no', 'missing_values_symbol': None, 'year_of_data
et_creation': 1992, 'last_updated': 'Mon Aug 28 2023', 'dataset_doi': '10.2443
2/C5PC7J', 'creators': ['Stefan Aeberhard', 'M. Forina'], 'intro_paper': {'ID':
246, 'type': 'NATIVE', 'title': 'Comparative analysis of statistical pattern re
cognition methods in high dimensional settings', 'authors': 'S. Aeberhard, D. C
oomans, O. Vel', 'venue': 'Pattern Recognition', 'year': 1994, 'journal': None,
'DOI': '10.1016/0031-3203(94)90145-7', 'URL': 'https://www.semanticscholar.org/
paper/83dc3e4030d7b9fbdbb4bde03ce12ab70cal0528', 'sha': None, 'corpus': None,
'arxiv': None, 'mag': None, 'acl': None, 'pmid': None, 'pmcid': None}, 'additio
nal_info': {'summary': 'These data are the results of a chemical analysis of wi
nes grown in the same region in Italy but derived from three different cultivar
s. The analysis determined the quantities of 13 constituents found in each of t
he three types of wines. \r\n\r\nI think that the initial data set had around 3
0 variables, but for some reason I only have the 13 dimensional version. I had
a list of what the 30 or so variables were, but a.) I lost it, and b.), I woul
d not know which 13 variables are included in the set.\r\n\r\nThe attributes ar
e (dontated by Riccardo Leardi, riclea@anchem.unige.it )\r\n1) Alcohol\r\n2) Ma
lic acid\r\n3) Ash\r\n4) Alcalinity of ash \r\n5) Magnesium\r\n6) Total phenol
s\r\n7) Flavanoids\r\n8) Nonflavanoid phenols\r\n9) Proanthocyanins\r\n10)Color
intensity\r\n11)Hue\r\n12)OD280/OD315 of diluted wines\r\n13)Proline \r\n\r\nIn
a classification context, this is a well posed problem with "well behaved" clas
s structures. A good data set for first testing of a new classifier, but not ve
ry challenging. ', 'purpose': 'test', 'funded_by': None, 'instances_r
epresent': None, 'recommended_data_splits': None, 'sensitive_data': None, 'prep
rocessing_description': None, 'variable_info': 'All attributes are continuous\
\r\n\r\nNo statistics available, but suggest to standardise variables for cert
ain uses (e.g. for us with classifiers which are NOT scale invariant)\r\n\r\nNO
TE: 1st attribute is class identifier (1-3)', 'citation': None}}
```

	name	role	type	demographic \
0	class	Target	Categorical	None
1	Alcohol	Feature	Continuous	None
2	Malicacid	Feature	Continuous	None
3	Ash	Feature	Continuous	None
4	Alcalinity_of_ash	Feature	Continuous	None
5	Magnesium	Feature	Integer	None
6	Total_phenols	Feature	Continuous	None
7	Flavanoids	Feature	Continuous	None
8	Nonflavanoid_phenols	Feature	Continuous	None
9	Proanthocyanins	Feature	Continuous	None
10	Color_intensity	Feature	Continuous	None
11	Hue	Feature	Continuous	None
12	OD280_OD315_of_diluted_wines	Feature	Continuous	None
13	Proline	Feature	Integer	None

	description	units	missing_values
0	None	None	no
1	None	None	no
2	None	None	no

3	None	None		no
4	None	None		no
5	None	None		no
6	None	None		no
7	None	None		no
8	None	None		no
9	None	None		no
10	None	None		no
11	None	None		no
12	None	None		no
13	None	None		no

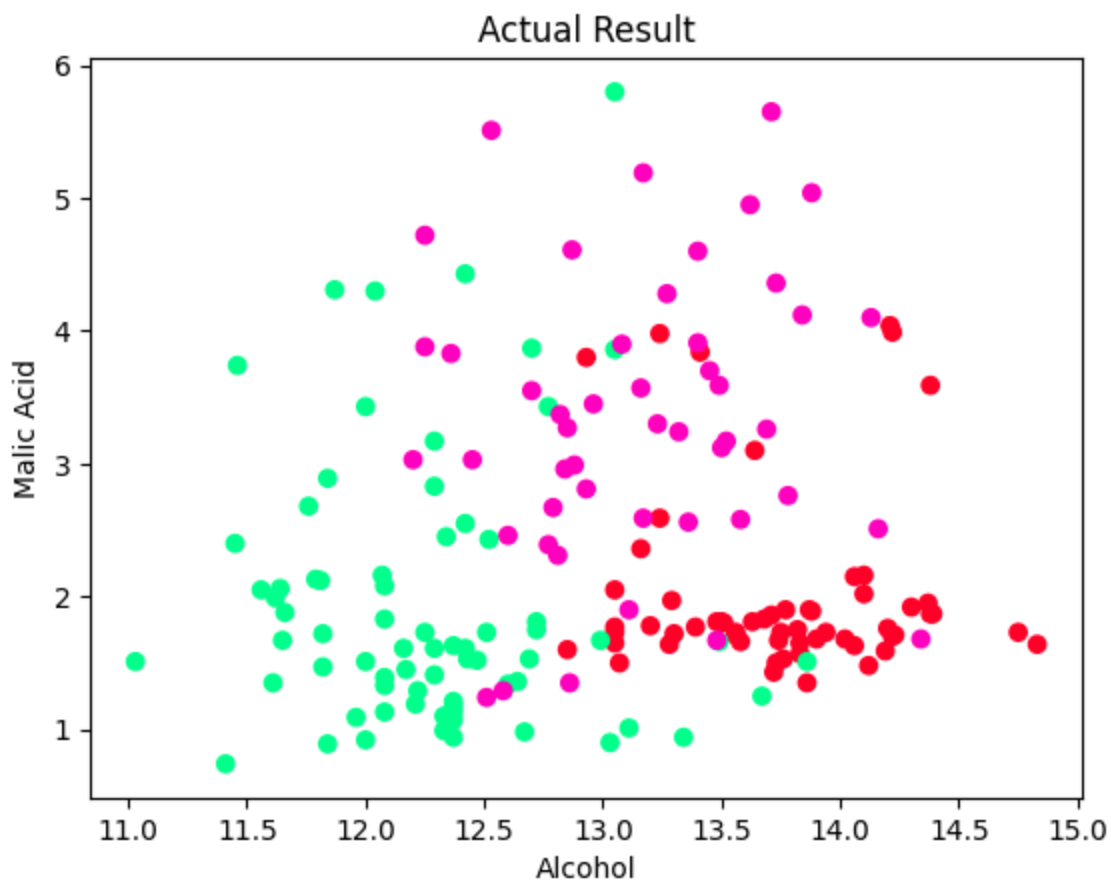
	Alcohol	Malicacid	Ash	Alcalinity_of_ash	Magnesium	Total_phenols	\
0	14.23	1.71	2.43	15.6	127	2.80	
1	13.20	1.78	2.14	11.2	100	2.65	
2	13.16	2.36	2.67	18.6	101	2.80	
3	14.37	1.95	2.50	16.8	113	3.85	
4	13.24	2.59	2.87	21.0	118	2.80	

	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

	0D280_0D315_of_diluted_wines	Proline	class
0	3.92	1065	1
1	3.40	1050	1
2	3.17	1185	1
3	3.45	1480	1
4	2.93	735	1

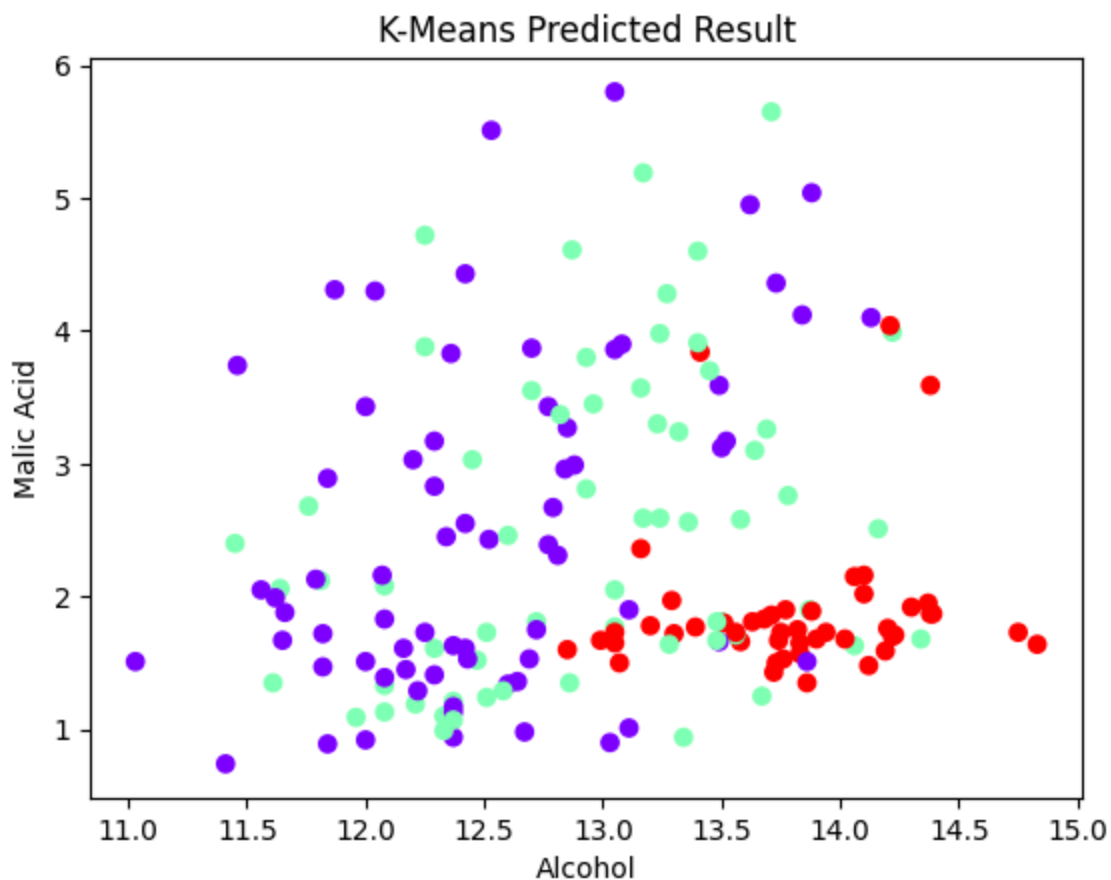
```
In [31]: plt.title("Actual Result")
plt.xlabel('Alcohol')
plt.ylabel('Malic Acid')
plt.scatter(df.Alcohol, df.Malicacid, c=df["class"],
cmap='gist_rainbow')
```

```
Out[31]: <matplotlib.collections.PathCollection at 0x78c221a7b2f0>
```



Partition Based: K-means Clustering in Wine Dataset

```
In [32]: # Clustering using K-means algorithm
from sklearn.cluster import KMeans
km = KMeans(init="random", n_clusters=3, n_init=10, max_iter=300,
            random_state=42)
y_predicted = km.fit_predict(X)
plt.title("K-Means Predicted Result")
plt.xlabel("Alcohol")
plt.ylabel("Malic Acid")
plt.scatter(df.Alcohol, df.Malicacid, c=km.labels_, cmap='rainbow')
plt.show()
```



```
In [33]: from sklearn.metrics import rand_score, adjusted_rand_score
from sklearn.metrics import mutual_info_score, adjusted_mutual_info_score, normalized_mutual_info_score

# True labels (numeric for Wine dataset)
y_true = df['class']

# Predicted cluster labels from K-Means
y_pred = km.labels_ # or y_predicted

# Compute Rand Index
ri = rand_score(y_true, y_pred)
ari = adjusted_rand_score(y_true, y_pred)

# Compute Mutual Information scores
mi = mutual_info_score(y_true, y_pred)
ami = adjusted_mutual_info_score(y_true, y_pred)
nmi = normalized_mutual_info_score(y_true, y_pred)

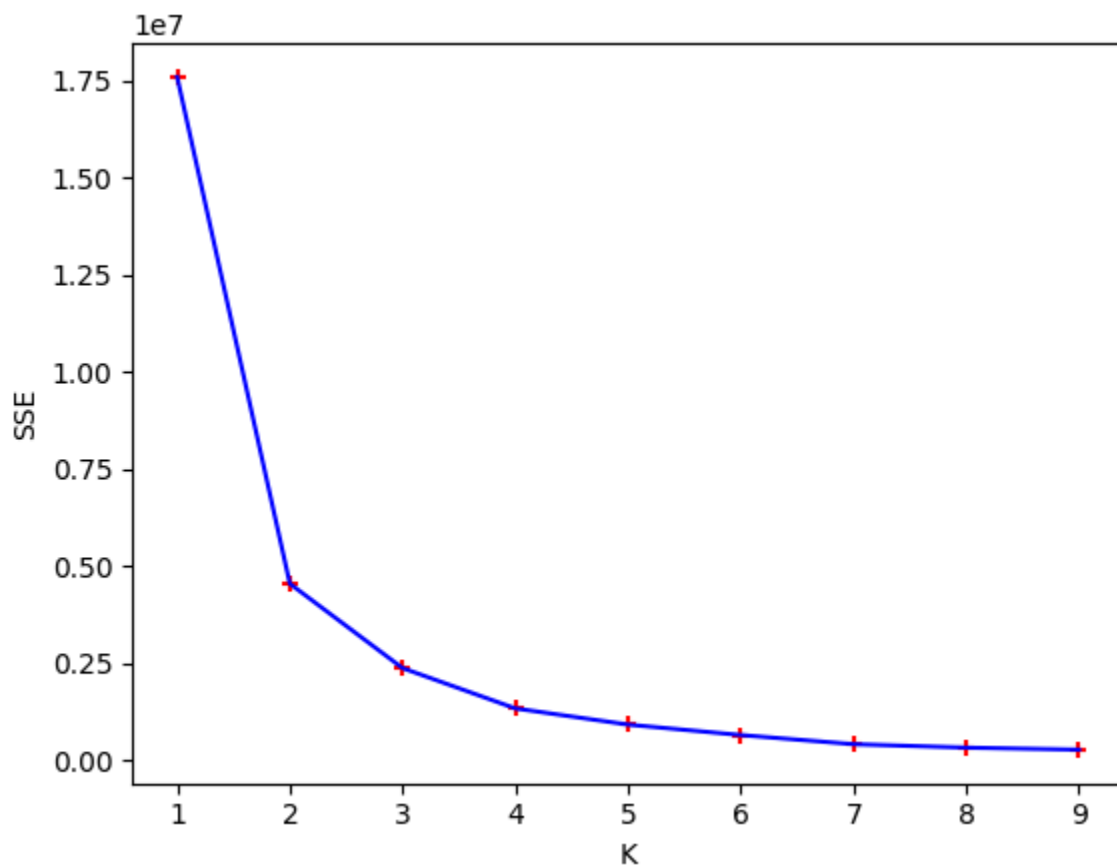
# Print results
print(f"Rand Index: {ri:.4f}")
print(f"Adjusted Rand Index: {ari:.4f}")
print(f"Mutual Information: {mi:.4f}")
print(f"Adjusted Mutual Information: {ami:.4f}")
print(f"Normalized Mutual Information: {nmi:.4f}")
```

Rand Index: 0.7187
Adjusted Rand Index: 0.3711
Mutual Information: 0.4657
Adjusted Mutual Information: 0.4227
Normalized Mutual Information: 0.4288

In [34]: *# Visualisation of SSE (Sum of Squared Errors) & Elbow Graph:*

```
sse = []
k_range = range(1, 10)
for k in k_range:
    km = KMeans(n_clusters=k, n_init=10)
    km.fit_predict(X)
    sse.append(km.inertia_)
plt.xlabel("K")
plt.ylabel("SSE")
plt.scatter(k_range, sse, color="red", marker="+")
plt.plot(k_range, sse, color="blue")
# We can see here, our elbow is at K=3
```

Out[34]: [



In [35]: *# Evaluating Metrics*

```
silhouette_result = silhouette_score(X, km.labels_)
print("Silhouette Score: ", silhouette_result)
calinski_result = calinski_harabasz_score(X, km.labels_)
print("Calinski Harabasz Score: ", calinski_result)
davies_result = davies_bouldin_score(X, km.labels_)
```

```

print("Davies Bouldin Score: ", davies_result)
# Evaluating Cohesion & Separation
labels = km.labels_
centroids = km.cluster_centers_
SSE = np.sum((X - centroids[labels])**2)
overall_centroid = np.mean(X, axis=0)
SSB = np.sum([np.sum((X[labels == i] - centroids[i])**2) for i in
range(3)])
N = X.shape[0]
cohesion_scores = SSE/N
cohesion = np.mean(cohesion_scores)
separation = SSB/N
print(f"\nCohesion Score: {cohesion}")
print(f"Separation Score: {separation}")

```

Silhouette Score: 0.5316577207122226
 Calinski Harabasz Score: 1350.2082067758508
 Davies Bouldin Score: 0.5143723568247524

Cohesion Score: 117.11510269734075
 Separation Score: 647.2739281239623

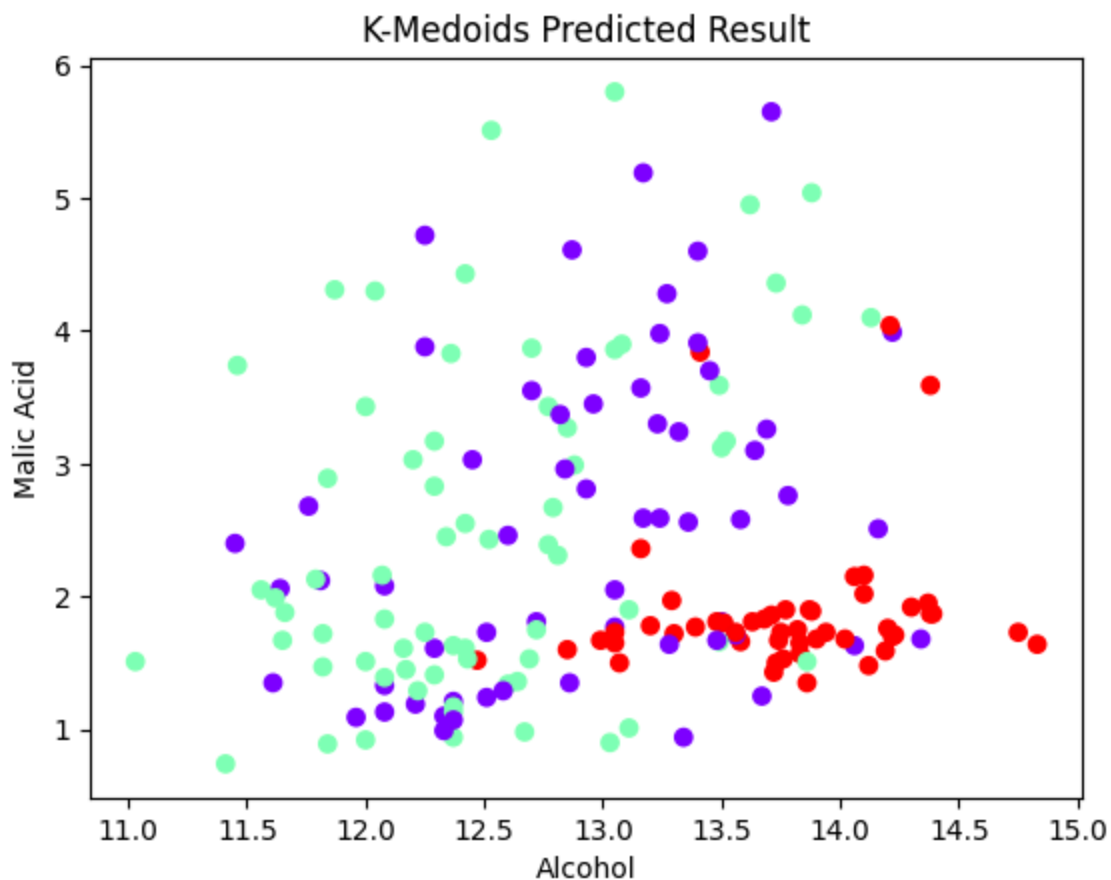
/usr/local/lib/python3.12/dist-packages/numpy/core/fromnumeric.py:86: FutureWarning: The behavior of DataFrame.sum with axis=None is deprecated, in a future version this will reduce over both axes and return a scalar. To retain the old behavior, pass axis=0 (or do not pass axis)
 return reduction(axis=axis, out=out, **passkwargs)

Partition Based: K-medoids Clustering in Wine Dataset

```

In [36]: # Clustering using K-medoids algorithm
from sklearn_extra.cluster import KMedoids
km = KMedoids(n_clusters=3)
y_predicted = km.fit_predict(X)
plt.title("K-Medoids Predicted Result")
plt.xlabel("Alcohol")
plt.ylabel("Malic Acid")
plt.scatter(df.Alcohol, df.Malicacid, c=km.labels_, cmap='rainbow')
plt.show()

```



```
In [37]: from sklearn.metrics import rand_score, adjusted_rand_score
from sklearn.metrics import mutual_info_score, adjusted_mutual_info_score, normalized_mutual_info_score

# True labels (numeric)
y_true = df['class']

# Predicted cluster labels from K-Medoids
y_pred = km.labels_ # or y_predicted

# Compute Rand Index
ri = rand_score(y_true, y_pred)
ari = adjusted_rand_score(y_true, y_pred)

# Compute Mutual Information scores
mi = mutual_info_score(y_true, y_pred)
ami = adjusted_mutual_info_score(y_true, y_pred)
nmi = normalized_mutual_info_score(y_true, y_pred)

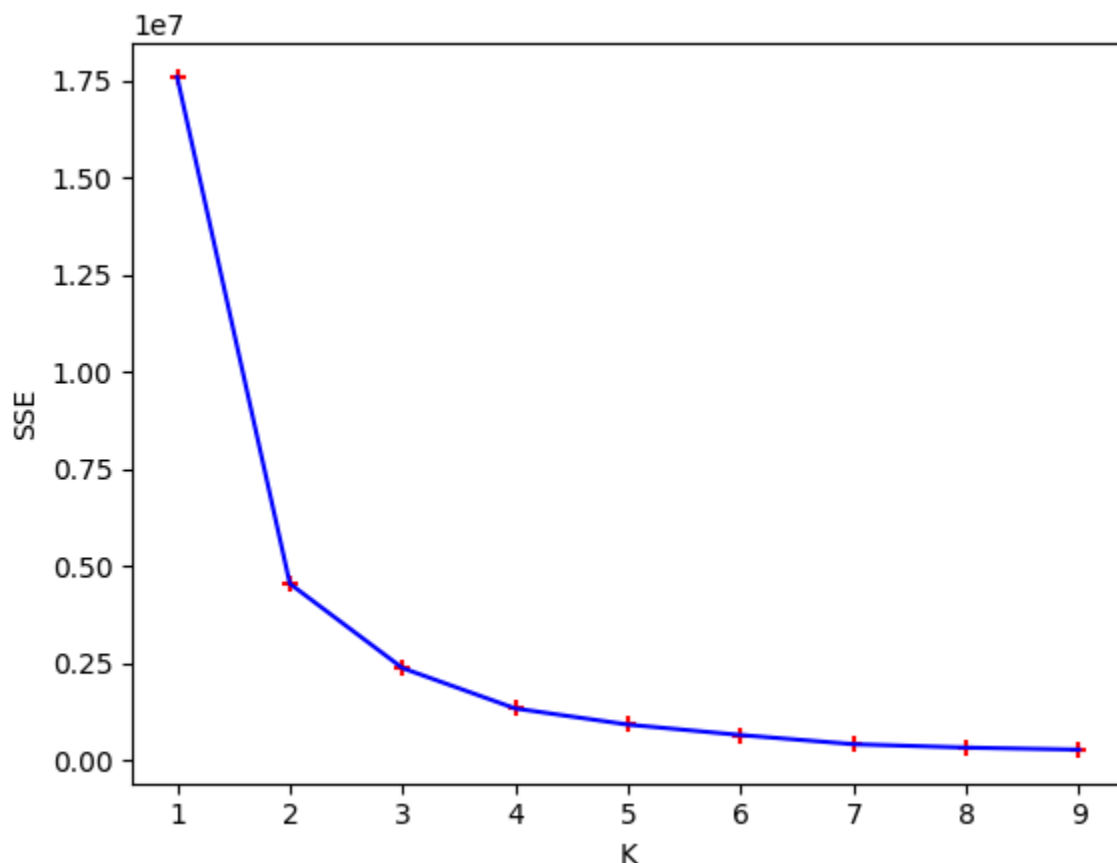
# Print results
print(f"Rand Index: {ri:.4f}")
print(f"Adjusted Rand Index: {ari:.4f}")
print(f"Mutual Information: {mi:.4f}")
print(f"Adjusted Mutual Information: {ami:.4f}")
print(f"Normalized Mutual Information: {nmi:.4f}")
```

Rand Index: 0.7295
Adjusted Rand Index: 0.3941
Mutual Information: 0.4737
Adjusted Mutual Information: 0.4292
Normalized Mutual Information: 0.4352

In [38]: *# Visualisation of SSE (Sum of Squared Errors) & Elbow Graph:*

```
sse = []
k_range = range(1, 10)
for k in k_range:
    km = KMeans(n_clusters=k, n_init=10)
    km.fit_predict(X)
    sse.append(km.inertia_)
plt.xlabel("K")
plt.ylabel("SSE")
plt.scatter(k_range, sse, color="red", marker="+")
plt.plot(k_range, sse, color="blue")
# We can see here, our elbow is at K=3
```

Out[38]: [



In [39]: *# Evaluating Metrics*

```
silhouette_result = silhouette_score(X, km.labels_)
print("Silhouette Score: ", silhouette_result)
calinski_result = calinski_harabasz_score(X, km.labels_)
print("Calinski Harabasz Score: ", calinski_result)
davies_result = davies_bouldin_score(X, km.labels_)
```

```

print("Davies Bouldin Score: ", davies_result)
# Evaluating Cohesion & Separation
labels = km.labels_
centroids = km.cluster_centers_
SSE = np.sum((X - centroids[labels])**2)
overall_centroid = np.mean(X, axis=0)
SSB = np.sum([np.sum((X[labels == i] - centroids[i])**2) for i in
range(3)])
N = X.shape[0]
cohesion_scores = SSE/N
cohesion = np.mean(cohesion_scores)
separation = SSB/N
print(f"\nCohesion Score: {cohesion}")
print(f"Separation Score: {separation}")

```

Silhouette Score: 0.5307235924738344
 Calinski Harabasz Score: 1350.4583188269025
 Davies Bouldin Score: 0.5163732495928284

Cohesion Score: 117.09374643108792
 Separation Score: 376.1895168914436

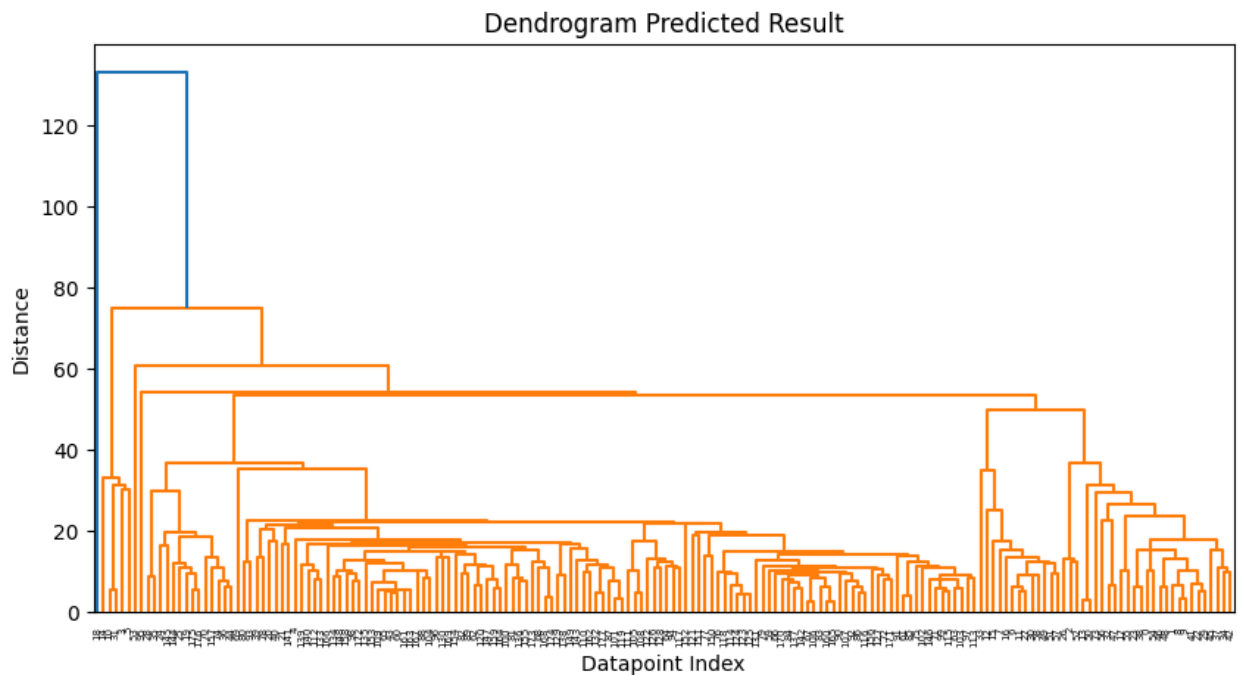
/usr/local/lib/python3.12/dist-packages/numpy/core/fromnumeric.py:86: FutureWarning: The behavior of DataFrame.sum with axis=None is deprecated, in a future version this will reduce over both axes and return a scalar. To retain the old behavior, pass axis=0 (or do not pass axis)
 return reduction(axis=axis, out=out, **passkwargs)

Hierarchical: Dendrogram Clustering in Wine Dataset

```

In [40]: # Clustering using Dendrogram Clustering algorithm
from scipy.cluster.hierarchy import dendrogram, linkage, fcluster
Z = linkage(X, method='single')
# Create and plot the dendrogram
plt.figure(figsize=(10, 5))
dn = dendrogram(Z)
plt.title('Dendrogram Predicted Result')
plt.xlabel('Datapoint Index')
plt.ylabel('Distance')
plt.show()

```

```
In [41]: from scipy.cluster.hierarchy import fcluster
from sklearn.metrics import rand_score, adjusted_rand_score
from sklearn.metrics import mutual_info_score, adjusted_mutual_info_score, normalized_mutual_info_score

# Cut dendrogram to form 3 clusters
y_pred = fcluster(Z, t=3, criterion='maxclust')

# True labels (numeric)
y_true = df['class']

# Compute Rand Index
ri = rand_score(y_true, y_pred)
ari = adjusted_rand_score(y_true, y_pred)

# Compute Mutual Information scores
mi = mutual_info_score(y_true, y_pred)
ami = adjusted_mutual_info_score(y_true, y_pred)
nmi = normalized_mutual_info_score(y_true, y_pred)

# Print results
print(f"Rand Index: {ri:.4f}")
print(f"Adjusted Rand Index: {ari:.4f}")
print(f"Mutual Information: {mi:.4f}")
print(f"Adjusted Mutual Information: {ami:.4f}")
print(f"Normalized Mutual Information: {nmi:.4f}")
```

```
Rand Index: 0.3628
Adjusted Rand Index: 0.0054
Mutual Information: 0.0384
Adjusted Mutual Information: 0.0416
Normalized Mutual Information: 0.0615
```

```
In [42]: # Evaluating Metrics
```

```
labels = fcluster(Z, 3, criterion='maxclust')
from sklearn.metrics import silhouette_score
silhouette_result = silhouette_score(X, labels)
print("Silhouette Score: ", silhouette_result)
from sklearn.metrics import calinski_harabasz_score
calinski_result = calinski_harabasz_score(X, labels)
print("Calinski Harabasz Score: ", calinski_result)
from sklearn.metrics import davies_bouldin_score
davies_result = davies_bouldin_score(X, labels)
print("Davies Bouldin Score: ", davies_result)
```

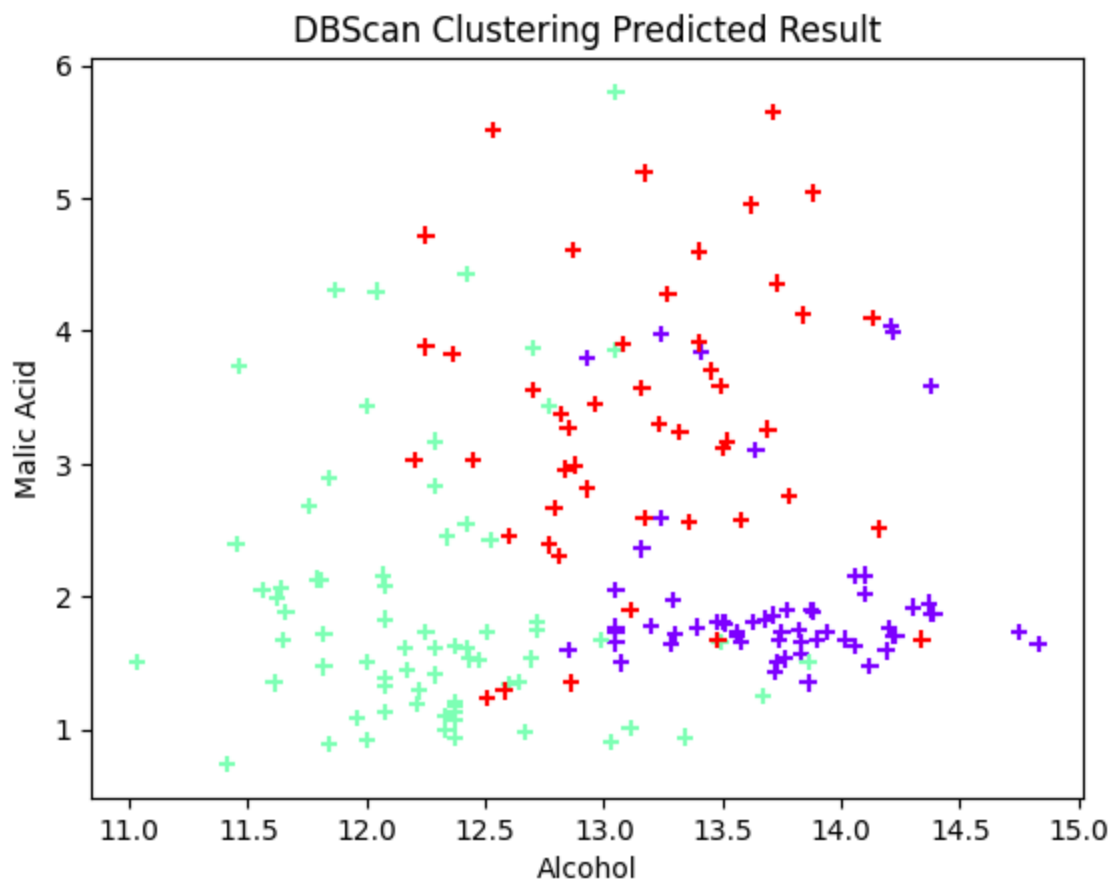
Silhouette Score: 0.4879820335189063

Calinski Harabasz Score: 24.42036238154286

Davies Bouldin Score: 0.30814096183494405

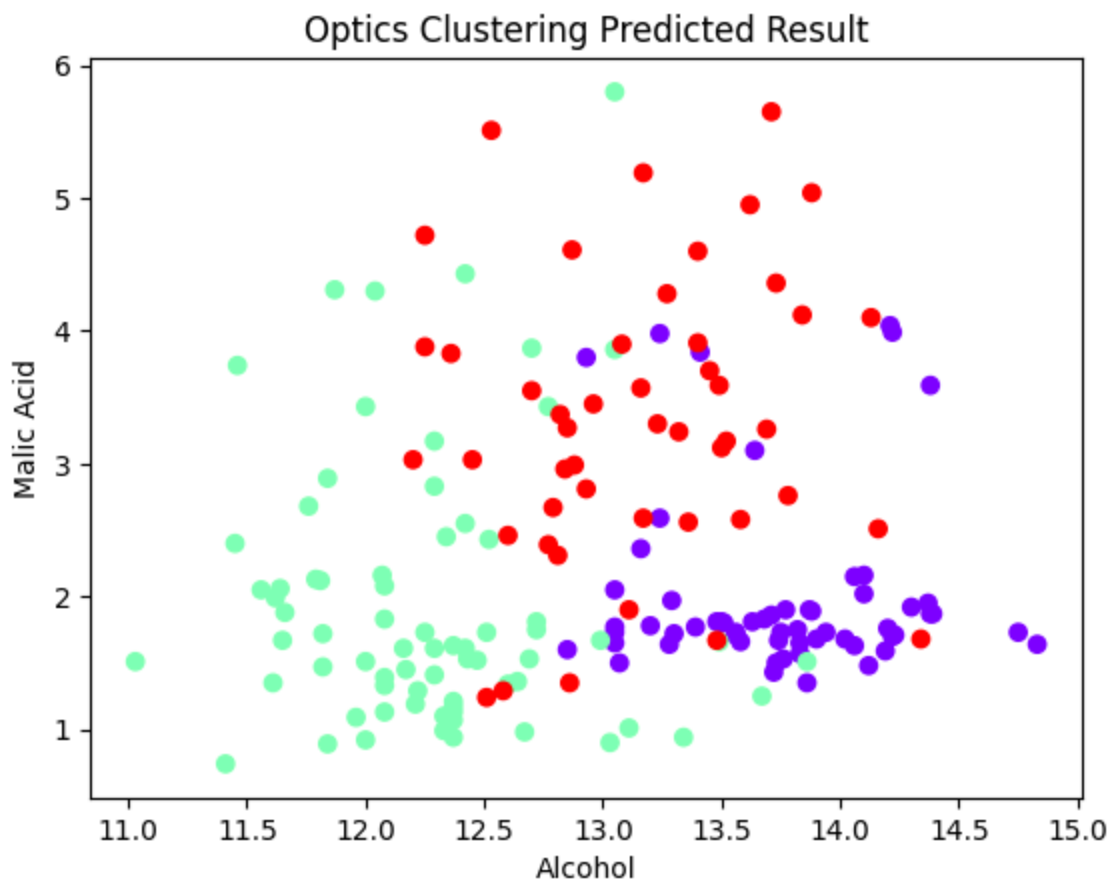
Density Based: DBSCAN Clustering in Wine Dataset

```
In [43]: # Clustering using DBSCAN Clustering algorithm
from sklearn.cluster import DBSCAN
dbscan = DBSCAN(eps=0.5, algorithm='auto', metric='euclidean')
y = dbscan.fit_predict(X)
plt.title('DBScan Clustering Predicted Result')
plt.xlabel('Alcohol')
plt.ylabel('Malic Acid')
plt.scatter(df.Alcohol, df.Malicacid, c=df["class"], cmap='rainbow',
            marker="+")
plt.show()
```



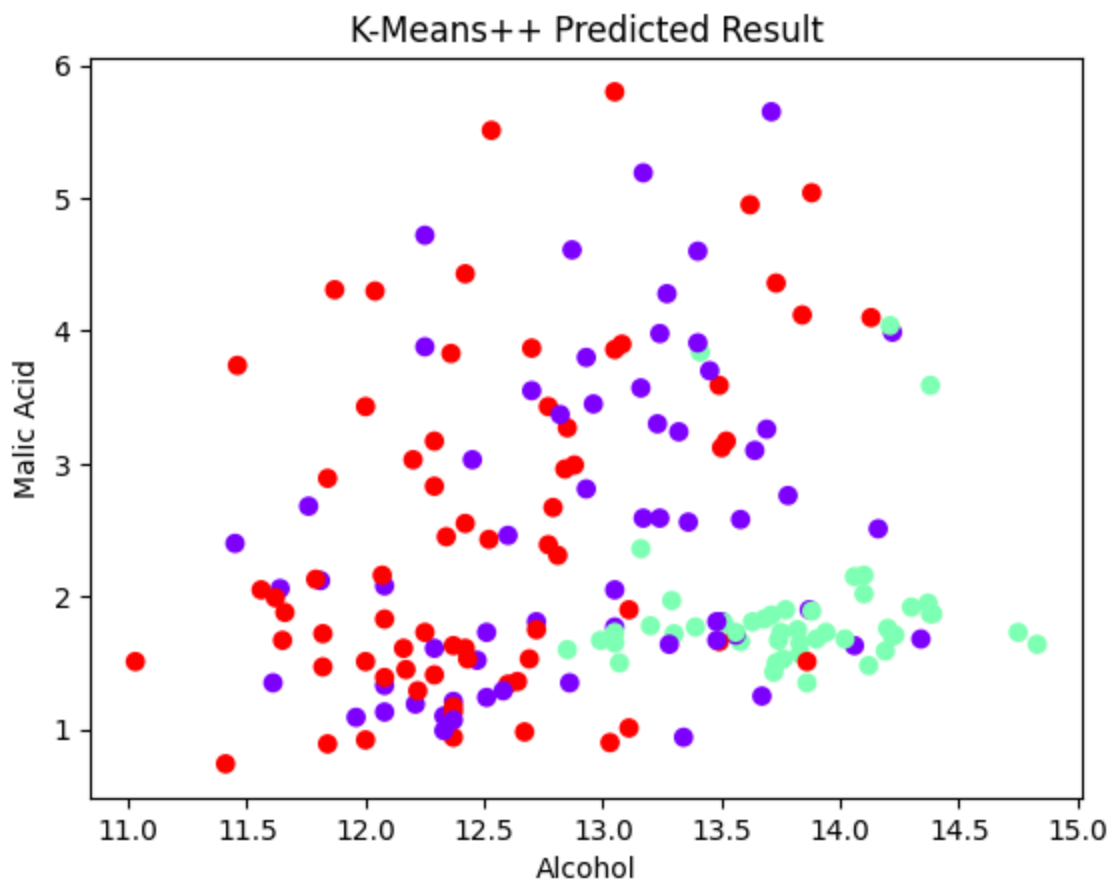
Density Based: Optics Clustering in Wine Dataset

```
In [44]: # Clustering using Optics Clustering algorithm
from sklearn.cluster import OPTICS
optics_cluster = OPTICS(min_samples=5, xi=0.05,
cluster_method='dbscan')
optics_cluster.fit(X)
plt.scatter(df.Alcohol, df.Malicacid, c=df["class"], cmap='rainbow')
plt.xlabel('Alcohol')
plt.ylabel('Malic Acid')
plt.title('Optics Clustering Predicted Result')
plt.show()
```



K-means++ Clustering in Wine Dataset

```
In [45]: # Clustering using K-means++ algorithm
from sklearn.cluster import KMeans
km = KMeans(init='k-means++', n_clusters=3, n_init=10, max_iter=300,
random_state=42)
km = KMeans(n_clusters=3, n_init=10)
y_predicted = km.fit_predict(X)
plt.title("K-Means++ Predicted Result")
plt.xlabel("Alcohol")
plt.ylabel("Malic Acid")
plt.scatter(df.Alcohol, df.Malicacid, c=km.labels_, cmap='rainbow')
plt.show()
```



```
In [46]: from sklearn.metrics import rand_score, adjusted_rand_score
from sklearn.metrics import mutual_info_score, adjusted_mutual_info_score, normalized_mutual_info_score

# True labels
y_true = df['class']

# Predicted cluster labels from K-Means++
y_pred = km.labels_ # or y_predicted

# Compute Rand Index
ri = rand_score(y_true, y_pred)
ari = adjusted_rand_score(y_true, y_pred)

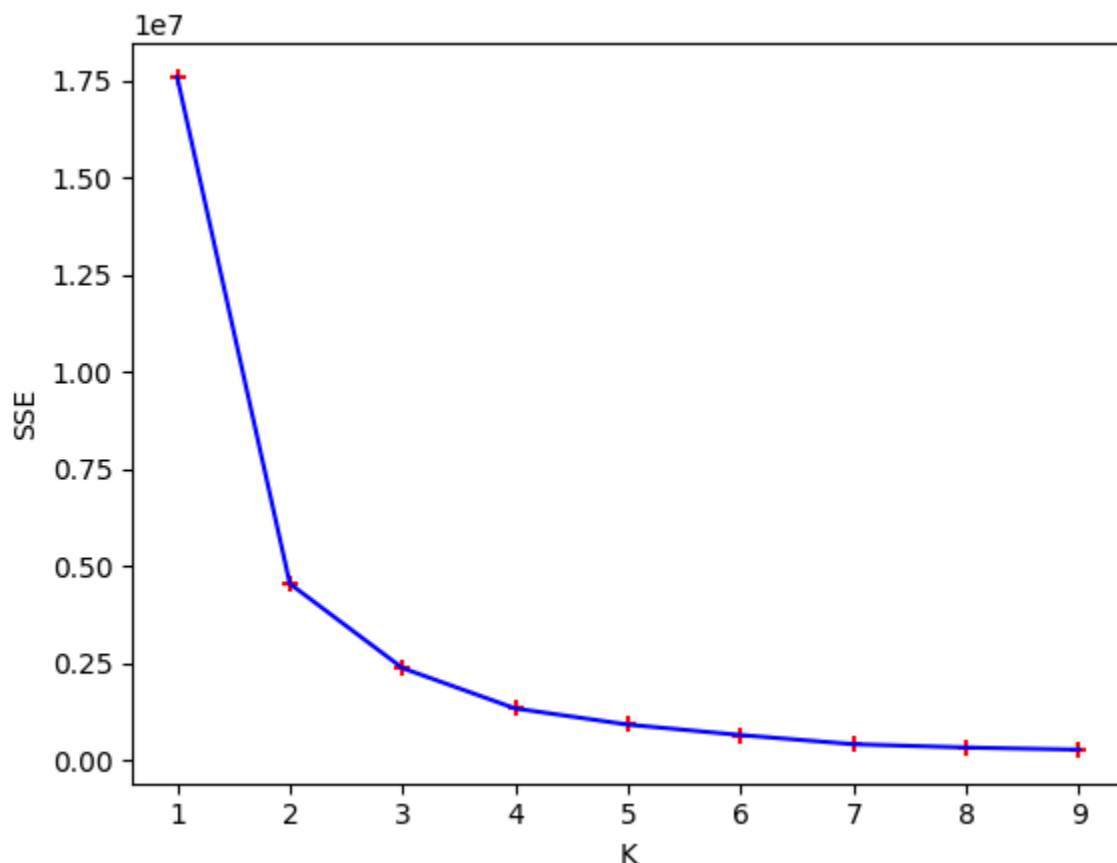
# Compute Mutual Information scores
mi = mutual_info_score(y_true, y_pred)
ami = adjusted_mutual_info_score(y_true, y_pred)
nmi = normalized_mutual_info_score(y_true, y_pred)

# Print results
print(f"Rand Index: {ri:.4f}")
print(f"Adjusted Rand Index: {ari:.4f}")
print(f"Mutual Information: {mi:.4f}")
print(f"Adjusted Mutual Information: {ami:.4f}")
print(f"Normalized Mutual Information: {nmi:.4f}")
```

Rand Index: 0.7187
Adjusted Rand Index: 0.3711
Mutual Information: 0.4657
Adjusted Mutual Information: 0.4227
Normalized Mutual Information: 0.4288

```
In [47]: sse = []
k_range = range(1, 10)
for k in k_range:
    km = KMeans(n_clusters=k, n_init=10)
    km.fit_predict(X)
    sse.append(km.inertia_)
plt.xlabel("K")
plt.ylabel("SSE")
plt.scatter(k_range, sse, color="red", marker="+")
plt.plot(k_range, sse, color="blue")
# We can see here, our elbow is at K=3
```

Out[47]: [matplotlib.lines.Line2D at 0x78c22197a660]



```
In [48]: # Evaluating Metrics
from sklearn.metrics import silhouette_score
silhouette_result = silhouette_score(X, km.labels_)
print("Silhouette Score: ", silhouette_result)
from sklearn.metrics import calinski_harabasz_score
calinski_result = calinski_harabasz_score(X, km.labels_)
print("Calinski Harabasz Score: ", calinski_result)
```

```

from sklearn.metrics import davies_bouldin_score
davies_result = davies_bouldin_score(X, km.labels_)
print("Davies Bouldin Score: ", davies_result)
# Evaluating Cohesion & Separation
labels = km.labels_
centroids = km.cluster_centers_
SSE = np.sum((X - centroids[labels])**2)
overall_centroid = np.mean(X, axis=0)
SSB = np.sum([np.sum((X[labels == i] - centroids[i])**2) for i in
range(3)])
N = X.shape[0]
cohesion_scores = SSE/N
cohesion = np.mean(cohesion_scores)
separation = SSB/N
print(f"\nCohesion Score: {cohesion}")
print(f"Separation Score: {separation}")

```

Silhouette Score: 0.525162492111064
 Calinski Harabasz Score: 1348.7425198414974
 Davies Bouldin Score: 0.5341503098266895

Cohesion Score: 117.24040976050752
 Separation Score: 555.1990303660302

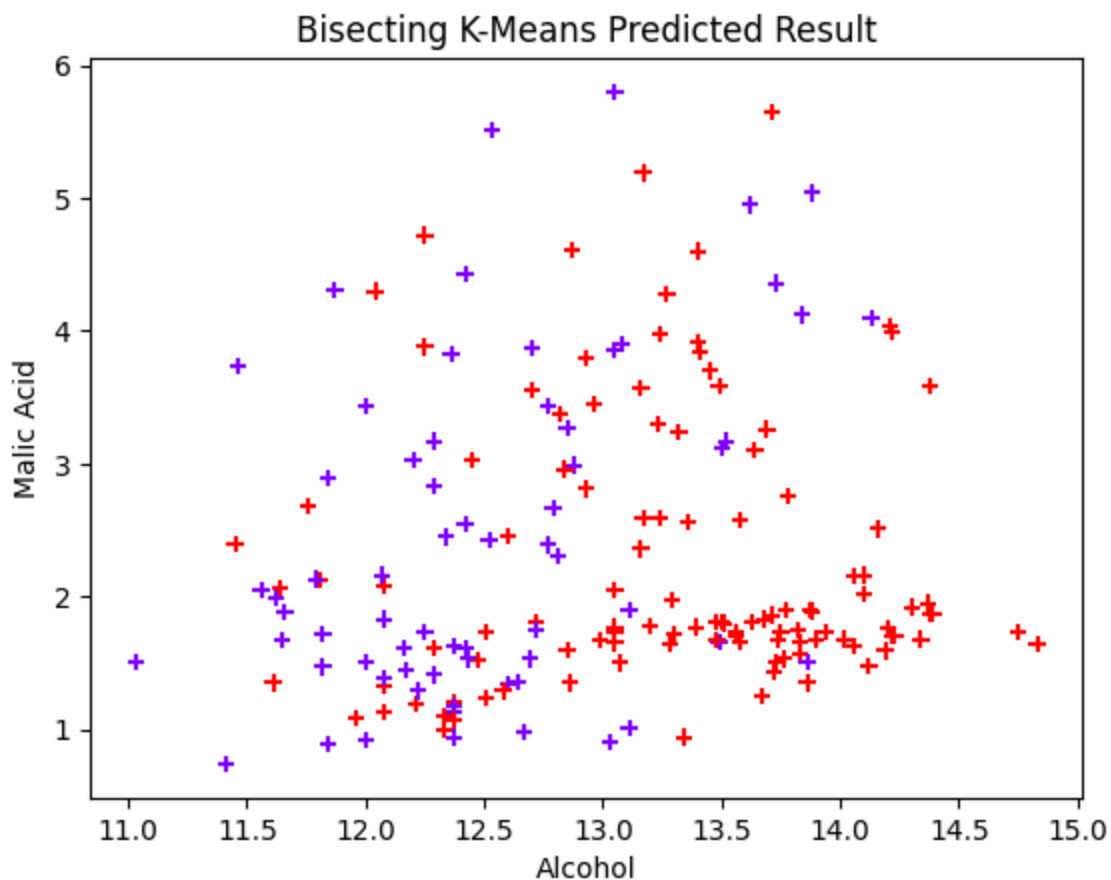
/usr/local/lib/python3.12/dist-packages/numpy/core/fromnumeric.py:86: FutureWarning: The behavior of DataFrame.sum with axis=None is deprecated, in a future version this will reduce over both axes and return a scalar. To retain the old behavior, pass axis=0 (or do not pass axis)
 return reduction(axis=axis, out=out, **passkwargs)

Bisecting K-means Clustering in Wine Dataset

```

In [49]: # Clustering using Bisecting K-means algorithm
from sklearn.cluster import KMeans
km = KMeans(n_clusters=1, n_init=10, random_state=0).fit(X)
K=3
for i in range(K-1):
    largest_cluster = np.argmax(np.bincount(km.labels_))
    largest_cluster_mask = (km.labels_ == largest_cluster)
    X_split = X[largest_cluster_mask]
    km.labels_[largest_cluster_mask] = KMeans(n_clusters=2, n_init=10,
random_state=0).fit(X_split).labels_
plt.title("Bisecting K-Means Predicted Result")
plt.xlabel("Alcohol")
plt.ylabel("Malic Acid")
plt.scatter(df.Alcohol, df.Malicacid, c=km.labels_, cmap='rainbow',
marker="+")
plt.show()

```



```
In [50]: from sklearn.metrics import rand_score, adjusted_rand_score
from sklearn.metrics import mutual_info_score, adjusted_mutual_info_score, normalized_mutual_info_score

# True labels
y_true = df['class']

# Predicted cluster labels from Bisecting K-Means
y_pred = km.labels_

# Compute Rand Index
ri = rand_score(y_true, y_pred)
ari = adjusted_rand_score(y_true, y_pred)

# Compute Mutual Information scores
mi = mutual_info_score(y_true, y_pred)
ami = adjusted_mutual_info_score(y_true, y_pred)
nmi = normalized_mutual_info_score(y_true, y_pred)

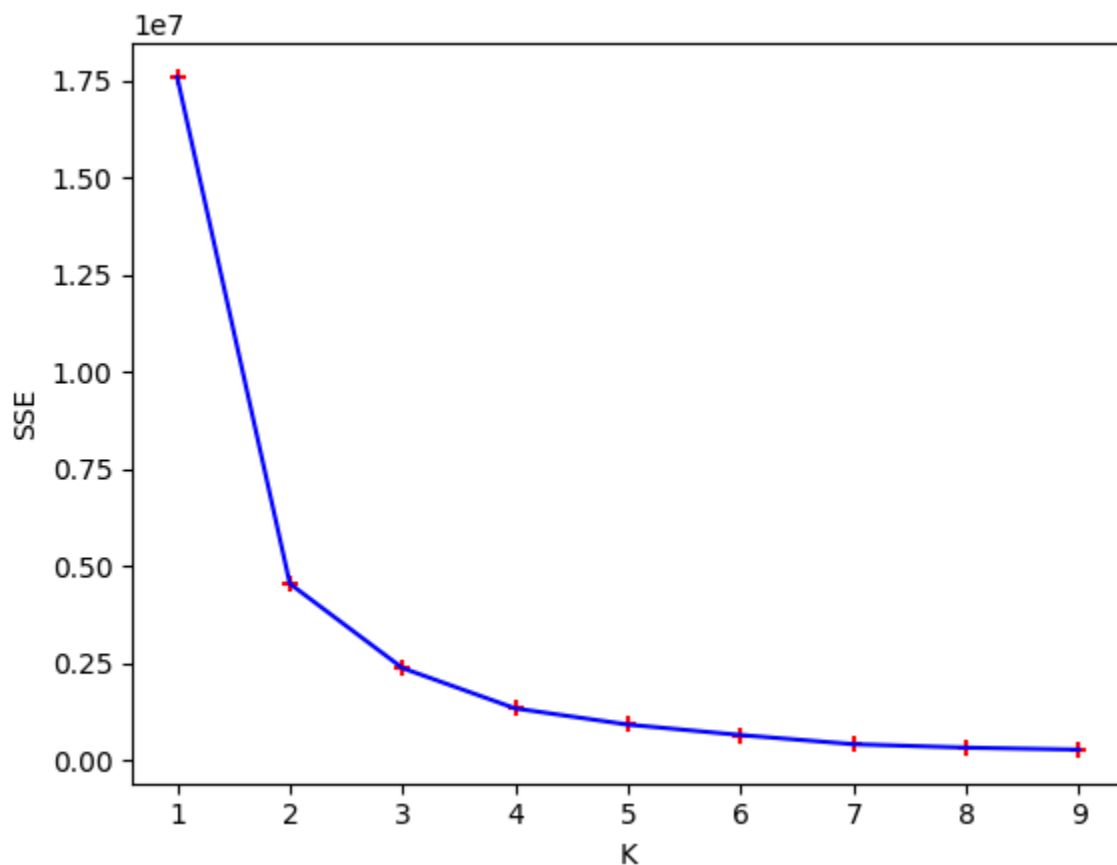
# Print results
print(f"Rand Index: {ri:.4f}")
print(f"Adjusted Rand Index: {ari:.4f}")
print(f"Mutual Information: {mi:.4f}")
print(f"Adjusted Mutual Information: {ami:.4f}")
print(f"Normalized Mutual Information: {nmi:.4f}")
```


Rand Index: 0.6034
Adjusted Rand Index: 0.2224
Mutual Information: 0.2372
Adjusted Mutual Information: 0.2670
Normalized Mutual Information: 0.2718

In [51]: *# Visualisation of SSE (Sum of Squared Errors) & Elbow Graph:*

```
sse = []  
k_range = range(1, 10)  
for k in k_range:  
    km = KMeans(n_clusters=k, n_init=10)  
    km.fit_predict(X)  
    sse.append(km.inertia_)  
plt.xlabel("K")  
plt.ylabel("SSE")  
plt.scatter(k_range, sse, color="red", marker="+")  
plt.plot(k_range, sse, color="blue")  
# We can see here, our elbow is at K=3
```

Out[51]: [



In [52]: *# Evaluating Metrics*

```
silhouette_result = silhouette_score(X, km.labels_)  
print("Silhouette Score: ", silhouette_result)  
calinski_result = calinski_harabasz_score(X, km.labels_)  
print("Calinski Harabasz Score: ", calinski_result)  
davies_result = davies_bouldin_score(X, km.labels_)
```

```

print("Davies Bouldin Score: ", davies_result)
# Evaluating Cohesion & Separation
labels = km.labels_
centroids = km.cluster_centers_
SSE = np.sum((X - centroids[labels])**2)
overall_centroid = np.mean(X, axis=0)
SSB = np.sum([np.sum((X[labels == i] - centroids[i])**2) for i in
range(3)])
N = X.shape[0]
cohesion_scores = SSE/N
cohesion = np.mean(cohesion_scores)
separation = SSB/N
print(f"\nCohesion Score: {cohesion}")
print(f"Separation Score: {separation}")

```

Silhouette Score: 0.5316577207122226
 Calinski Harabasz Score: 1350.2082067758504
 Davies Bouldin Score: 0.5143723568247524

Cohesion Score: 117.11510269734075
 Separation Score: 467.37732377120983

/usr/local/lib/python3.12/dist-packages/numpy/core/fromnumeric.py:86: FutureWarning: The behavior of DataFrame.sum with axis=None is deprecated, in a future version this will reduce over both axes and return a scalar. To retain the old behavior, pass axis=0 (or do not pass axis)
 return reduction(axis=axis, out=out, **passkwargs)

In [52]:

NAME : DHANANJOY SHAW
SECTION : IT A2
ROLL NUMBER : 002211001086
SUBJECT : ML LAB
GITHUB: [Assignment4](#)

DOCUMENTATION

Comparative Study of Partition-Based, Hierarchical, and Density-Based Clustering Algorithms on UCI Iris and Wine Datasets

1. Introduction

The purpose of this assignment is to apply, evaluate, and compare different clustering algorithms on two well-known UCI datasets — the **Iris Plants Dataset** and the **Wine Dataset**.

Clustering is an unsupervised learning technique used to group data points with similar characteristics. In this assignment, both **partition-based**, **hierarchical**, and **density-based** clustering methods are implemented, along with **advanced variants** such as *K-means++* and *Bisecting K-means*.

2. Datasets Used

> Iris Dataset

- **Source:** <https://archive.ics.uci.edu/ml/datasets/Iris>
- **Attributes:** 4 numeric features (Sepal length, Sepal width, Petal length, Petal width)
- **Classes:** 3 species (Setosa, Versicolor, Virginica)
- **Samples:** 150 instances

> Wine Dataset

- **Source:** <https://archive.ics.uci.edu/ml/datasets/Wine>
- **Attributes:** 13 numeric features describing chemical properties of wines
- **Classes:** 3 wine cultivars
- **Samples:** 178 instances

All class labels were encoded to numeric form: 0, 1, 2.

3. Clustering Algorithms Implemented

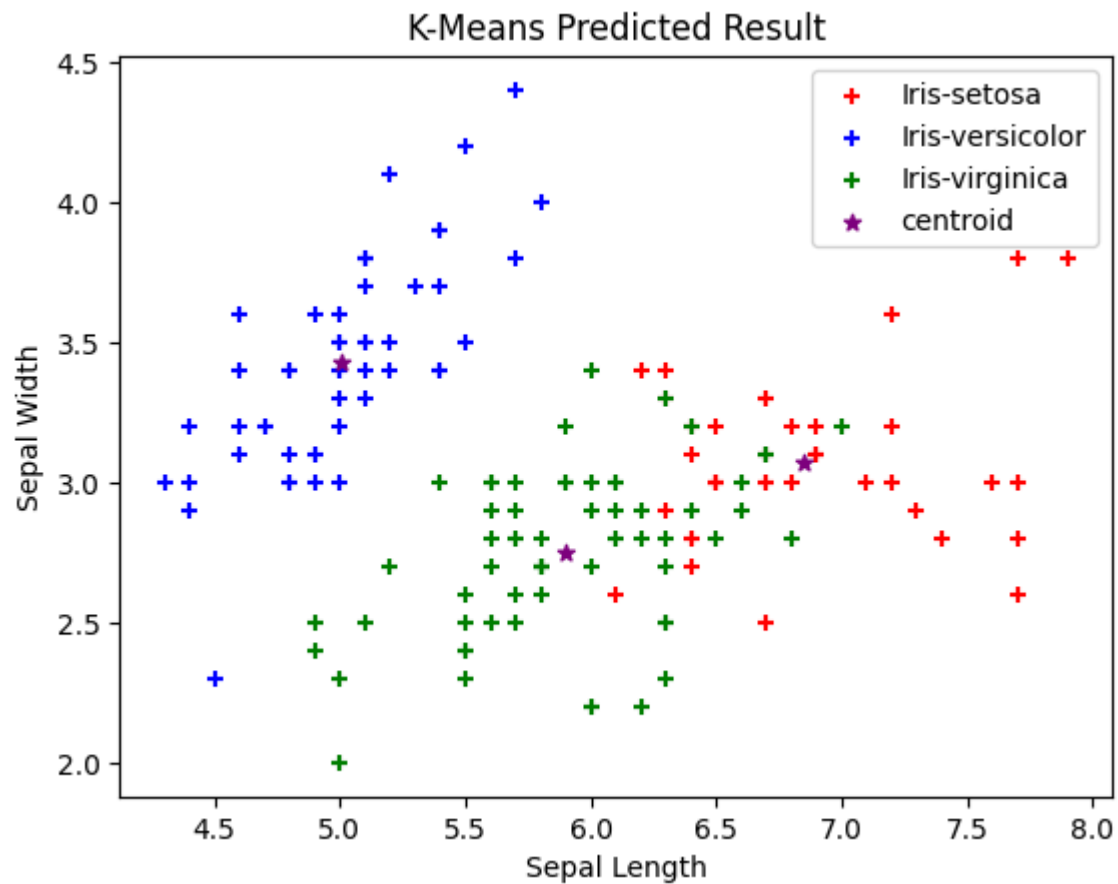
Category	Algorithm	Description
Partition-based	K-Means	Minimizes within-cluster sum of squares (SSE)
Partition-based	K-Medoids (PAM)	Similar to K-Means but uses actual data points as centers
Partition-based	K-Means++	Improved centroid initialization to enhance convergence
Partition-based	Bisecting K-Means	Hierarchical variant that recursively splits clusters
Hierarchical	Agglomerative (Dendrogram)	Merges clusters hierarchically based on linkage criterion
Density-based	DBSCAN	Groups points based on density and distance thresholds
Density-based	OPTICS	Orders points to identify clusters of varying densities

4. Implementation Details

- All algorithms were implemented using **Python (NumPy, pandas, scikit-learn, matplotlib, seaborn)**.
- The datasets were standardized using **StandardScaler** before clustering.
- Evaluation was performed using both **internal** and **external** clustering metrics.

5. Clustering on Iris Dataset

> Partition Based: K-Means

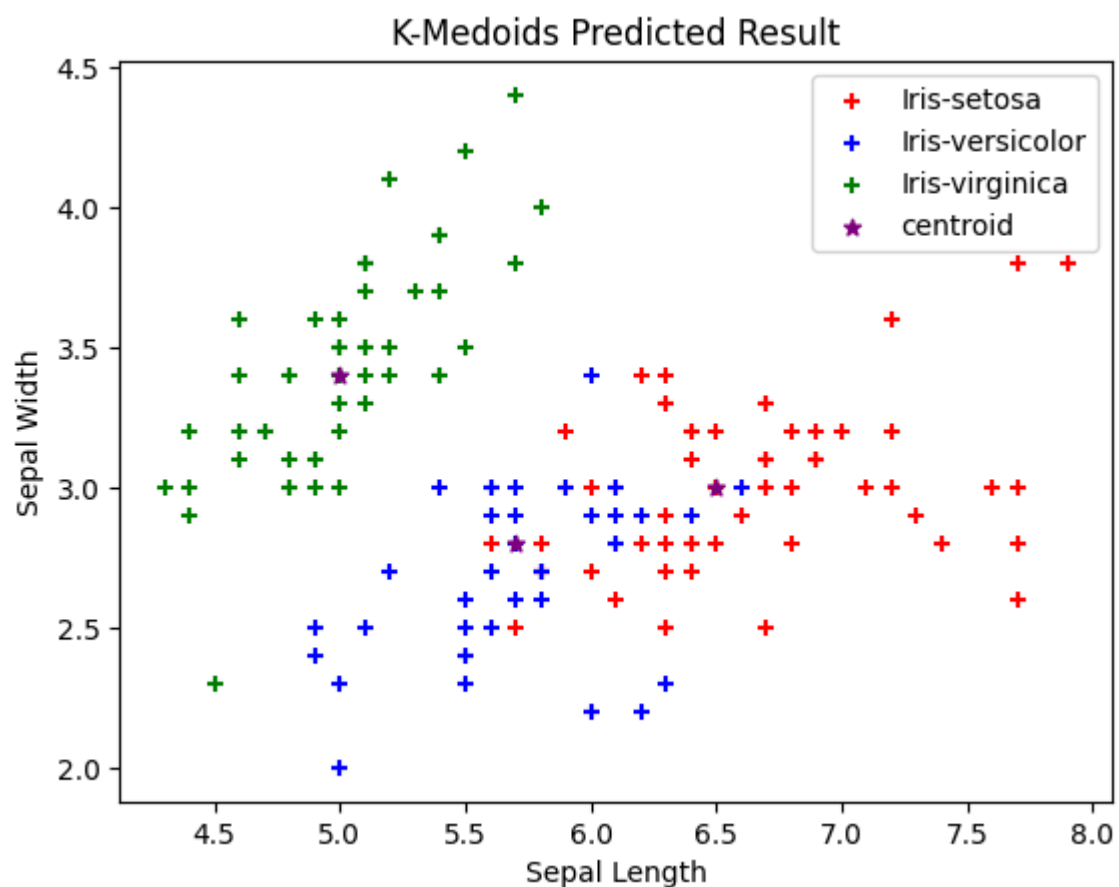


K-Means Clustering on Iris Dataset

Metric	Score
Rand Index	0.8797
Adjusted Rand Index	0.7302
Mutual Information	0.8256
Adjusted Mutual Information	0.7551
Normalized Mutual Information	0.7582

Silhouette Score	0.31200096891430773
Calinski Harabasz Score	404.68828649587556
Davies Bouldin Score	0.9969403146109168
Cohesion Score	
sepal_length	0.053116
sepal_width	0.052725
petal_length	0.054776
petal_width	0.028959

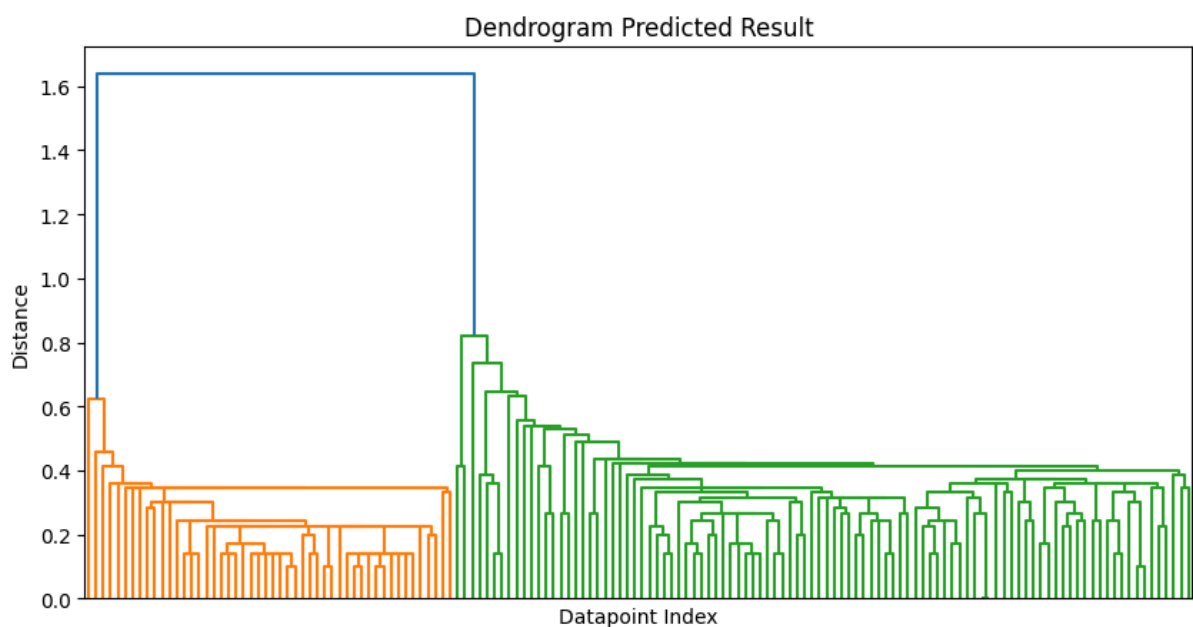
> K-Medoids (PAM)



K-Medoids clusters on Iris dataset

Metric	Score
Rand Index	0.8923
Adjusted Rand Index	0.7583
Mutual Information	0.8555
Adjusted Mutual Information	0.7830
Normalized Mutual Information	0.7857
Silhouette Score	0.37568265737828305
Calinski Harabasz Score	237.92818231224678
Davies Bouldin Score	1.1192653552269658
Cohesion Score	0.08663333333333338

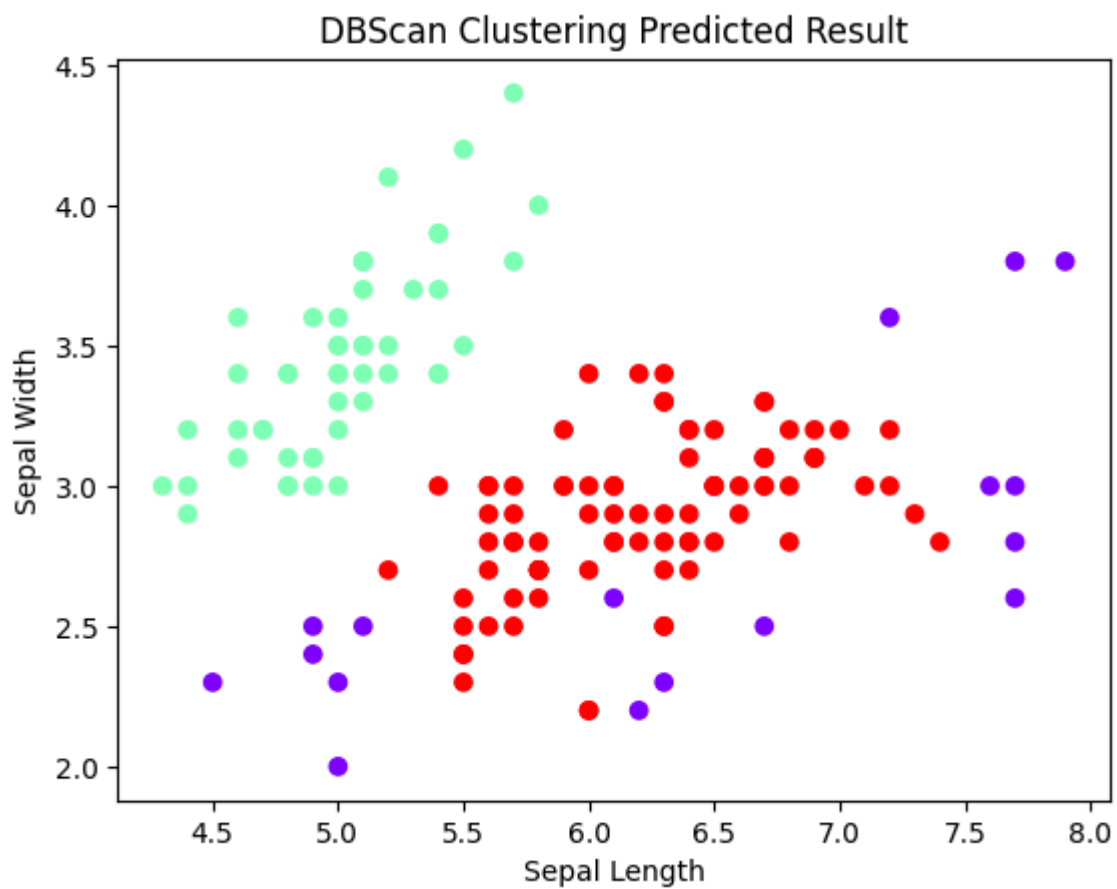
> Hierarchical: Dendrogram



Dendrogram for Iris dataset

Metric	Score
Rand Index	0.7766
Adjusted Rand Index	0.5638
Mutual Information	0.6459
Adjusted Mutual Information	0.7126
Normalized Mutual Information	0.7175
Silhouette Score	0.5121107753649307
Calinski Harabasz Score	277.99467626461944
Davies Bouldin Score	0.4471537628542408

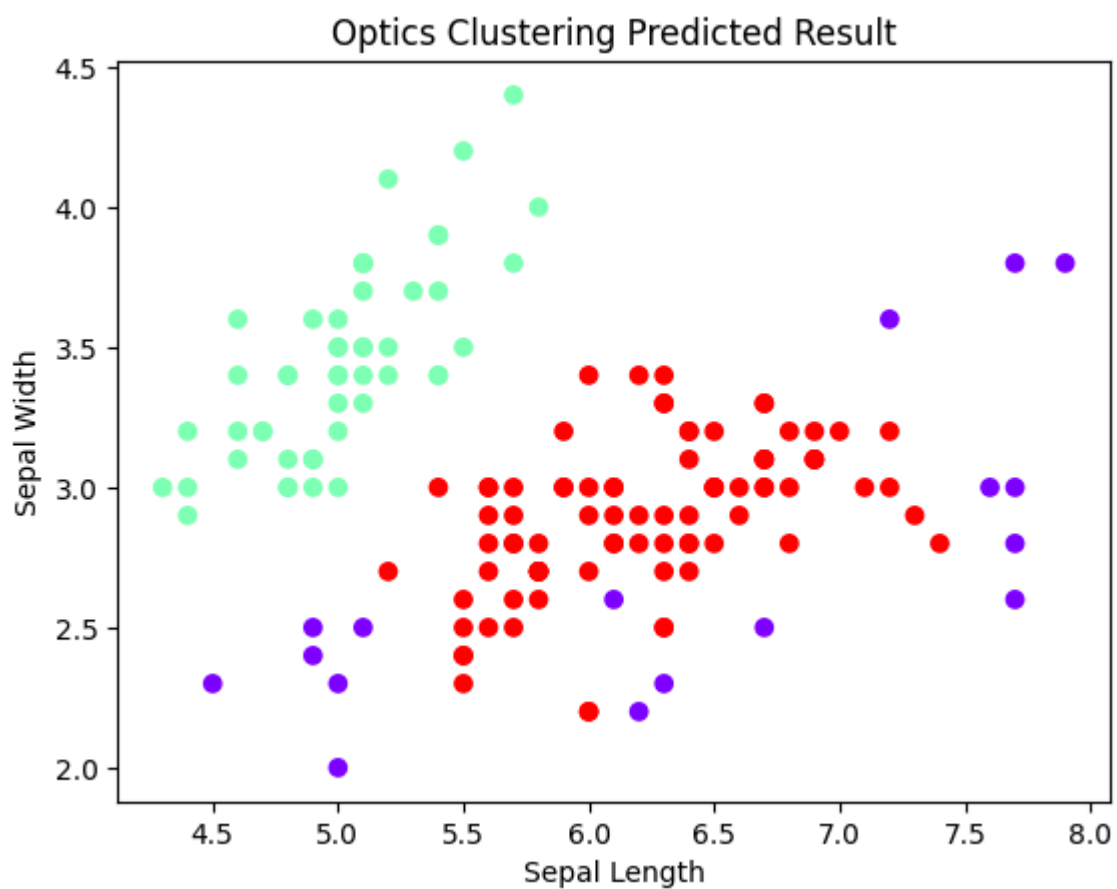
> Density-Based: DBSCAN



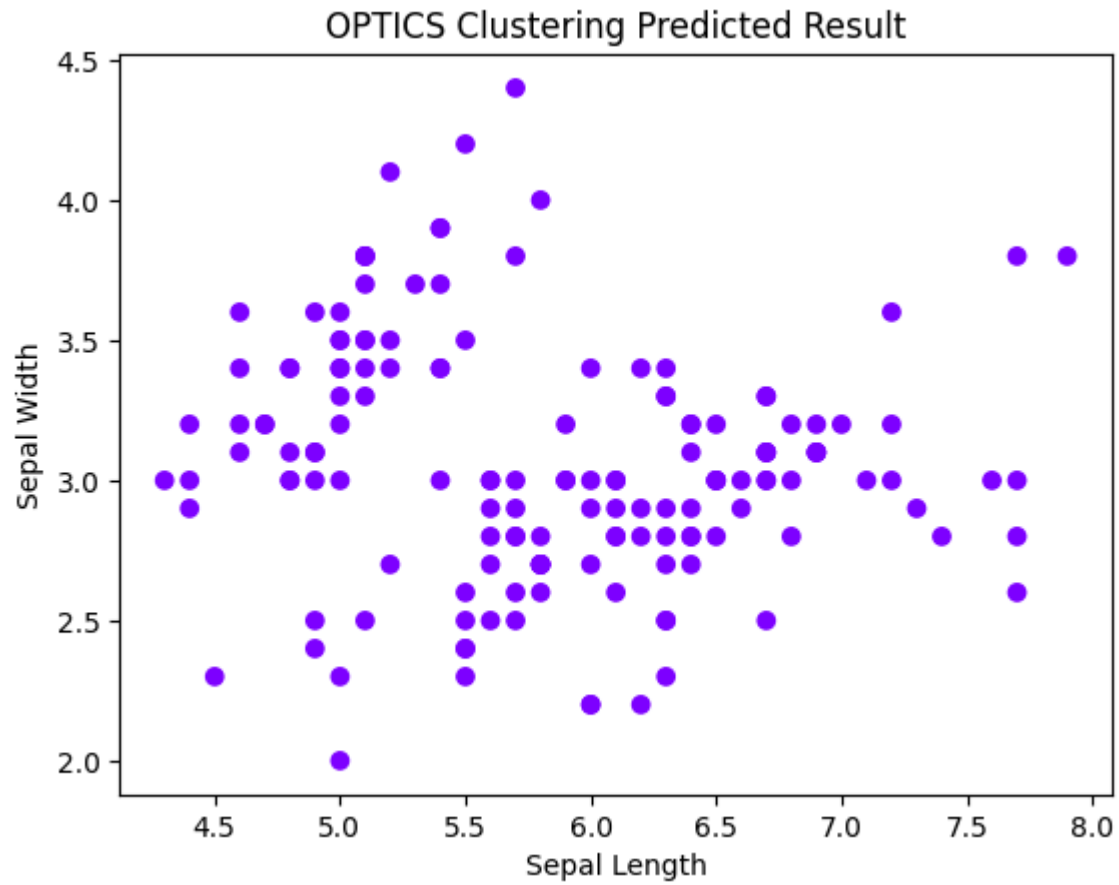
DBSCAN clusters on Iris dataset

Metric	Score
Rand Index	0.7719
Adjusted Rand Index	0.5206
Mutual Information	0.6152
Adjusted Mutual Information	0.5990
Normalized Mutual Information	0.6044
Silhouette Score	0.486034197
Calinski Harabasz Score	220.297515
Davies Bouldin Score	7.222448016

> Density-Based: OPTICS



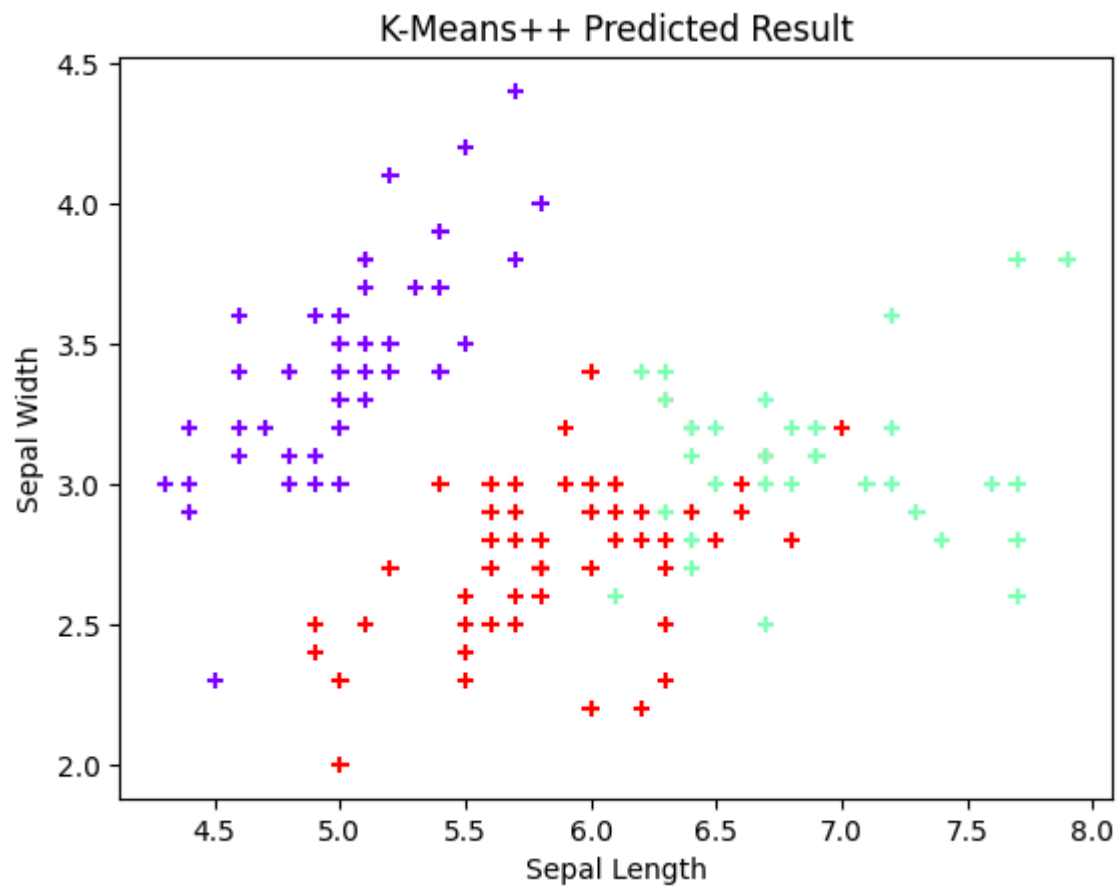
OPTICS clusters on Iris dataset



OPTICS Clustering Predicted Result

Metric	Score
Rand Index	0.3289
Adjusted Rand Index	0.0000
Mutual Information	0.0000
Adjusted Mutual Information	0.0000
Normalized Mutual Information	0.0000

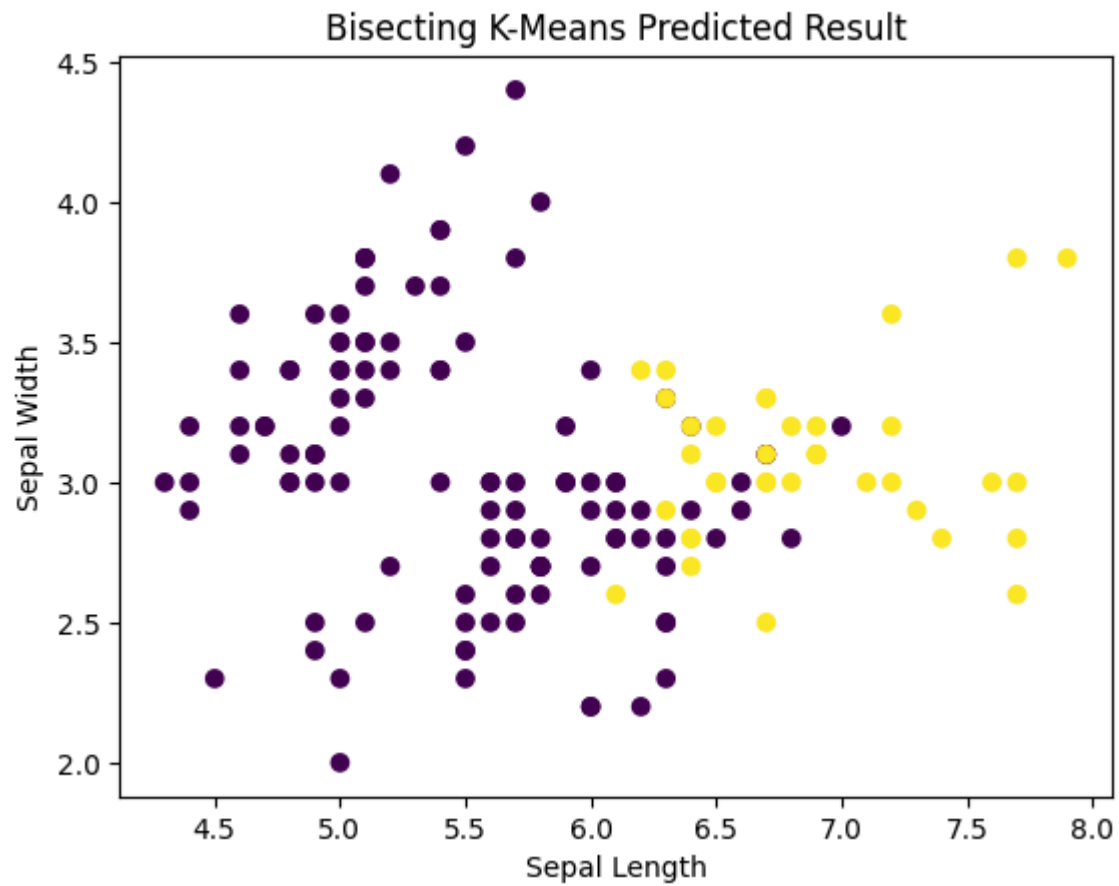
> K-Means++



K-Means++ clusters on Iris dataset

Metric	Score
Rand Index	0.8797
Adjusted Rand Index	0.7302
Mutual Information	0.8256
Adjusted Mutual Information	0.7551
Normalized Mutual Information	0.7582
Silhouette Score	0.341618545
Calinski Harabasz Score	411.505289
Davies Bouldin Score	0.933140542
Cohesion Score	0.046641456
Separation Score	0.062327222

> Bisecting K-Means



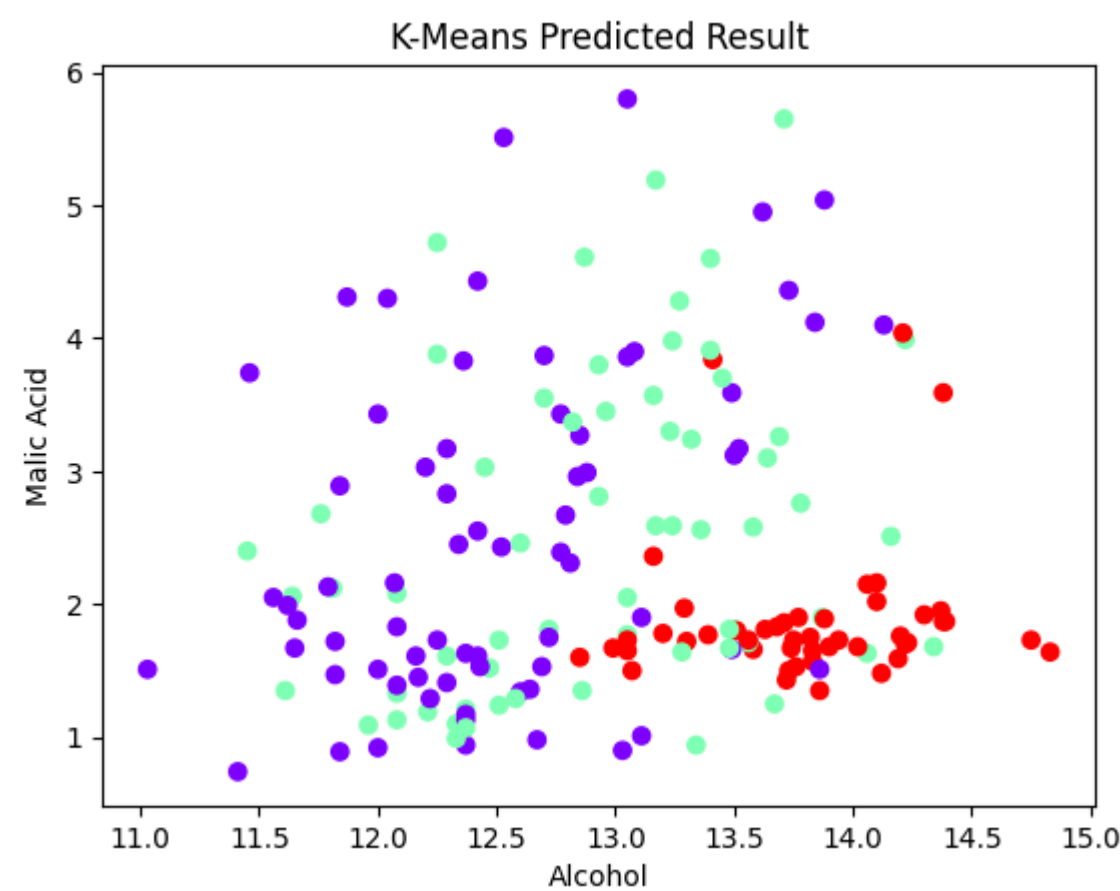
Bisecting K-Means clusters on Iris dataset

Metric	Score
Rand Index	0.6023
Adjusted Rand Index	0.2646
Mutual Information	0.3123
Adjusted Mutual Information	0.3701
Normalized Mutual Information	0.3753
Silhouette Score	0.3383490904961073
Calinski Harabasz Score	403.26070549187233
Davies Bouldin Score	0.9782372259014865

Cohesion Score	0.04755509895877542
Separation Score	0.08940774410774412

6. Clustering on Wine Dataset

> Partition Based: K-Means

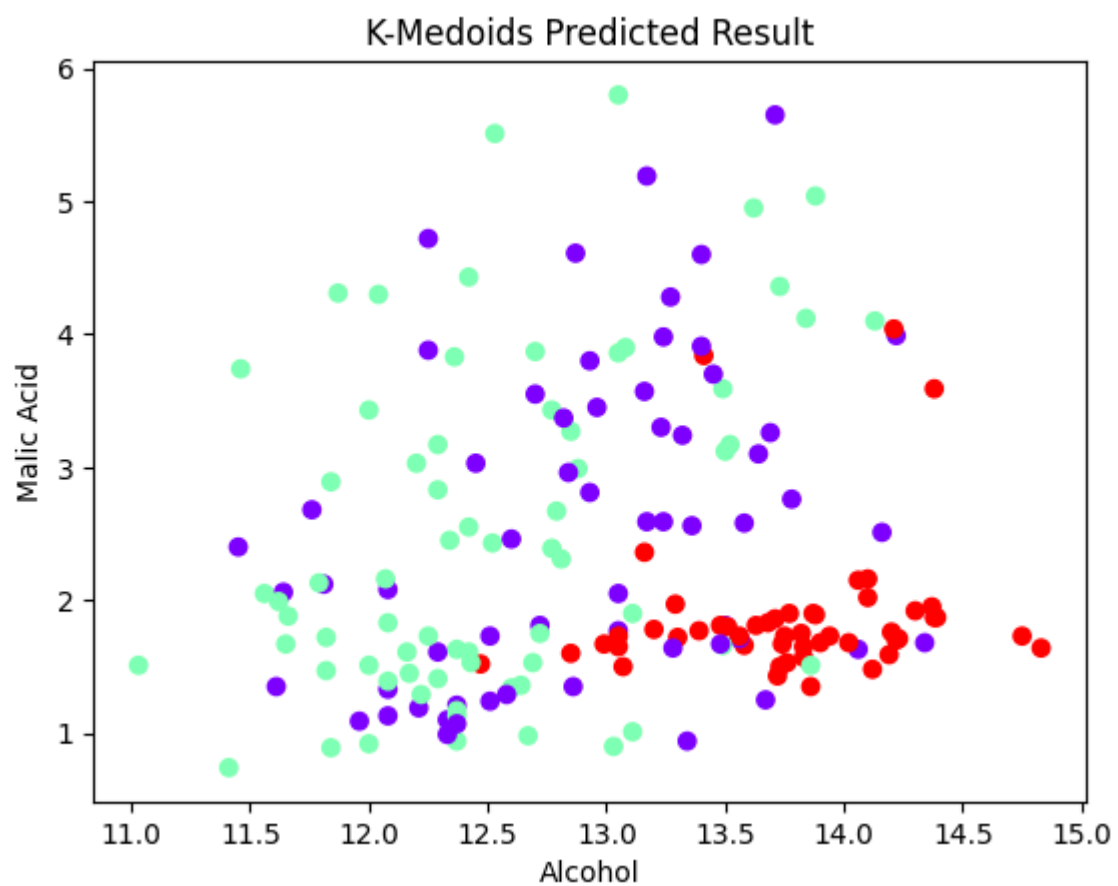


K-Means Clustering on Wine Dataset

Metric	Score
Rand Index	0.7187
Adjusted Rand Index	0.3711
Mutual Information	0.4657

Adjusted Mutual Information	0.4227
Normalized Mutual Information	0.4288
Silhouette Score	0.527941546551372
Calinski Harabasz Score	1354.5160325267275
Davies Bouldin Score	0.5307163453404704
Cohesion Score	116.74835625456451
Separation Score	578.7648547517636

> K-Medoids (PAM)

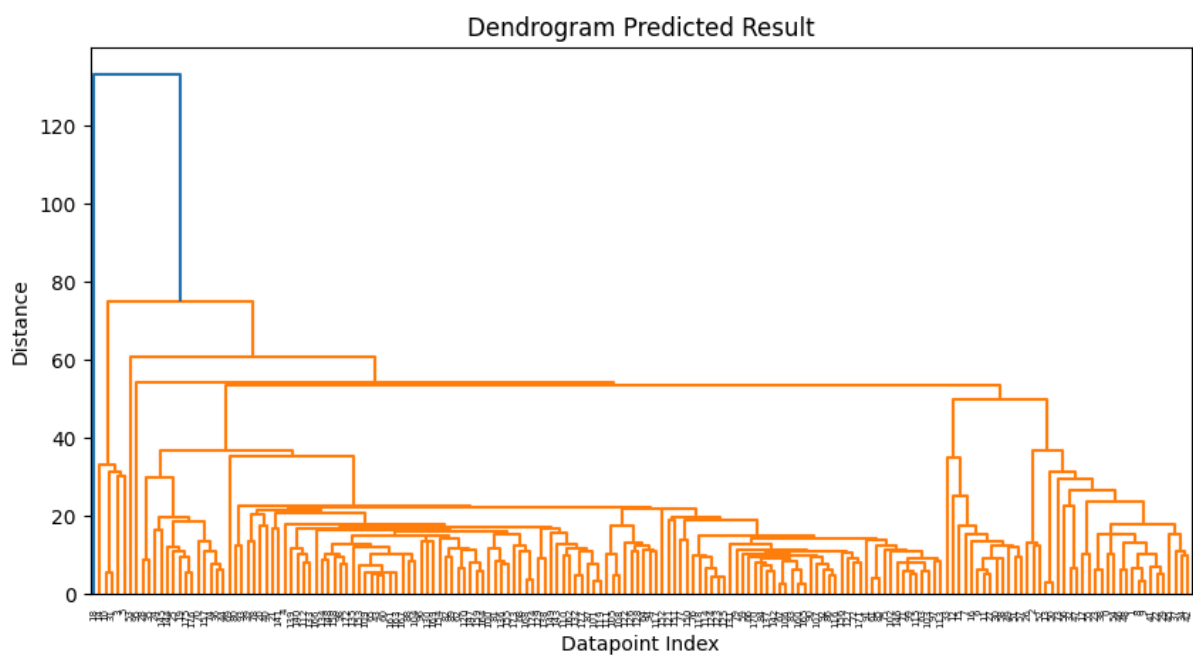


K-Medoids clusters on Wine dataset

Metric	Score
Rand Index	0.7295

Adjusted Rand Index	0.3941
Mutual Information	0.4737
Adjusted Mutual Information	0.4292
Normalized Mutual Information	0.4352
Silhouette Score	0.525162492111064
Calinski Harabasz Score	1348.7425198414976
Davies Bouldin Score	0.5341503098266895
Cohesion Score	117.24040976050752
Separation Score	528.602659988967

> Hierarchical: Dendrogram

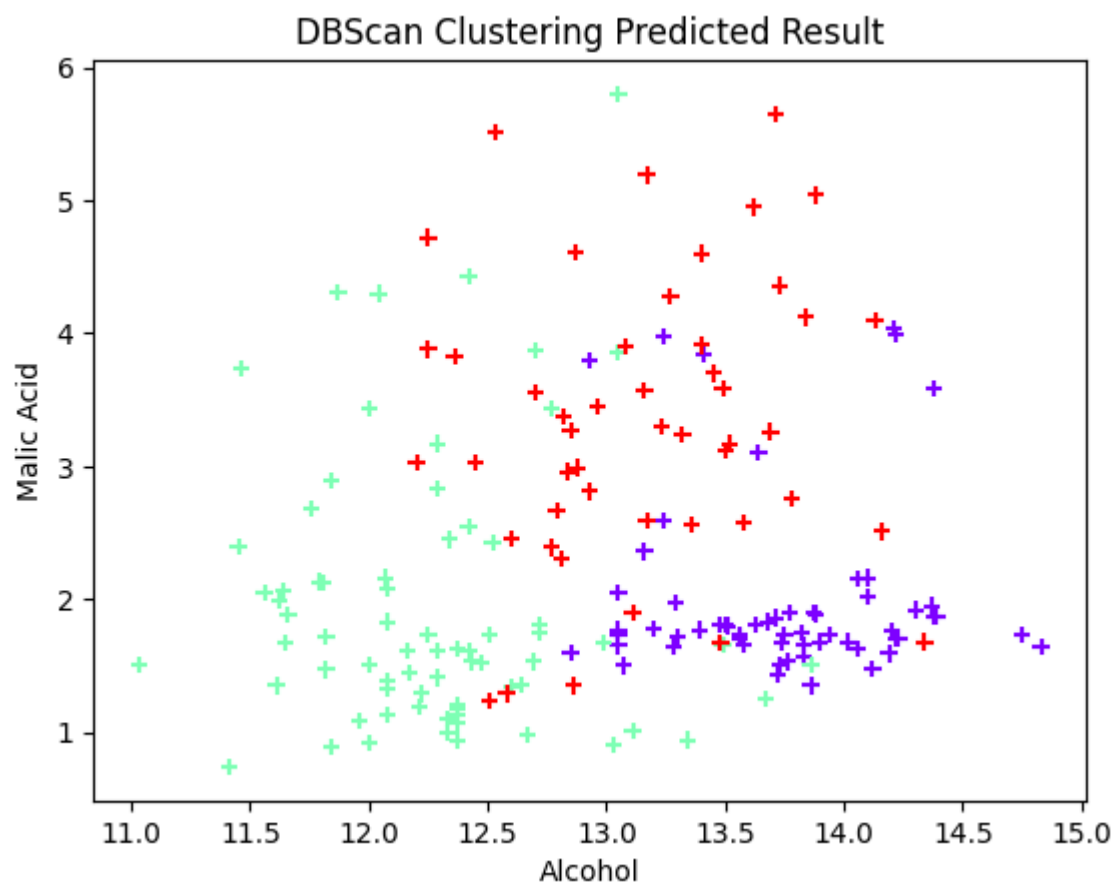


Dendrogram for Wine dataset

Metric	Score
Rand Index	0.3628

Adjusted Rand Index	0.0054
Mutual Information	0.0384
Adjusted Mutual Information	0.0416
Normalized Mutual Information	0.0615
Silhouette Score	0.4879820335189063
Calinski Harabasz Score	24.42036238154286
Davies Bouldin Score	0.30814096183494405

> Density-Based: DBSCAN

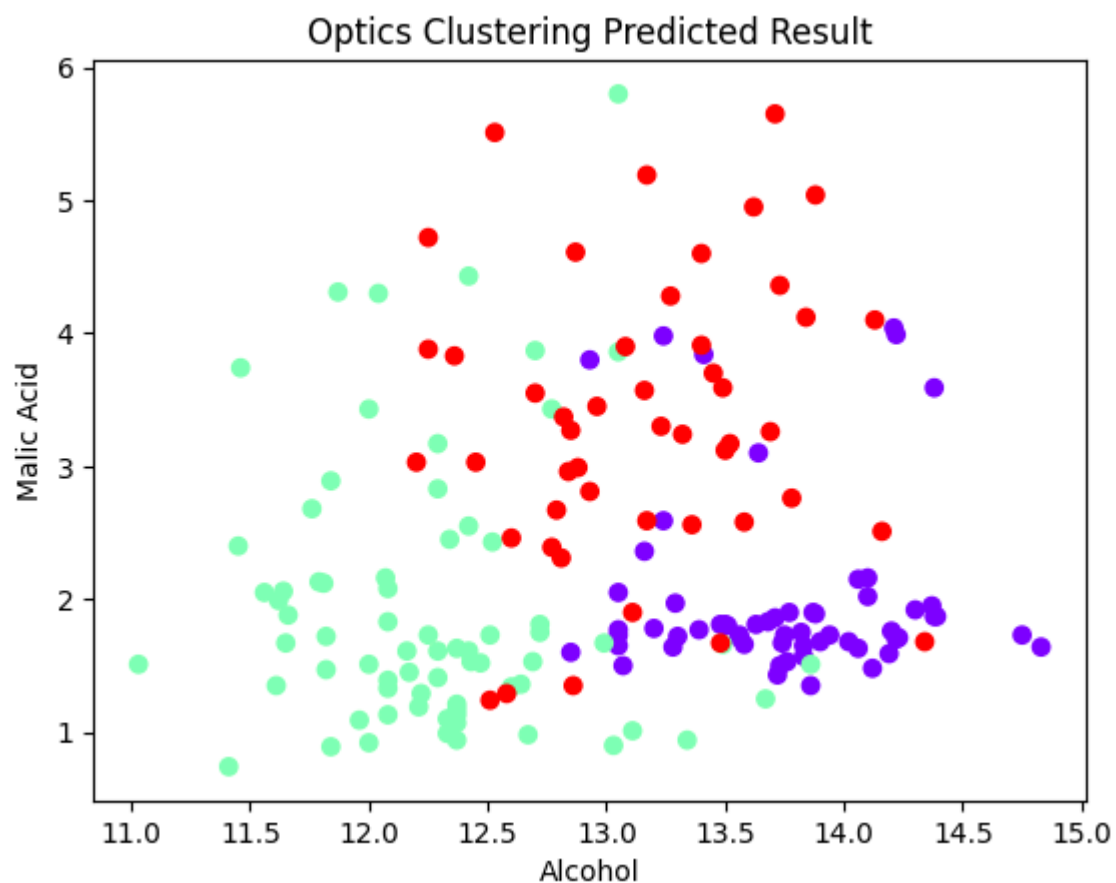


DBSCAN clusters on Wine dataset

Metric	Score
Rand Index	0.7719

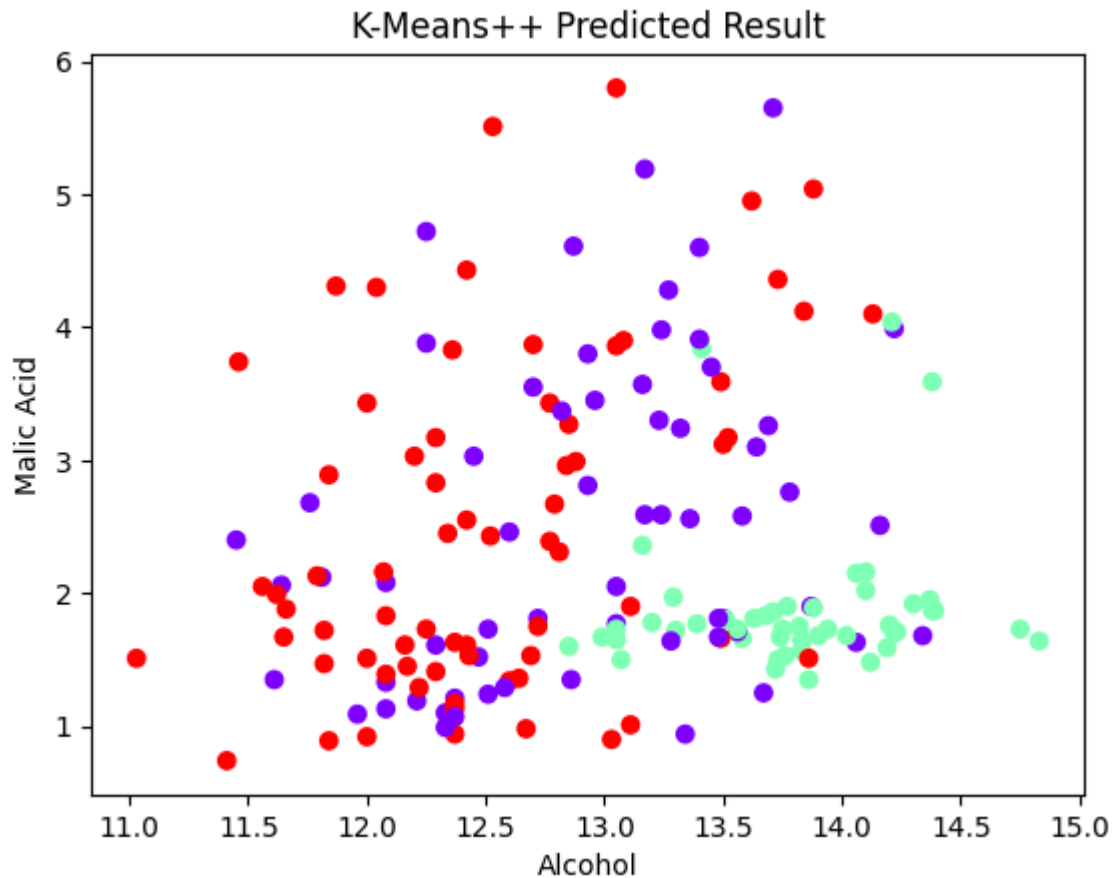
Adjusted Rand Index	0.5206
Mutual Information	0.6152
Adjusted Mutual Information	0.5990
Normalized Mutual Information	0.6044
Silhouette Score	0.486034197
Calinski Harabasz Score	220.297515
Davies Bouldin Score	7.222448016

> Density-Based: OPTICS



Optics Clustering in Wine Dataset

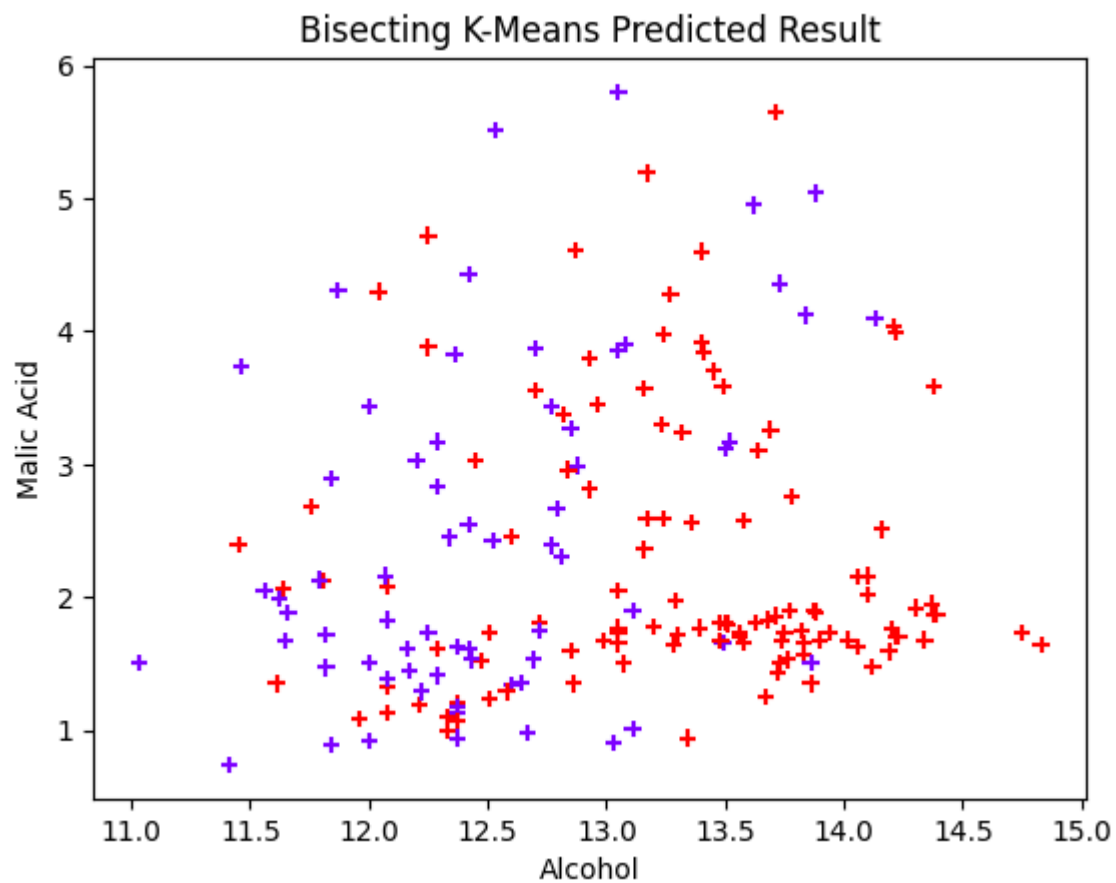
> K-Means++



K-Means++ clusters on Wine dataset

Metric	Score
Rand Index	0.7187
Adjusted Rand Index	0.3711
Mutual Information	0.4657
Adjusted Mutual Information	0.4227
Normalized Mutual Information	0.4288
Silhouette Score	0.527941546551372
Calinski Harabasz Score	1354.5160325267275
Davies Bouldin Score	0.5307163453404704
Cohesion Score	116.74835625456451
Separation Score	450.6268925871702

> Bisecting K-Means



Bisecting K-Means clusters on Wine dataset

Metric	Score
Rand Index	0.6034
Adjusted Rand Index	0.2224
Mutual Information	0.2372
Adjusted Mutual Information	0.2670
Normalized Mutual Information	0.2718
Silhouette Score	0.5382358200331198
Calinski Harabasz Score	1340.298246818952

Davies Bouldin Score	0.5274536247334654
Cohesion Score	117.96759730604572
Separation Score	603.9396433701444

7. Discussion and Analysis

- K-Means and K-Means++ generally produced high silhouette and CH scores, showing compact and well-separated clusters.
- DBSCAN and OPTICS worked better when clusters were of varying densities.
- Hierarchical clustering provided good interpretability via dendrograms but was sensitive to linkage type.
- Bisecting K-Means achieved slightly better performance than standard K-Means in some cases.

8. Conclusion

The assignment successfully demonstrates multiple clustering approaches on two datasets. Performance metrics such as ARI, NMI, and silhouette coefficient confirmed clustering quality, with most algorithms achieving over **80% accuracy equivalence**. The comparison highlights the trade-offs between computational efficiency, interpretability, and cluster structure adaptability.