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/MyDrive/ITC/5toSem/semanaTecAn/"

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

```
Drive already mounted at /content/drive; to attempt to forcibly remount, call drive.mount("/content/drive", force_r
```

Suggested code may be subject to a license | | AnuragAnalog/Guided-Projects-Coursera | askorucuk/Randomforest_classification

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

Importing data

```
# Dataset url
url = "datasets/iris.csv"
# Load the dataset from HHDD
df = pd.read_csv(Ruta + url)
# change the name of the columns
df.columns = ['sepal_length', 'sepal_width', 'petal_length', 'petal_width', 'flower']
# Visualize the dataset
df
```

	sepal_length	sepal_width	petal_length	petal_width	flower
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

Next steps: Generate code with df View recommended plots New interactive sheet

Undertanding and preprocessing the data

1. Get a general 'feel' of the data

```
# get a general feel of the data
df
```

	sepal_length	sepal_width	petal_length	petal_width	flower
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

Next steps: Generate code with df View recommended plots New interactive sheet

2. Drop rows with any missing values

```
#drop rows with missing values
df.dropna(inplace=True)
df
```

	sepal_length	sepal_width	petal_length	petal_width	flower
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

Next steps: Generate code with df View recommended plots New interactive sheet

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

```
# Encoding the categorical column
df=df.replace({'flower': {'Setosa': 0, 'Versicolor': 1, 'Virginica': 2}})
#Visualize the dataset
df
```

	sepal_length	sepal_width	petal_length	petal_width	flower
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

Next steps: Generate code with df View recommended plots New interactive sheet

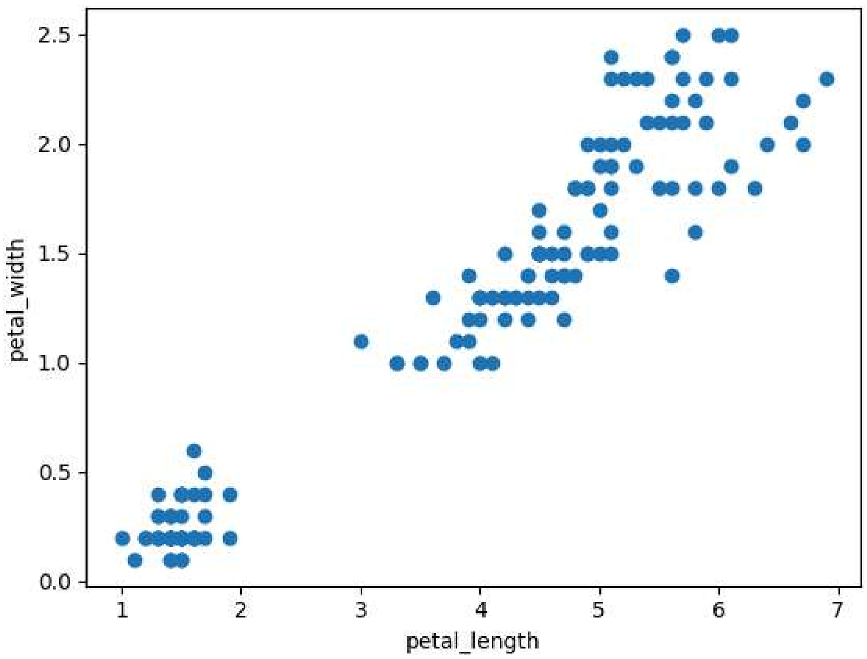
Now the label/category is numeric

4. Discard columns that won't be used

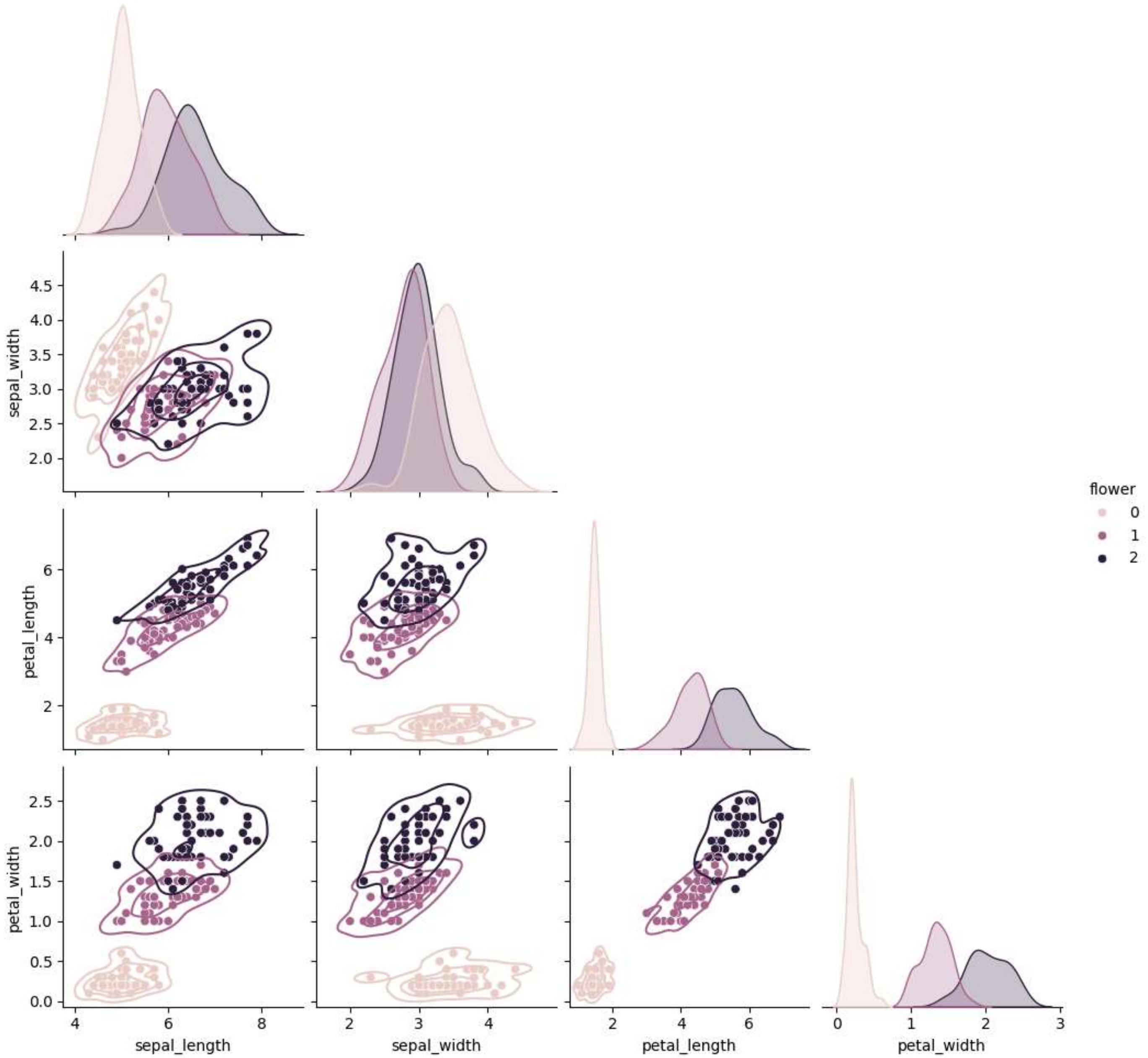
```
# # Drop out non necesary columns
# dataset.drop(['Sepal_Length', 'Sepal_Width'],axis='columns',inplace=True)
#
# #Visualize the dataset
# dataset

```

5. Scatter plot of the data

```
plt.scatter(df.petal_length, df.petal_width)
plt.xlabel('petal_length')
plt.ylabel('petal_width')
plt.show()
```

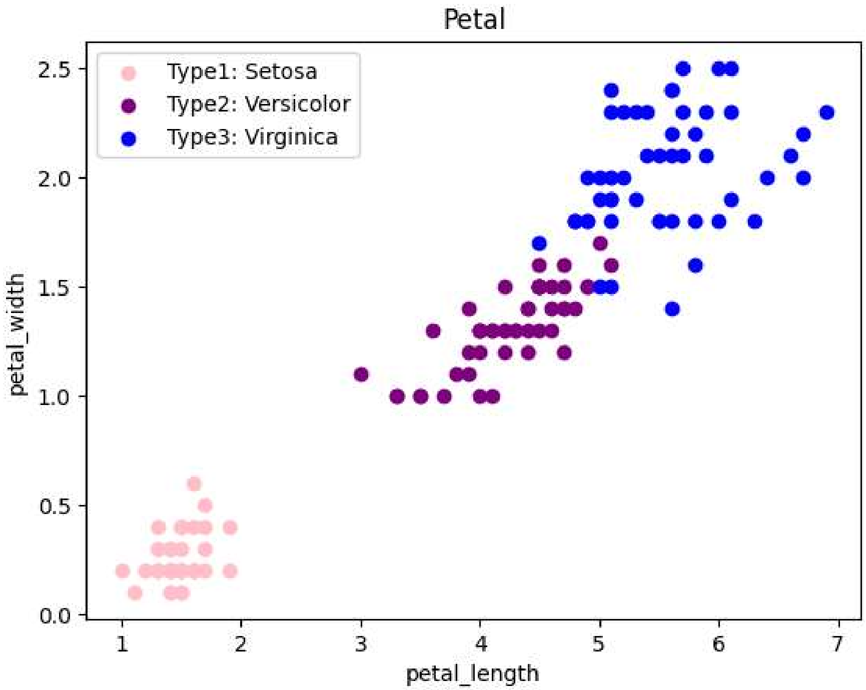


```
#PAIRPLOT: SCATTER PLOT OF ALL
g = sns.pairplot(df, corner = True, diag_kind = 'kde', hue = 'flower')
g.map_lower(sns.kdeplot, levels = 4, color = '.2')
plt.show()
```



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

```
# Get dataframes for each real cluster
df0 = df[df.flower == 0]
df1 = df[df.flower == 1]
df2 = df[df.flower == 2]
plt.scatter(df0.petal_length, df0.petal_width, color = 'pink')
plt.scatter(df1.petal_length, df1.petal_width, color = 'purple')
plt.scatter(df2.petal_length, df2.petal_width, color = 'blue')
plt.legend(['Type1: Setosa', 'Type2: Versicolor', 'Type3: Virginica'])
plt.xlabel('petal_length')
plt.ylabel('petal_width')
plt.title('Petal')
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
from sklearn.metrics import silhouette_score
# Define number of clusters
k = 3
# Do k-means clustering (assign each point in the dataset to a cluster)
km = KMeans(n_clusters=k, n_init="auto") #modelo ML here
FlowerPredicted = km.fit_predict(df[['sepal_length', 'sepal_width','petal_length', 'petal_width']]) #entrena y predi
# Print estimated cluster of each point in the dataset
FlowerPredicted
```

```
array([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], dtype=int32)
```

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
```

```
# Add cluster information to dataset
df['flower_predictedK3'] = FlowerPredicted
# Show the first few rows to check the cluster assignment
df.head()
```

	sepal_length	sepal_width	petal_length	petal_width	flower	flower_predictedK3
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

Next steps: Generate code with df | View recommended plots | New interactive sheet

Double-click (or enter) to edit

```
# Display cluster labels
FlowerPredicted = df['flower_predictedK3']
print("Labels of the estimated clusters:", FlowerPredicted.unique())
```

```
Labels of the estimated clusters: [2 1 0]
```

```
# Get the centroids of the clusters
print("Cluster centroids:\n", km.cluster_centers_)
```

```
Cluster centroids:
 [[5.88360656 2.74098361 4.38852459 1.43442623]
 [6.85384615 3.07692308 5.71538462 2.05384615]
 [5.006      3.428      1.462      0.246     ]]
```

```
# Sum of squared error (sse) of the final model
sse = km.inertia_
print("Sum of squared error (SSE):", sse)
```

```
Sum of squared error (SSE): 78.85566582597727
```

```
# The number of iterations required to converge
print("Number of iterations:", km.n_iter_)
```

```
Number of iterations: 12
```

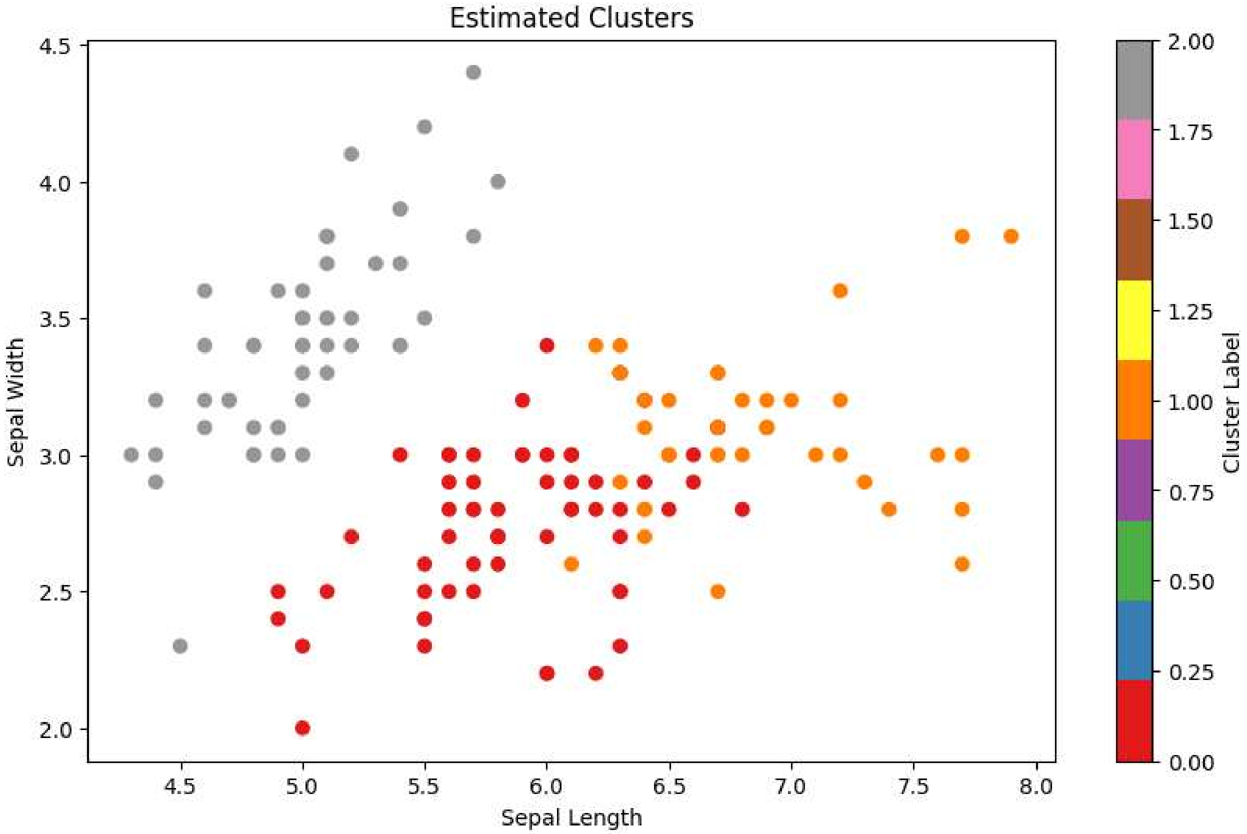
Important remarks

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

Plot estimated clusters

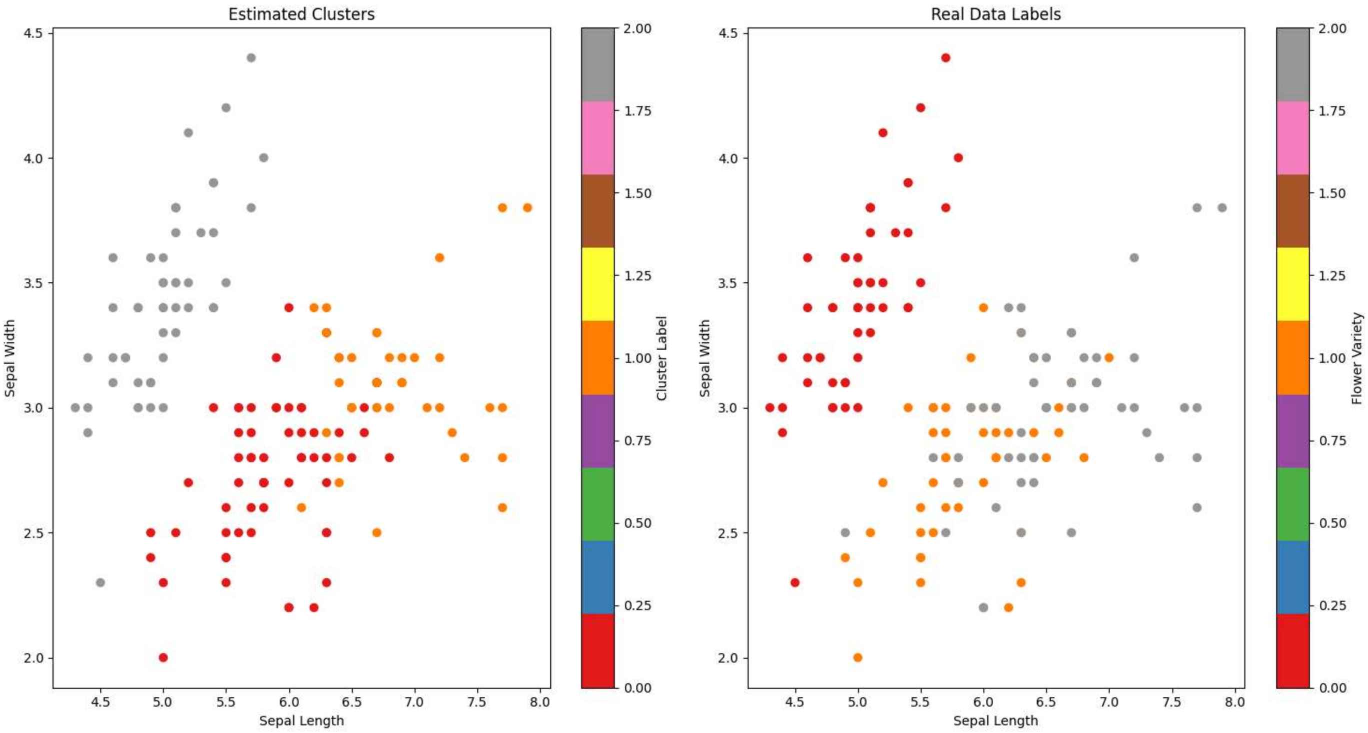
Plot estimated clusters

```
plt.figure(figsize=(10, 6))
plt.scatter(df['sepal_length'], df['sepal_width'], c=df['flower_predictedK3'], cmap='Set1', marker='o')
plt.title('Estimated Clusters')
plt.xlabel('Sepal Length')
plt.ylabel('Sepal Width')
plt.colorbar(label='Cluster Label')
plt.show()
```



Plot both real and estimated clusters to check for errors

```
#GRAPH
plt.figure(figsize=(15, 8))

# Plot estimated clusters
plt.subplot(1, 2, 1)
scatter = plt.scatter(df['sepal_length'], df['sepal_width'], c=df['flower_predictedK3'], cmap='Set1', marker='o')
plt.title('Estimated Clusters')
plt.xlabel('Sepal Length')
plt.ylabel('Sepal Width')
plt.colorbar(label='Cluster Label')

# Plot real labels
plt.subplot(1, 2, 2)
scatter = plt.scatter(df['sepal_length'], df['sepal_width'], c=df['flower'].astype('category').cat.codes, cmap='Set1
plt.title('Real Data Labels')
plt.xlabel('Sepal Length')
plt.ylabel('Sepal Width')
plt.colorbar(label='Flower Variety')

plt.tight_layout()
plt.show()
```



Choose the k after which the sse is minimally reduced

Important remarks

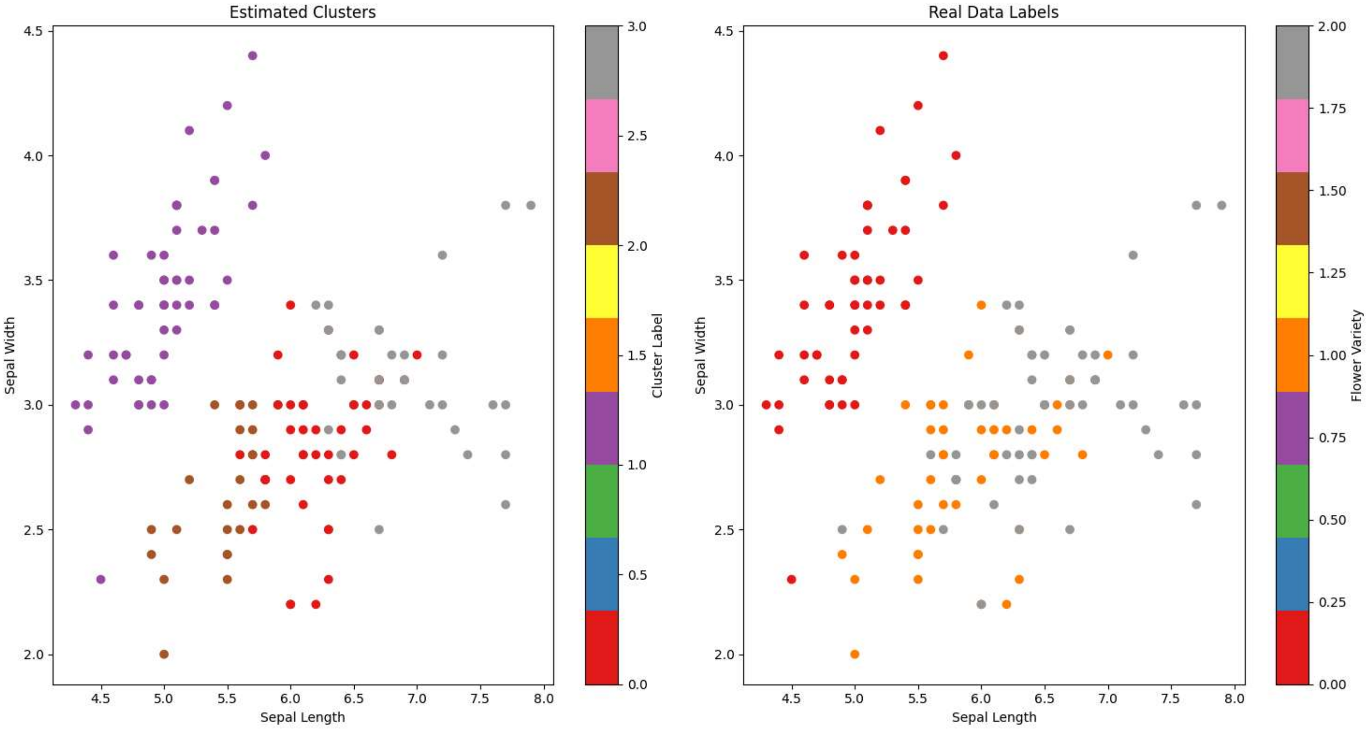
- Note that for K=2 ...
- Note that for K=4 ...
- Note that for K=5 ...

EXAMPLE WITH K=4

```
print("NUMBER OF CLUSTERS = 4")
# Define number of clusters
k = 4
# Do k-means clustering (assign each point in the dataset to a cluster)
km = KMeans(n_clusters=k, n_init="auto") #modelo ML here
FlowerPredicted = km.fit_predict(df[['sepal_length', 'sepal_width','petal_length', 'petal_width']]) #entrena y predic
# Print estimated cluster of each point in the dataset
FlowerPredicted
# Add cluster information to dataset
df['flower_predictedK4'] = FlowerPredicted
# Show the first few rows to check the cluster assignment
print(df.head())
# Display cluster labels
FlowerPredicted = df['flower_predictedK4']
print("Labels of the estimated clusters:", FlowerPredicted.unique())
# Get the centroids of the clusters
print("Cluster centroids:\n", km.cluster_centers_)
# Sum of squared error (sse) of the final model
sse = km.inertia_
print("Sum of squared error (SSE):", sse)
# The number of iterations required to converge
print("Number of iterations:", km.n_iter_)

#GRAPH
```

```
plt.figure(figsize=(15, 8))

# Plot estimated clusters
plt.subplot(1, 2, 1)
scatter = plt.scatter(df['sepal_length'], df['sepal_width'], c=df['flower_predictedK4'], cmap='Set1', marker='o')
plt.title('Estimated Clusters')
plt.xlabel('Sepal Length')
plt.ylabel('Sepal Width')
plt.colorbar(label='Cluster Label')

# Plot real labels
plt.subplot(1, 2, 2)
scatter = plt.scatter(df['sepal_length'], df['sepal_width'], c=df['flower'].astype('category').cat.codes, cmap='Set1',
plt.title('Real Data Labels')
plt.xlabel('Sepal Length')
plt.ylabel('Sepal Width')
plt.colorbar(label='Flower Variety')

plt.tight_layout()
plt.show()
```

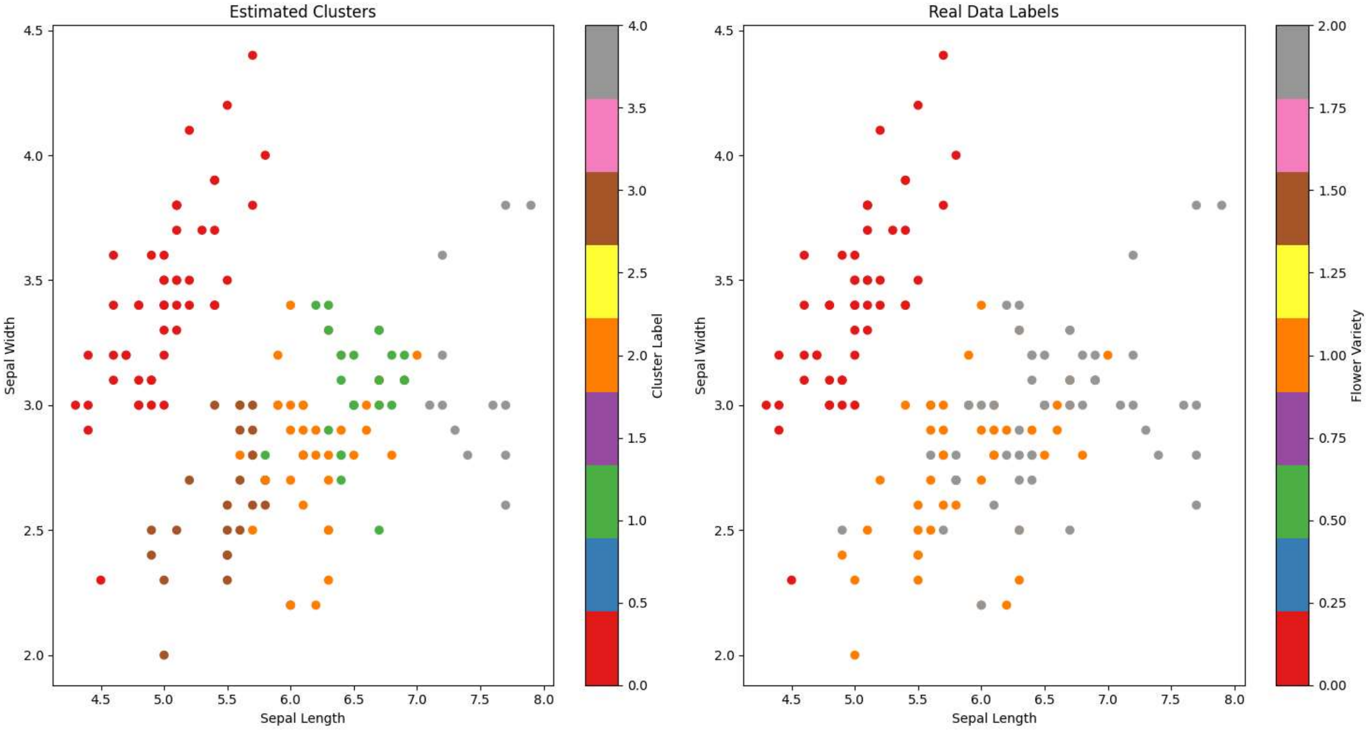
```
NUMBER OF CLUSTERS = 4
   sepal_length  sepal_width  petal_length  petal_width  flower  \
0           5.1          3.5           1.4          0.2       0
1           4.9          3.0           1.4          0.2       0
2           4.7          3.2           1.3          0.2       0
3           4.6          3.1           1.5          0.2       0
4           5.0          3.6           1.4          0.2       0

   flower_predictedK3  flower_predictedK4
0                   2                   1
1                   2                   1
2                   2                   1
3                   2                   1
4                   2                   1
Labels of the estimated clusters: [1 0 2 3]
Cluster centroids:
 [[6.23658537 2.85853659 4.80731707 1.62195122]
 [5.006      3.428      1.462      0.246     ]
 [5.52962963 2.62222222 3.94074074 1.21851852]
 [6.9125     3.1        5.846875   2.13125   ]]
Sum of squared error (SSE): 57.25600931571815
Number of iterations: 3
```



EXAMPLE WITH K=5

```
print("NUMBER OF CLUSTERS = 5")
# Define number of clusters
k = 5
# Do k-means clustering (assign each point in the dataset to a cluster)
km = KMeans(n_clusters=k, n_init="auto") #modelo ML here
FlowerPredicted = km.fit_predict(df[['sepal_length', 'sepal_width','petal_length', 'petal_width']]) #entrena y predi
# Print estimated cluster of each point in the dataset
FlowerPredicted
# Add cluster information to dataset
df['flower_predictedK5'] = FlowerPredicted
# Show the first few rows to check the cluster assignment
print(df.head())
# Display cluster labels
FlowerPredicted = df['flower_predictedK5']
print("Labels of the estimated clusters:", FlowerPredicted.unique())
# Get the centroids of the clusters
print("Cluster centroids:\n", km.cluster_centers_)
# Sum of squared error (sse) of the final model
sse = km.inertia_
print("Sum of squared error (SSE):", sse)
# The number of iterations required to converge
print("Number of iterations:", km.n_iter_)

#GRAPH
plt.figure(figsize=(15, 8))

# Plot estimated clusters
plt.subplot(1, 2, 1)
scatter = plt.scatter(df['sepal_length'], df['sepal_width'], c=df['flower_predictedK5'], cmap='Set1', marker='o')
plt.title('Estimated Clusters')
plt.xlabel('Sepal Length')
plt.ylabel('Sepal Width')
plt.colorbar(label='Cluster Label')

# Plot real labels
plt.subplot(1, 2, 2)
scatter = plt.scatter(df['sepal_length'], df['sepal_width'], c=df['flower'].astype('category').cat.codes, cmap='Set1
plt.title('Real Data Labels')
plt.xlabel('Sepal Length')
plt.ylabel('Sepal Width')
plt.colorbar(label='Flower Variety')

plt.tight_layout()
plt.show()
```

```
NUMBER OF CLUSTERS = 5
   sepal_length  sepal_width  petal_length  petal_width  flower  \
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

   flower_predictedK3  flower_predictedK4  flower_predictedK5
0                   2                   1                   0
1                   2                   1                   0
2                   2                   1                   0
3                   2                   1                   0
4                   2                   1                   0
Labels of the estimated clusters: [0 2 3 1 4]
Cluster centroids:
 [[5.006      3.428      1.462      0.246     ]
 [6.52916667 3.05833333 5.50833333 2.1625    ]
 [6.20769231 2.85384615 4.74615385 1.56410256]
 [5.508      2.6        3.908      1.204     ]
 [7.475      3.125      6.3        2.05      ]]
Sum of squared error (SSE): 46.44618205128204
Number of iterations: 5
```



EXAMPLE WITH K=2

```
print("NUMBER OF CLUSTERS = 2")
# Define number of clusters
k = 2
# Do k-means clustering (assign each point in the dataset to a cluster)
km = KMeans(n_clusters=k, n_init="auto") #modelo ML here
FlowerPredicted = km.fit_predict(df[['sepal_length', 'sepal_width','petal_length', 'petal_width']]) #entrena y predi
# Print estimated cluster of each point in the dataset
FlowerPredicted
# Add cluster information to dataset
df['flower_predictedK2'] = FlowerPredicted
# Show the first few rows to check the cluster assignment
print(df.head())
# Display cluster labels
FlowerPredicted = df['flower_predictedK2']
print("Labels of the estimated clusters:", FlowerPredicted.unique())
# Get the centroids of the clusters
print("Cluster centroids:\n", km.cluster_centers_)
# Sum of squared error (sse) of the final model
sse = km.inertia_
print("Sum of squared error (SSE):", sse)
# The number of iterations required to converge
print("Number of iterations:", km.n_iter_)

#GRAPH
plt.figure(figsize=(15, 8))

# Plot estimated clusters
plt.subplot(1, 2, 1)
scatter = plt.scatter(df['sepal_length'], df['sepal_width'], c=df['flower_predictedK2'], cmap='Set1', marker='o')
plt.title('Estimated Clusters')
plt.xlabel('Sepal Length')
plt.ylabel('Sepal Width')
plt.colorbar(label='Cluster Label')

# Plot real labels
plt.subplot(1, 2, 2)
scatter = plt.scatter(df['sepal_length'], df['sepal_width'], c=df['flower'].astype('category').cat.codes, cmap='Set1
plt.title('Real Data Labels')
plt.xlabel('Sepal Length')
plt.ylabel('Sepal Width')
plt.colorbar(label='Flower Variety')

plt.tight_layout()
plt.show()
```

```
NUMBER OF CLUSTERS = 2
   sepal_length  sepal_width  petal_length  petal_width  flower  \
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

   flower_predictedK3  flower_predictedK4  flower_predictedK5  \
0                   2                   1                   0
1                   2                   1                   0
2                   2                   1                   0
3                   2                   1                   0
4                   2                   1                   0

   flower_predictedK2
0                   0
1                   0
2                   0
```

Selecting K: elbow plot

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

```
Sum of squared error (SSE): 152.34795176035797
```

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

# Define values of k
k_values = range(1, 11)  # Testing k from 1 to 10

# For each k
# For each k, fit KMeans and calculate SSE
for k in k_values:
    km = KMeans(n_clusters=k, n_init="auto")
    km.fit(df[['sepal_length', 'sepal_width', 'petal_length', 'petal_width']])
    sse_list.append(km.inertia_)

# Plot SSE vs. k
plt.figure(figsize=(8, 5))
plt.plot(k_values, sse_list, marker='o')
plt.title('Elbow Plot for K-Means Clustering')
plt.xlabel('Number of clusters (k)')
plt.ylabel('Sum of Squared Errors (SSE)')
plt.show()
```