K-means clustering

The notebook aims to study and implement a k-means clustering using "sklearn". The iris dataset will be used to identify clusters automatically using the K-means method.

Acknowledgments

- Used dataset: https://archive.ics.uci.edu/ml/datasets/iris
- Inquiries: mauricio.antelis@tec.mx

Importing libraries

```
# Define where you are running the code: colab or local
RunInColab          = True     # (False: no  | True: yes)

# If running in colab:
if RunInColab:
    # Mount your google drive in google colab
    from google.colab import drive
    drive.mount('/content/drive')

    # Find location
    #!pwd
    #!ls
    #!ls "/content/drive/My Drive/Colab Notebooks/MachineLearningWithPython/"

    # Define path del proyecto
    Ruta            = "/content/drive/My Drive/Colab Notebooks/MachineLearningWithPython/"

else:
    # Define path del proyecto
    Ruta            = ""
```

```
Drive already mounted at /content/drive; to attempt to forcibly remount, call drive.mount("/content/drive", force_remount=True).
```

```
# Import the packages that we will be using
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
```

Importing data

```
# Load the Iris dataset from seaborn
dataset = sns.load_dataset('iris')
```

Undertanding and preprocessing the data

1. Get a general 'feel' of the data

```
dataset
```

	sepal_length	sepal_width	petal_length	petal_width	species
0	5.1	3.5	1.4	0.2	setosa
1	4.9	3.0	1.4	0.2	setosa
2	4.7	3.2	1.3	0.2	setosa
3	4.6	3.1	1.5	0.2	setosa
4	5.0	3.6	1.4	0.2	setosa
...	...	...	...	...	...
145	6.7	3.0	5.2	2.3	virginica
146	6.3	2.5	5.0	1.9	virginica
147	6.5	3.0	5.2	2.0	virginica
148	6.2	3.4	5.4	2.3	virginica
149	5.9	3.0	5.1	1.8	virginica

150 rows × 5 columns

Pasos siguientes: Generar código con `dataset` Ver gráficos recomendados New interactive sheet

2. Drop rows with any missing values

```
# Check for missing data
missing_data = dataset.isnull().sum()
print("Missing Data:\n", missing_data)

# Create a new dataset without missing data (if any)
dataset.dropna()
```

```
Missing Data:
 sepal_length    0
sepal_width     0
petal_length    0
petal_width     0
species         0
dtype: int64
```

	sepal_length	sepal_width	petal_length	petal_width	species
0	5.1	3.5	1.4	0.2	setosa
1	4.9	3.0	1.4	0.2	setosa
2	4.7	3.2	1.3	0.2	setosa
3	4.6	3.1	1.5	0.2	setosa
4	5.0	3.6	1.4	0.2	setosa
...	...	...	...	...	...
145	6.7	3.0	5.2	2.3	virginica
146	6.3	2.5	5.0	1.9	virginica
147	6.5	3.0	5.2	2.0	virginica
148	6.2	3.4	5.4	2.3	virginica
149	5.9	3.0	5.1	1.8	virginica

150 rows × 5 columns

3. Encoding the class label categorical column: from string to num

```
# Encoding the categorical column
dataset['species'] = dataset['species'].astype('category')
dataset['species'] = dataset['species'].cat.codes
#Visualize the dataset
dataset
```

	sepal_length	sepal_width	petal_length	petal_width	species
0	5.1	3.5	1.4	0.2	0
1	4.9	3.0	1.4	0.2	0
2	4.7	3.2	1.3	0.2	0
3	4.6	3.1	1.5	0.2	0
4	5.0	3.6	1.4	0.2	0
...	...	...	...	...	...
145	6.7	3.0	5.2	2.3	2
146	6.3	2.5	5.0	1.9	2
147	6.5	3.0	5.2	2.0	2
148	6.2	3.4	5.4	2.3	2
149	5.9	3.0	5.1	1.8	2

150 rows × 5 columns

Pasos siguientes: Generar código con `dataset` Ver gráficos recomendados New interactive sheet

Now the label/category is numeric

4. Discard columns that won't be used

```
# Drop out non necesary columns
petals = dataset.drop(['sepal_length', 'sepal_width'],axis='columns')

#Visualize the dataset
petals
```

	petal_length	petal_width	species
0	1.4	0.2	0
1	1.4	0.2	0
2	1.3	0.2	0
3	1.5	0.2	0
4	1.4	0.2	0
...	...	...	...
145	5.2	2.3	2
146	5.0	1.9	2
147	5.2	2.0	2
148	5.4	2.3	2
149	5.1	1.8	2

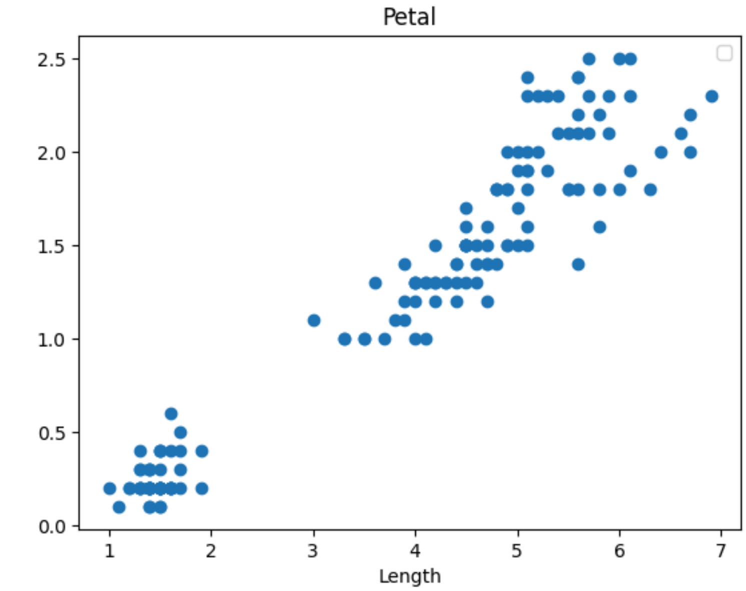
150 rows × 3 columns

Pasos siguientes: Generar código con `petals` Ver gráficos recomendados New interactive sheet

5. Scatter plot of the data

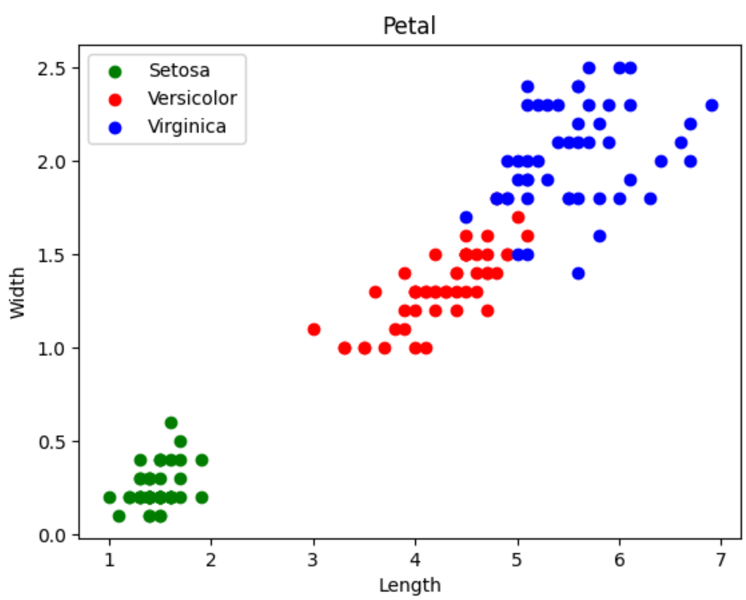
```
# Scatter plot of each real cluster
plt.scatter(petals['petal_length'],petals['petal_width'])

# Plot labels
plt.title('Petal')
plt.xlabel('Length')
plt.ylabel('Width')
plt.legend()
plt.show()
```

```
NING:matplotlib.legend:No artists with labels found to put in legend.  Note that artists whose label start with an underscore are ign
```



6. Scatter plot of the data asigning each point to the cluster it belongs to ¡¡

```
# Get dataframes for each real cluster
df1 = petals[petals['species'] == 0]
df2 = petals[petals['species'] == 1]
df3 = petals[petals['species'] == 2]

# Scatter plot of each real cluster
plt.scatter(df1['petal_length'],df1['petal_width'],color='green')
plt.scatter(df2['petal_length'],df2['petal_width'],color='red')
plt.scatter(df3['petal_length'],df3['petal_width'],color='blue')

# Plot labels
plt.title('Petal')
plt.xlabel('Length')
plt.ylabel('Width')
plt.legend(['Setosa','Versicolor','Virginica'])
plt.show()
```



Recall that for this dataset we know in advance the class to which each point belongs to

Kmeans clustering

Kmeans clustering

```
# Import sklearn KMeans
from sklearn.cluster import KMeans
# Define number of clusters
k=3
km = KMeans(n_clusters=k, n_init="auto")
# Do K-means clustering (assing each point in the dataset to a cluster)
FlowePRedicted = km.fit_predict(dataset[['petal_length','petal_width','sepal_length', 'sepal_width']])

# Print estimated cluster of each point in the dataset
FlowePRedicted
```

```
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, 2, 0, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2,
       2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 0, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2,
       2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 0, 2, 0, 0, 0, 0, 2, 0, 0, 0,
       0, 0, 0, 2, 2, 0, 0, 0, 0, 2, 0, 2, 0, 2, 0, 0, 2, 2, 0, 0, 0, 0,
       0, 2, 0, 0, 0, 0, 2, 0, 0, 0, 2, 0, 0, 0, 2, 0, 0, 2], dtype=int32)
```

Empieza a programar o a crear código con IA.

NOTE: the lables of the estimated clusters do not agree with the lables in the real labels, therefore, it will be important to pair the labels of the real and estimated clusters

```
# Manual pairing the labels of the real and estimated clusters
for i in range(len(FlowePRedicted)):
    if FlowePRedicted[i] == 0:
        FlowePRedicted[i] = 1
    elif FlowePRedicted[i] == 1:
        FlowePRedicted[i] = 2
    elif FlowePRedicted[i] == 2:
        FlowePRedicted[i] = 0
```

```
# Add a new column to the dataset with the cluster information
dataset['Cluster'] = FlowePRedicted
dataset
```

	sepal_length	sepal_width	petal_length	petal_width	species	Cluster
0	5.1	3.5	1.4	0.2	0	2
1	4.9	3.0	1.4	0.2	0	2
2	4.7	3.2	1.3	0.2	0	2
3	4.6	3.1	1.5	0.2	0	2
4	5.0	3.6	1.4	0.2	0	2
...	...	...	...	...	...	...
145	6.7	3.0	5.2	2.3	2	1
146	6.3	2.5	5.0	1.9	2	0
147	6.5	3.0	5.2	2.0	2	1
148	6.2	3.4	5.4	2.3	2	1
149	5.9	3.0	5.1	1.8	2	0

150 rows × 6 columns

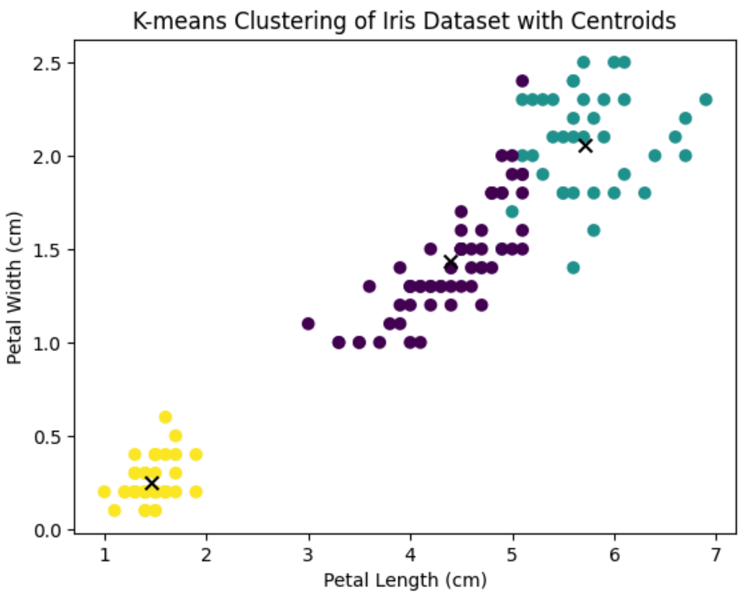
Pasos siguientes: Generar código con dataset | Ver gráficos recomendados | New interactive sheet

```
# Laber of the estimated clusters
print(km.labels_)
```

```
[2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
 2 2 2 2 2 2 2 2 2 2 2 2 2 1 0 1 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 0 0 0 0 0 0 0 0 0 0 0 0 1 0 1 1 1 1 0 1 1 1 1
```

```
 1 1 0 0 1 1 1 1 0 1 0 1 0 1 1 0 0 1 1 1 1 1 0 1 1 1 1 0 1 1 1 0 1 1 1 0 1
 1 0]
```

```
# Cluster centroides
plt.scatter(dataset['petal_length'], dataset['petal_width'], c=dataset['Cluster'])

centroids = km.cluster_centers_
plt.scatter(centroids[:, 0], centroids[:, 1], c='black', marker='x', s=50)

plt.title("K-means Clustering of Iris Dataset with Centroids")
plt.xlabel("Petal Length (cm)")
plt.ylabel("Petal Width (cm)")
plt.show()
```




```
# Sum of squared error (sse) of the final model
print(km.inertia_)
```

```
78.85566582597727
```

```
# The number of iterations required to converge
print(km.n_iter_)
```

```
4
```

Important remarks

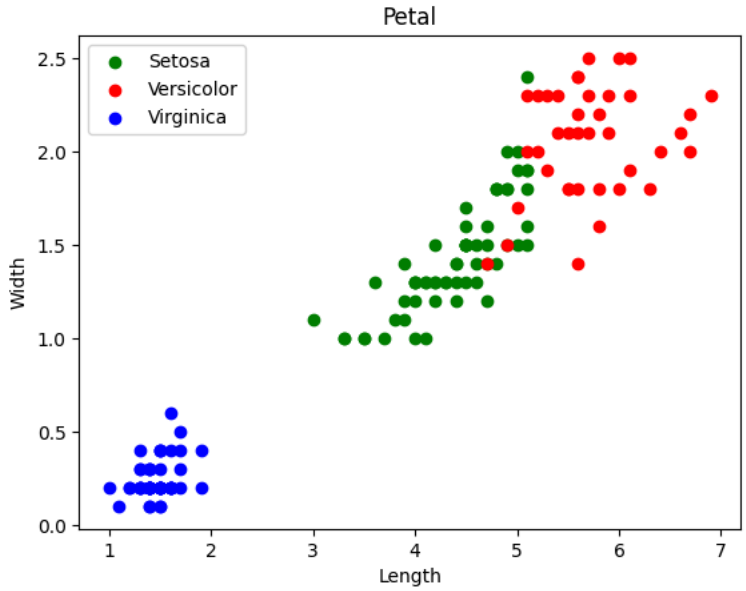
- The number of each cluster is randomly assigned
- The order of the numer in each cluster is random

Plot estimated clusters

Plot estimated clusters

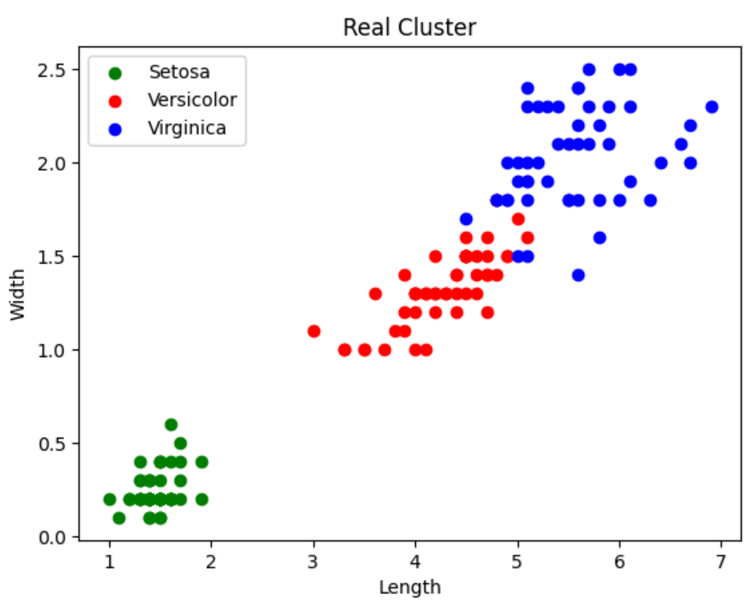
```
df1 = dataset[dataset['Cluster'] == 0]
df2 = dataset[dataset['Cluster'] == 1]
df3 = dataset[dataset['Cluster'] == 2]

plt.scatter(df1['petal_length'],df1['petal_width'],color='green')
plt.scatter(df2['petal_length'],df2['petal_width'],color='red')
plt.scatter(df3['petal_length'],df3['petal_width'],color='blue')

plt.title('Petal')
plt.xlabel('Length')
plt.ylabel('Width')
plt.legend(['Setosa','Versicolor','Virginica'])
```

```
<matplotlib.legend.Legend at 0x7f46ee6c4970>
```



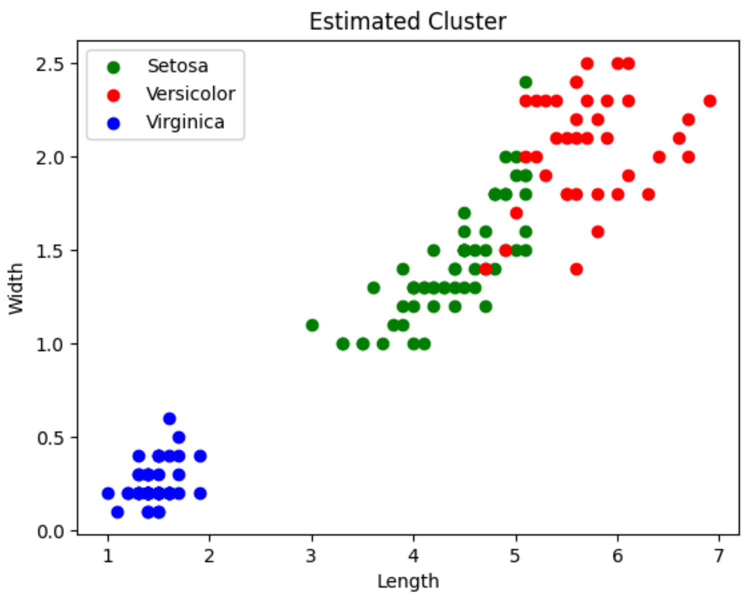
Plot both real and estimated clusters to check for errors

```
# Get dataframes for each real cluster
df1 = petals[petals['species'] == 0]
df2 = petals[petals['species'] == 1]
df3 = petals[petals['species'] == 2]

# Scatter plot of each real cluster
plt.scatter(df1['petal_length'],df1['petal_width'],color='green')
plt.scatter(df2['petal_length'],df2['petal_width'],color='red')
plt.scatter(df3['petal_length'],df3['petal_width'],color='blue')

# Plot labels
plt.title('Real Cluster')
plt.xlabel('Length')
plt.ylabel('Width')
plt.legend(['Setosa','Versicolor','Virginica'])
plt.show()
```



```
df1 = dataset[dataset['Cluster'] == 0]
df2 = dataset[dataset['Cluster'] == 1]
df3 = dataset[dataset['Cluster'] == 2]

plt.scatter(df1['petal_length'],df1['petal_width'],color='green')
plt.scatter(df2['petal_length'],df2['petal_width'],color='red')
plt.scatter(df3['petal_length'],df3['petal_width'],color='blue')

plt.title('Estimated Cluster')
plt.xlabel('Length')
plt.ylabel('Width')
plt.legend(['Setosa','Versicolor','Virginica'])
```

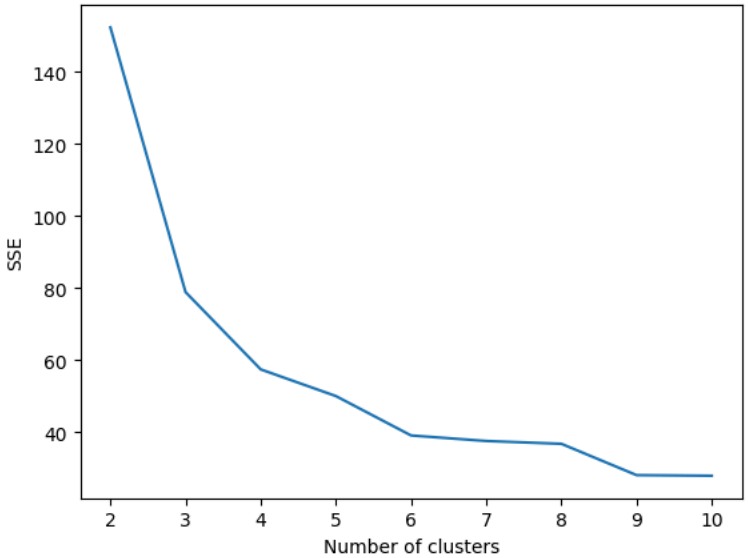
```
<matplotlib.legend.Legend at 0x7f46ee643be0>
```



Selecting K: elbow plot

Check the acurracy of the model using k-fold cross-validation

```
# Intialize a list to hold sum of squared error (sse)
sse = []

# Define values of k
k = [2,3,4,5,6,7,8,9,10]

# For each k
for i in k:
    # Initialize
    km = KMeans(n_clusters=i, n_init="auto")
    # Do K-means clustering
    km.fit(dataset[['petal_length','petal_width','sepal_length', 'sepal_width']])
    # Append sse to the list
    sse.append(km.inertia_)


# Plot sse versus k
plt.plot(k, sse)
plt.xticks(k)
plt.xlabel('Number of clusters')
plt.ylabel('SSE')
plt.show()
```



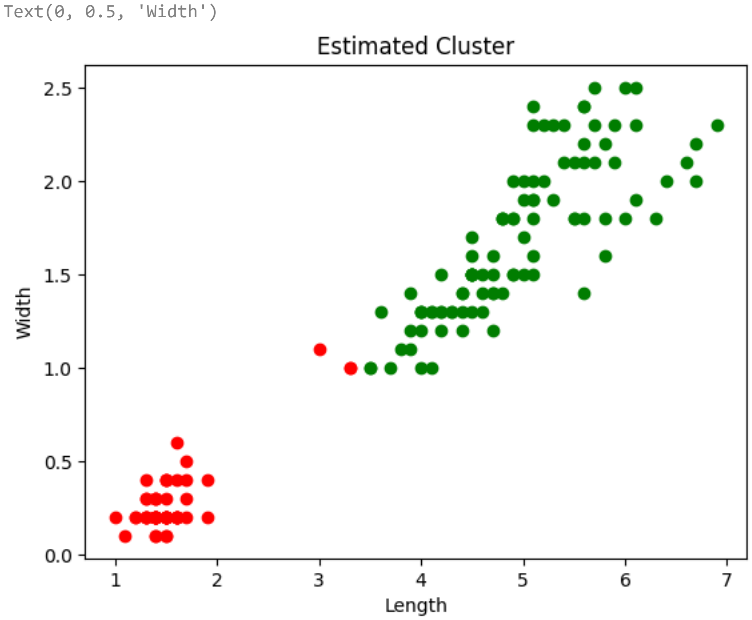
Choose the k after which the sse is minimally reduced

Important remarks

- Note that for K=2 ...
- Note that for K=3 ...

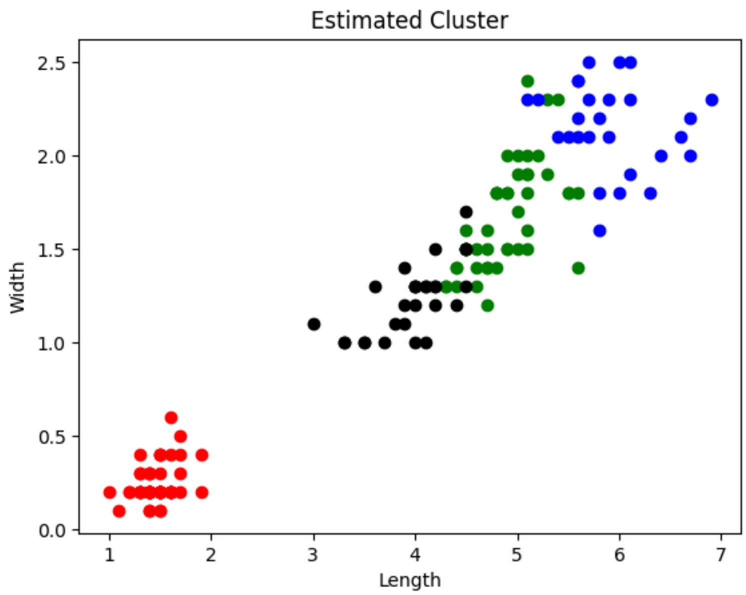
```
k=2
km = KMeans(n_clusters=k, n_init="auto")
# Do K-means clustering (assing each point in the dataset to a cluster)
FlowePRedicted = km.fit_predict(dataset[['petal_length','petal_width','sepal_length', 'sepal_width']])

dataset['Cluster'] = FlowePRedicted

df1 = dataset[dataset['Cluster'] == 0]
df2 = dataset[dataset['Cluster'] == 1]

plt.scatter(df1['petal_length'],df1['petal_width'],color='green')
plt.scatter(df2['petal_length'],df2['petal_width'],color='red')

plt.title('Estimated Cluster')
plt.xlabel('Length')
plt.ylabel('Width')
```

```
Text(0, 0.5, 'Width')
```



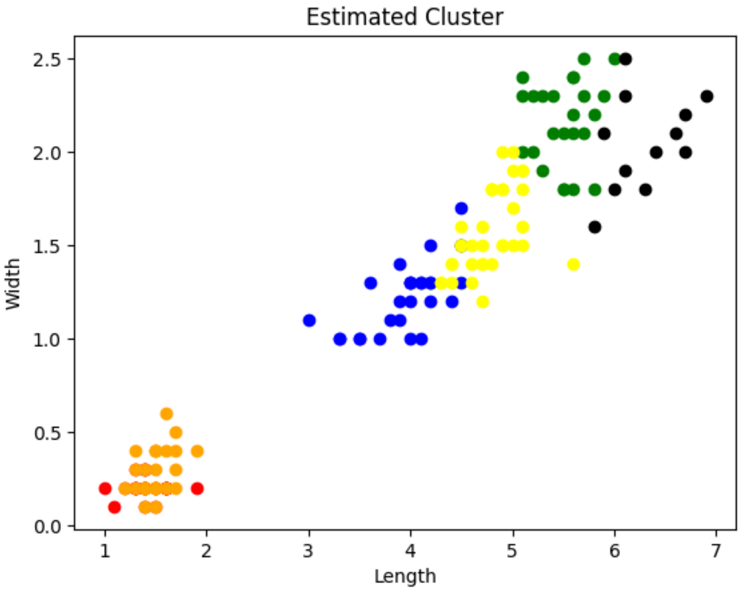
```
k=4
km = KMeans(n_clusters=k, n_init="auto")
# Do K-means clustering (assing each point in the dataset to a cluster)
FlowePRedicted = km.fit_predict(dataset[['petal_length','petal_width','sepal_length', 'sepal_width']])

dataset['Cluster'] = FlowePRedicted

df1 = dataset[dataset['Cluster'] == 0]
df2 = dataset[dataset['Cluster'] == 1]
df3 = dataset[dataset['Cluster'] == 2]
df4 = dataset[dataset['Cluster'] == 3]

plt.scatter(df1['petal_length'],df1['petal_width'],color='green')
plt.scatter(df2['petal_length'],df2['petal_width'],color='red')
plt.scatter(df3['petal_length'],df3['petal_width'],color='blue')
plt.scatter(df4['petal_length'],df4['petal_width'],color='black')

plt.title('Estimated Cluster')
plt.xlabel('Length')
plt.ylabel('Width')
```

```
Text(0, 0.5, 'Width')
```




```
k=6
km = KMeans(n_clusters=k, n_init="auto")
# Do K-means clustering (assing each point in the dataset to a cluster)
FlowePRedicted = km.fit_predict(dataset[['petal_length','petal_width','sepal_length', 'sepal_width']])

dataset['Cluster'] = FlowePRedicted

df1 = dataset[dataset['Cluster'] == 0]
df2 = dataset[dataset['Cluster'] == 1]
df3 = dataset[dataset['Cluster'] == 2]
df4 = dataset[dataset['Cluster'] == 3]
df5 = dataset[dataset['Cluster'] == 4]
df6 = dataset[dataset['Cluster'] == 5]

plt.scatter(df1['petal_length'],df1['petal_width'],color='green')
plt.scatter(df2['petal_length'],df2['petal_width'],color='red')
plt.scatter(df3['petal_length'],df3['petal_width'],color='blue')
plt.scatter(df4['petal_length'],df4['petal_width'],color='black')
plt.scatter(df5['petal_length'],df5['petal_width'],color='yellow')
plt.scatter(df6['petal_length'],df6['petal_width'],color='orange')

plt.title('Estimated Cluster')
plt.xlabel('Length')
plt.ylabel('Width')
```

```
Text(0, 0.5, 'Width')
```




```
k=7
km = KMeans(n_clusters=k, n_init="auto")
# Do K-means clustering (assing each point in the dataset to a cluster)
FlowePRedicted = km.fit_predict(dataset[['petal_length','petal_width','sepal_length', 'sepal_width']])

dataset['Cluster'] = FlowePRedicted

df1 = dataset[dataset['Cluster'] == 0]
df2 = dataset[dataset['Cluster'] == 1]
df3 = dataset[dataset['Cluster'] == 2]
df4 = dataset[dataset['Cluster'] == 3]
df5 = dataset[dataset['Cluster'] == 4]
df6 = dataset[dataset['Cluster'] == 5]
df7 = dataset[dataset['Cluster'] == 6]

plt.scatter(df1['petal_length'],df1['petal_width'],color='green')
plt.scatter(df2['petal_length'],df2['petal_width'],color='red')
plt.scatter(df3['petal_length'],df3['petal_width'],color='blue')
plt.scatter(df4['petal_length'],df4['petal_width'],color='black')
plt.scatter(df5['petal_length'],df5['petal_width'],color='yellow')
plt.scatter(df6['petal_length'],df6['petal_width'],color='orange')
plt.scatter(df7['petal_length'],df7['petal_width'],color='purple')

plt.title('Estimated Cluster')
plt.xlabel('Length')
plt.ylabel('Width')
```

```
Text(0, 0.5, 'Width')
```

Estimated Cluster