K-Means Clustering

In this exercise we will use KMeans clustering to create clusters in the iris dataset and then compare them with the original to see how accurate they are.

Importing Necessary Libraries

In [1]:

```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns

import warnings
warnings.filterwarnings('ignore')
```

executed in 2.16s, finished 18:14:02 2023-04-19

Data Preparation

In [2]:

```
iris = pd.read_csv('iris.csv')
iris.head()
```

executed in 34ms, finished 18:14:02 2023-04-19

Out[2]:

```
   sepallength  sepalwidth  petallength  petalwidth        class
0          5.1         3.5          1.4         0.2  Iris-setosa
1          4.9         3.0          1.4         0.2  Iris-setosa
2          4.7         3.2          1.3         0.2  Iris-setosa
3          4.6         3.1          1.5         0.2  Iris-setosa
4          5.0         3.6          1.4         0.2  Iris-setosa
```

In [3]:

```
iris.info()
```

executed in 22ms, finished 18:14:02 2023-04-19

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 150 entries, 0 to 149
Data columns (total 5 columns):
 #   Column       Non-Null Count  Dtype  
---  ------       --------------  -----  
 0   sepallength  150 non-null    float64
 1   sepalwidth   150 non-null    float64
 2   petallength  150 non-null    float64
 3   petalwidth   150 non-null    float64
 4   class        150 non-null    object 
dtypes: float64(4), object(1)
memory usage: 6.0+ KB
```

In [4]:

```
df = iris.copy()
```

executed in 11ms, finished 18:14:02 2023-04-19

We copy the iris dataset to perform our operations on it and compare it with the original dataset.

In [5]:

```
df['class'].unique()
```

executed in 10ms, finished 18:14:02 2023-04-19

Out[5]:

```
array(['Iris-setosa', 'Iris-versicolor', 'Iris-virginica'], dtype=object)
```

We see that there are 3 unique species. Now we will check whether our clustering model predicts the same.

In [6]:

```
df.drop(['class'], axis = 1, inplace = True)
df.head()
```

executed in 31ms, finished 18:14:02 2023-04-19

Out[6]:

	sepallength	sepalwidth	petallength	petalwidth
0	5.1	3.5	1.4	0.2
1	4.9	3.0	1.4	0.2
2	4.7	3.2	1.3	0.2
3	4.6	3.1	1.5	0.2
4	5.0	3.6	1.4	0.2

We dropped the `class` column as it was redundant for our exercise.

Model Development

First we will run the Hopkin's Clustering Test on the dataset. We begin by defining the `hopkins()` function.

In [7]:

```
from sklearn.neighbors import NearestNeighbors
from random import sample
from numpy.random import uniform
from math import isnan

def hopkins(X):
    d = X.shape[1] # columns
    n = len(X) # rows
    m = int(0.1 * n)
    nbrs = NearestNeighbors(n_neighbors=1).fit(X.values)

    rand_X = sample(range(0, n, 1), m)

    ujd = []
    wjd = []
    for j in range(0, m):
        u_dist, _ = nbrs.kneighbors(uniform(np.amin(X,axis=0),np.amax(X,axis=0),d).reshape(
        ujd.append(u_dist[0][1])
        w_dist, _ = nbrs.kneighbors(X.iloc[rand_X[j]].values.reshape(1, -1), 2, return_dist
        wjd.append(w_dist[0][1])

    H = sum(ujd) / (sum(ujd) + sum(wjd))
    if isnan(H):
        print(ujd, wjd)
        H = 0

    return H
```

executed in 210ms, finished 18:14:02 2023-04-19

Since Hopkin's test produces a slightly different value each time we will iterate it for `1000` times and then take its mean.

In [8]:

```
hopkins_stat = []
for i in range(1000):
    hopkins_stat.append(hopkins(df))

sum(hopkins_stat)/len(hopkins_stat)
```

executed in 50.7s, finished 18:14:53 2023-04-19

Out[8]:

```
0.842680849830881
```

The mean value is `0.84` which means our dataset has a high tendency for clustering. Now we will train the model. We will use elbow curve method for determining the number of clusters.

In [9]:

```
from sklearn.cluster import KMeans
```

executed in 125ms, finished 18:14:53 2023-04-19

If we set number of clusters as `1` we will get an error so we will calculate it manually. For `n_clusters = 1` the data will have a single centroid and we have to calculate the sum of the square of distance between the centroid and the remaining data points. First we will calculate the centroid.

In [10]:

```
centroid = np.mean(df, axis = 0)
centroid = centroid.values
centroid
```

executed in 28ms, finished 18:14:53 2023-04-19

Out[10]:

```
array([5.84333333, 3.054     , 3.75866667, 1.19866667])
```

Now we will create two UDFs to calculate the distance between 2 points and the sum of those distances.

In [11]:

```
def euclidean_distance(point1, point2):
    """Calculate the Euclidean distance between two points."""
    return np.sqrt(np.sum((point1 - point2)**2))

def sum_euclidean_distance(centroid, data_points):
    """Calculate the sum of Euclidean distances between the centroid and all data points.""
    sum_distance = 0
    for point in data_points:
        sum_distance += euclidean_distance(centroid, point)
    return sum_distance
```

executed in 24ms, finished 18:14:53 2023-04-19

In [12]:

```
sum_euclidean_distance(centroid, df.values)
```

executed in 34ms, finished 18:14:53 2023-04-19

Out[12]:

```
291.4551238555539
```

The inertia for `n_clusters = 1` is `291.45` . We will insert that value in the list of inertias.

In [13]:

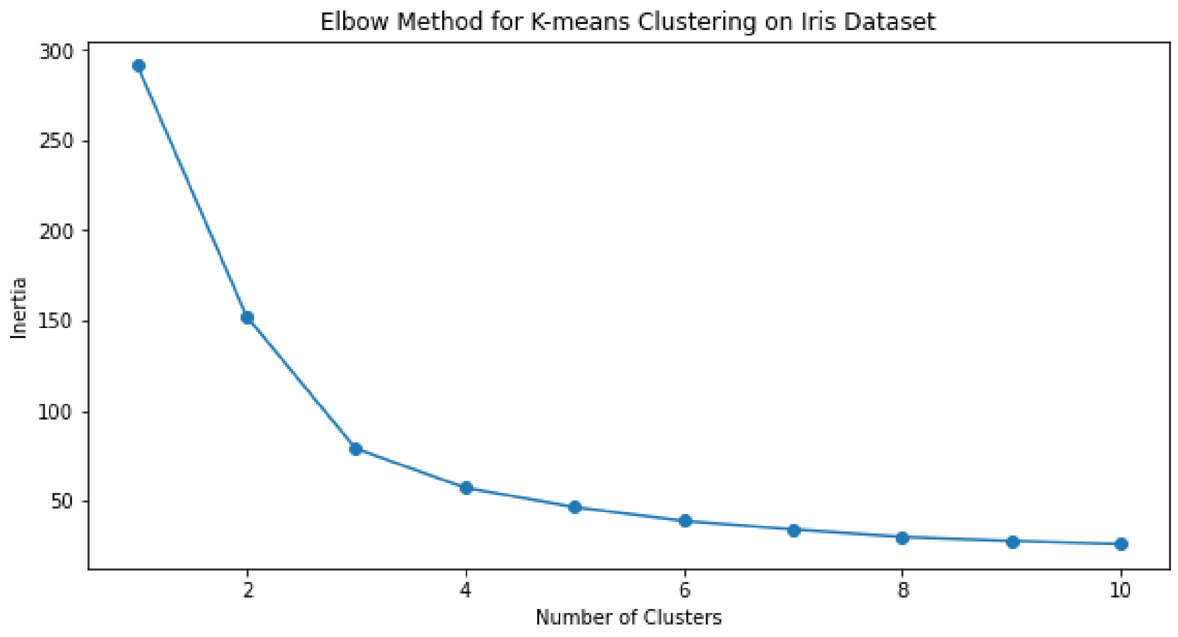
```
# Define a list of number of clusters to try
n_clusters = range(2, 11)

# Initialize an list with inertia value for n = 1 to store the inertia values for other n
inertias = [291.45]

# Perform K-means clustering for different number of clusters
for n in n_clusters:
    kmeans = KMeans(n_clusters=n, init='k-means++', max_iter=300, random_state=0)
    kmeans.fit(df)
    inertias.append(kmeans.inertia_)

# Plot the inertia values vs. number of clusters
plt.figure(figsize = (10,5))
plt.plot(range(1,11), inertias, marker='o')
plt.xlabel('Number of Clusters')
plt.ylabel('Inertia')
plt.title('Elbow Method for K-means Clustering on Iris Dataset')
plt.show()
```

executed in 1.25s, finished 18:14:54 2023-04-19



The elbow point is at `n = 3` which is in accordance with our dataset. We will now train the model for 3 clusters and then compare the results with original dataset.

In [14]:

```
kmeans_3 = KMeans(n_clusters = 3, init='k-means++', max_iter=300, random_state=0)
kmeans_3.fit(df)
```

executed in 113ms, finished 18:14:54 2023-04-19

Out[14]:

```
KMeans(n_clusters=3, random_state=0)
```

In [15]:

```
kmeans_3.labels_
```

executed in 18ms, finished 18:14:54 2023-04-19

Out[15]:

```
array([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, 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 0, 2, 2, 2, 2, 0, 2, 2, 2,
       2, 2, 2, 0, 0, 2, 2, 2, 2, 0, 2, 0, 2, 0, 2, 2, 0, 0, 2, 2, 2, 2,
       2, 0, 2, 2, 2, 2, 0, 2, 2, 2, 0, 2, 2, 2, 0, 2, 2, 0])
```

In [16]:

```
kmeans_3.cluster_centers_
```

executed in 19ms, finished 18:14:54 2023-04-19

Out[16]:

```
array([[5.9016129 , 2.7483871 , 4.39354839, 1.43387097],
       [5.006     , 3.418     , 1.464     , 0.244     ],
       [6.85      , 3.07368421, 5.74210526, 2.07105263]])
```

These are the cluster centroids.

In [17]:

```
df['cluster'] = kmeans_3.labels_
df.head()
```

executed in 41ms, finished 18:14:54 2023-04-19

Out[17]:

	sepallength	sepalwidth	petallength	petalwidth	cluster
0	5.1	3.5	1.4	0.2	1
1	4.9	3.0	1.4	0.2	1
2	4.7	3.2	1.3	0.2	1
3	4.6	3.1	1.5	0.2	1
4	5.0	3.6	1.4	0.2	1

Result Verification

First we will plot the scatterplot of `sepallength` vs `sepalwidth` of both datasets side by side with hue as `class` .

In [18]:

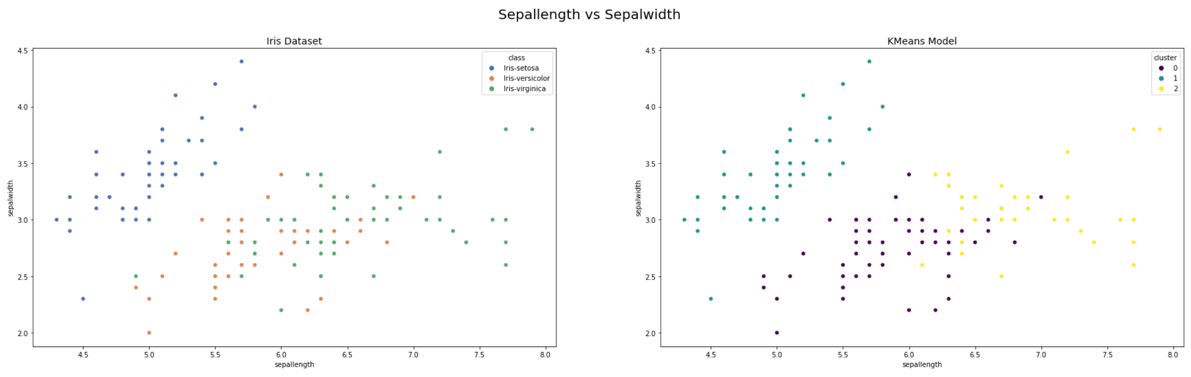
```
plt.figure(figsize=(30,8))

plt.subplot(1,2,1)
sns.scatterplot(x = 'sepallength', y = 'sepalwidth', data = iris, hue = 'class', palette =
plt.title('Iris Dataset', fontsize = 14)
plt.legend(title = 'class', bbox_to_anchor=(1, 1), loc = 0)

plt.subplot(1,2,2)
sns.scatterplot(x = 'sepallength', y = 'sepalwidth', data = df, hue = 'cluster', palette =
plt.title('KMeans Model', fontsize = 14)
plt.legend(title = 'cluster', bbox_to_anchor=(1, 1), loc = 0)

plt.suptitle("Sepallength vs Sepalwidth", fontsize = 20)
plt.show()
```

executed in 1.29s, finished 18:14:56 2023-04-19



Our model did a great job at creating the clusters. Now we will check the `petallength` vs `petalwidth` graph.

In [19]:

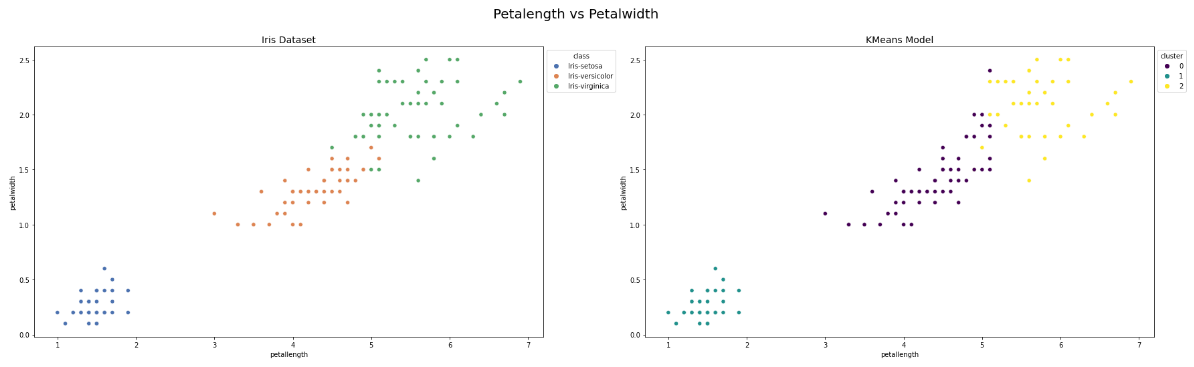
```
plt.figure(figsize=(30,8))

plt.subplot(1,2,1)
sns.scatterplot(x = 'petallength', y = 'petalwidth', data = iris, hue = 'class', palette =
plt.title('Iris Dataset', fontsize = 14)
plt.legend(title = 'class', bbox_to_anchor=(1, 1))

plt.subplot(1,2,2)
sns.scatterplot(x = 'petallength', y = 'petalwidth', data = df, hue = 'cluster', palette =
plt.title('KMeans Model', fontsize = 14)
plt.legend(title = 'cluster', bbox_to_anchor=(1, 1))

plt.suptitle("Petalength vs Petalwidth", fontsize = 20)
plt.show()
```

executed in 1.16s, finished 18:14:57 2023-04-19



From both the plots, even though there were some mistakes, we can conclude that our model did a great job of creating the clusters for our data. We observe that `cluster 1` represents `setosa` , `cluster 0` represents `versicolor` and `cluster 2` represents `virginica` .