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1. load the data and separate in X all the columns but the last one, in y the last column, then produce a pairplot of X and decide which pair of columns is most interesting for a 2d scatterplot, ad produce the scatterplot (5pt)
2. find the best clustering scheme for X with a method of your choice, plot ssd and global silhouette index for an appropriate range of parameters and show the chosen hyperparameter(s) (5pt)
3. consider carefully the number of clusters, simple optimisation of the silhouette will not be enough, consider also the elbow plot and decide visually the best number of clusters
4. fit the clustering scheme to y_km, then produce the confusion matrix comparing y and y_km with sklearn.metrics.confusion_matrix, the resulting confusion matrix must be "sorted" using the function max_diag provided below, producing the final confusion matrix cm_km (5pt)
5. in a comment explain why function max_diag is useful (2pt)
6. compute the accuracy a_km of y_km versus y as the ratio the sum of the main diagonal of cm_km and the number of samples in X (2pt)
7. rescale X using sklearn.preprocessing.MinMaxScaler, producing the scaled dataset X_mms (3pt)
8. repeat point 3 and 5 above, fitting X_mms to y_km_mms and producing the confusion matrix cm_km_mms reordered with max_diag and the accuracy a_km_mms as above (3pt)

1.1.1 1. load the data and separate in X all the columns but the last one, in y the last column, then produce a pairplot of X and decide which pair of columns is most interesting for a 2d scatterplot, ad produce the scatterplot (5pt)

[75]:
```python
# Imports
import pandas as pd
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt
from sklearn.cluster import KMeans
from sklearn.metrics import silhouette_score
from sklearn.metrics import confusion_matrix
from sklearn.preprocessing import MinMaxScaler
from plot_clusters import plot_clusters
from max_diag import max_diag
```

```
# Variables
file_name = 'seeds_dataset.txt'
separator = '\t'
random_state = 42
target = 7

# Directives
%matplotlib inline
np.random.seed(random_state)
```

We use numpy to load the dataset, then convert it to a Pandas DataFrame to operate on it. We'll also print the head of the dataframe to have a look at it.

[46]:
```
text = np.loadtxt(file_name, delimiter = separator)
df = pd.DataFrame(text)
df.head()
```

[46]:
```
       0      1       2      3      4      5      6    7
0  15.26  14.84  0.8710  5.763  3.312  2.221  5.220  0.0
1  14.88  14.57  0.8811  5.554  3.333  1.018  4.956  0.0
2  14.29  14.09  0.9050  5.291  3.337  2.699  4.825  0.0
3  13.84  13.94  0.8955  5.324  3.379  2.259  4.805  0.0
4  16.14  14.99  0.9034  5.658  3.562  1.355  5.175  0.0
```

We now separate the feature matrix from the target column

[47]:
```
X = df.drop(target, axis = 1)
y = df[target]

print(f"The feature matrix has {X.shape[0]} rows and {X.shape[1]} columns")
```

```
The feature matrix has 210 rows and 7 columns
```

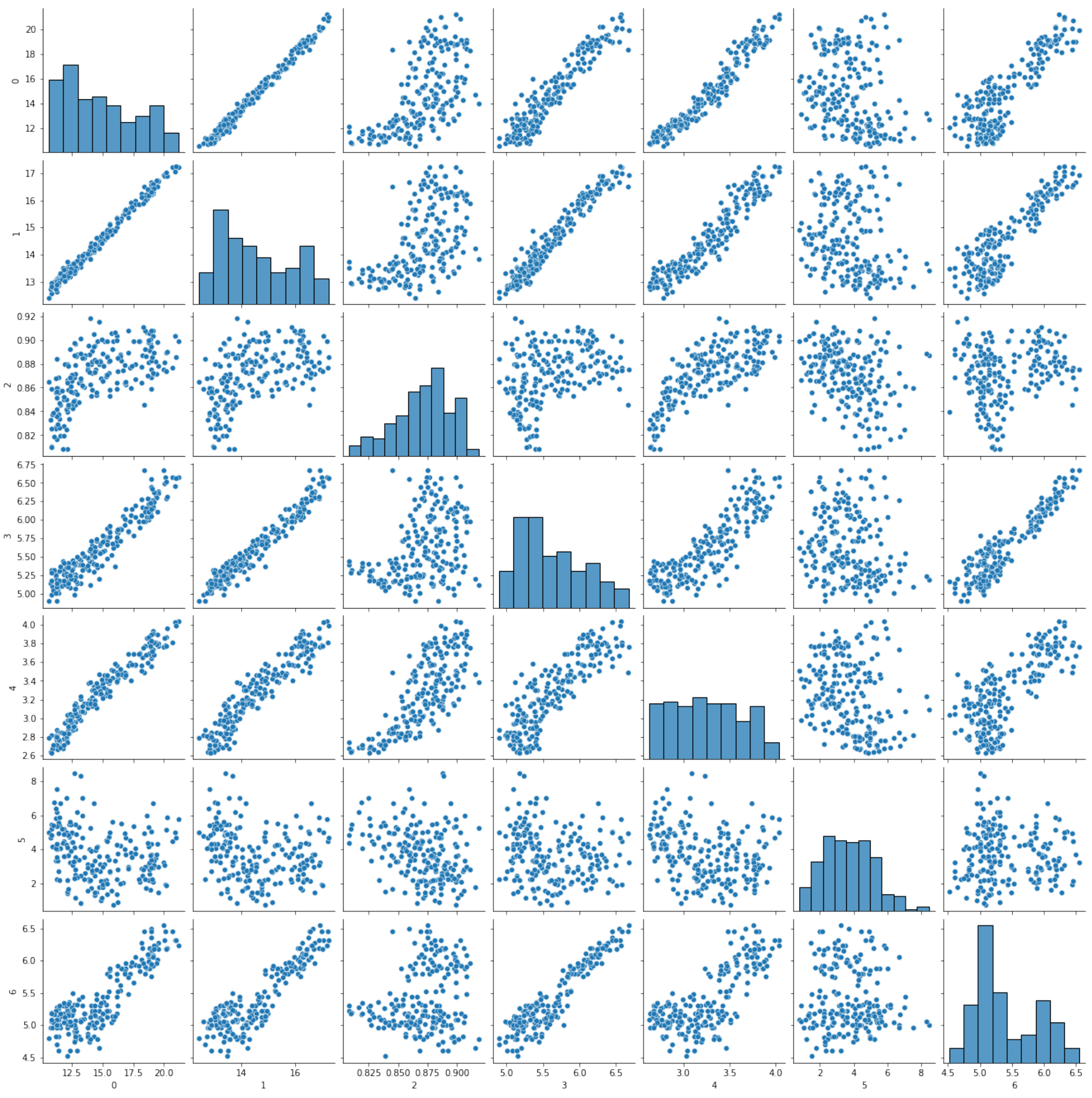
[69]:
```
print(f"There are {len(np.unique(y))} unique classes")
```

```
There are 3 unique classes
```

We will now produce a pairplot to look for possible interesting patterns.

[48]:
```
sns.pairplot(X)
```

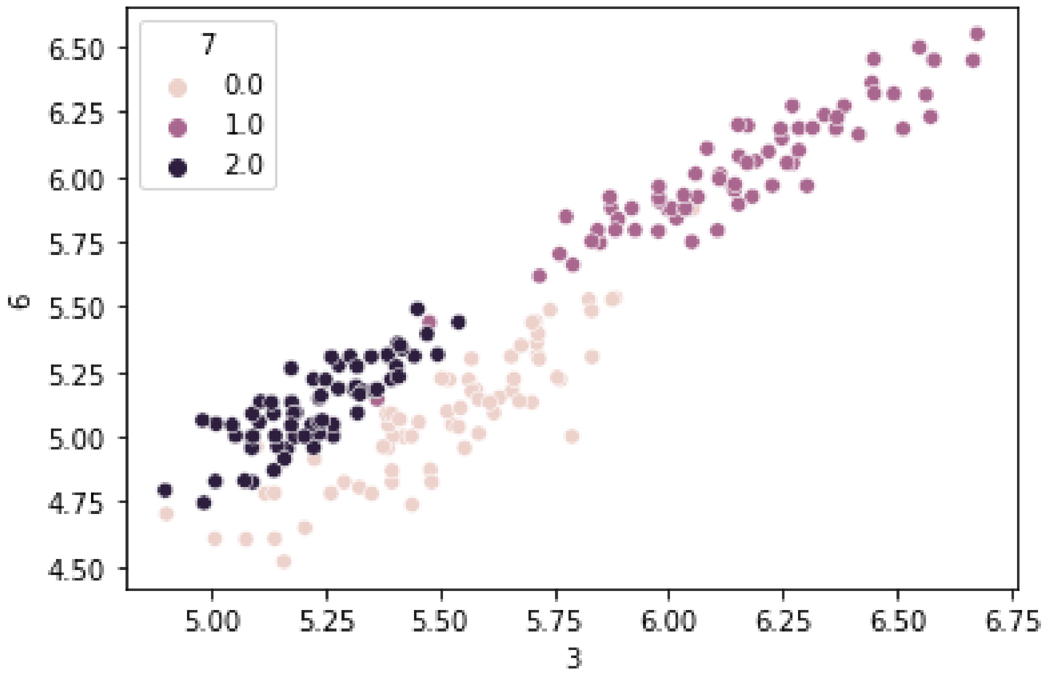
[48]:
```
<seaborn.axisgrid.PairGrid at 0x22e00d38e50>
```



Judging by the pairplots, we choose the columns with indexes 3,6, as they seem to create three distinct clusters, one for each of the classes that we have. We will plot a scatterplot using those two columns.

```
[68]: focus = [3,6]
      sns.scatterplot(x = focus[0], y = focus[1], data = df, hue = target)
```

```
[68]: <AxesSubplot:xlabel='3', ylabel='6'>
```



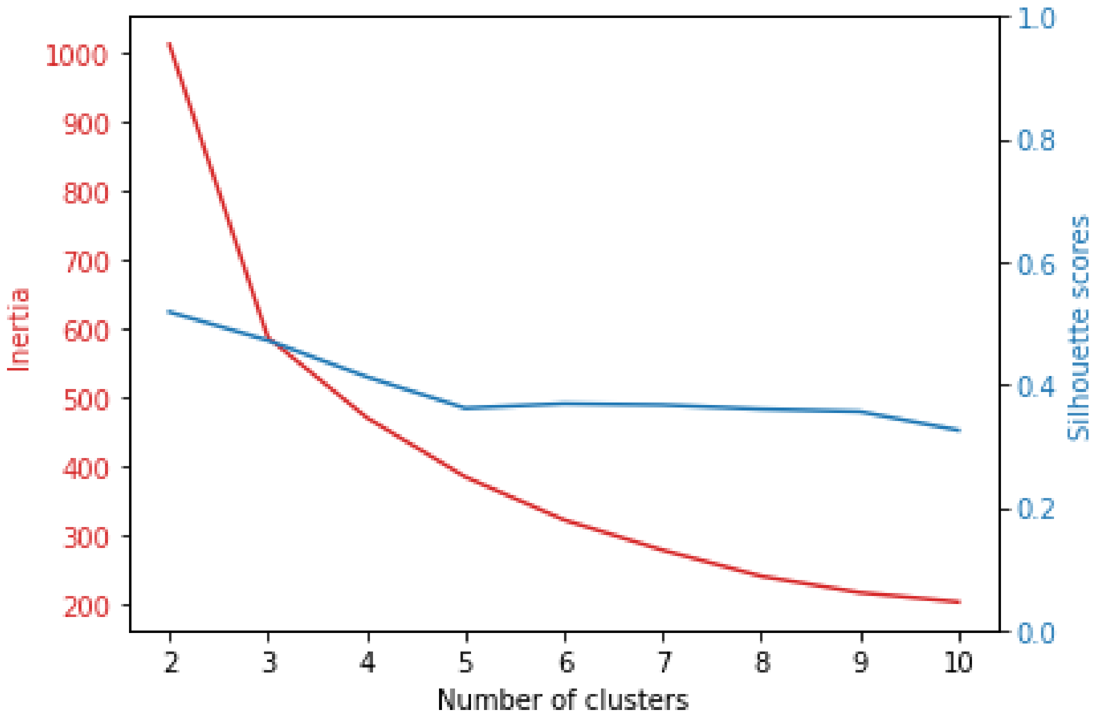
1.1.2 2. find the best clustering scheme for X with a method of your choice, plot ssd and global silhouhette index for an appropriate range of parameters and show the chosen hyperparameter(s) (5pt)

In order to find a clustering scheme, we will use K-means with the elbow method, ranging from 2 to 10 clusters

[50]:
```
# Range of possible clusters
k_range = range(2,11)

# Distortion and Silhouette Score as measures
distortions = []
silhouette_scores = []

for i in k_range:

    km = KMeans(n_clusters = i,
                init = 'k-means++',
                n_init = 10,
                max_iter = 300,
                random_state = random_state)

    y_km = km.fit_predict(X)
    distortions.append(km.inertia_)
    silhouette_scores.append(silhouette_score(X,y_km))
```

Plot distortion and silhouette indexes

```
[51]: fig, ax1 = plt.subplots()

color = 'tab:red'
ax1.set_xlabel('Number of clusters')
ax1.set_ylabel('Inertia', color=color)
ax1.plot(k_range, distortions, color=color)
ax1.tick_params(axis='y', labelcolor=color)

ax2 = ax1.twinx()  # instantiate a second axes that shares the same x-axis

color = 'tab:blue'
ax2.set_ylabel('Silhouette scores', color=color)  # we already handled the␣
 ↪x-label with ax1
ax2.plot(k_range, silhouette_scores, color=color)
ax2.tick_params(axis='y', labelcolor=color)
ax2.set_ylim(0,1) # the axis for silhouette is [0,1]

fig.tight_layout()  # otherwise the right y-label is slightly clipped
plt.show()
```



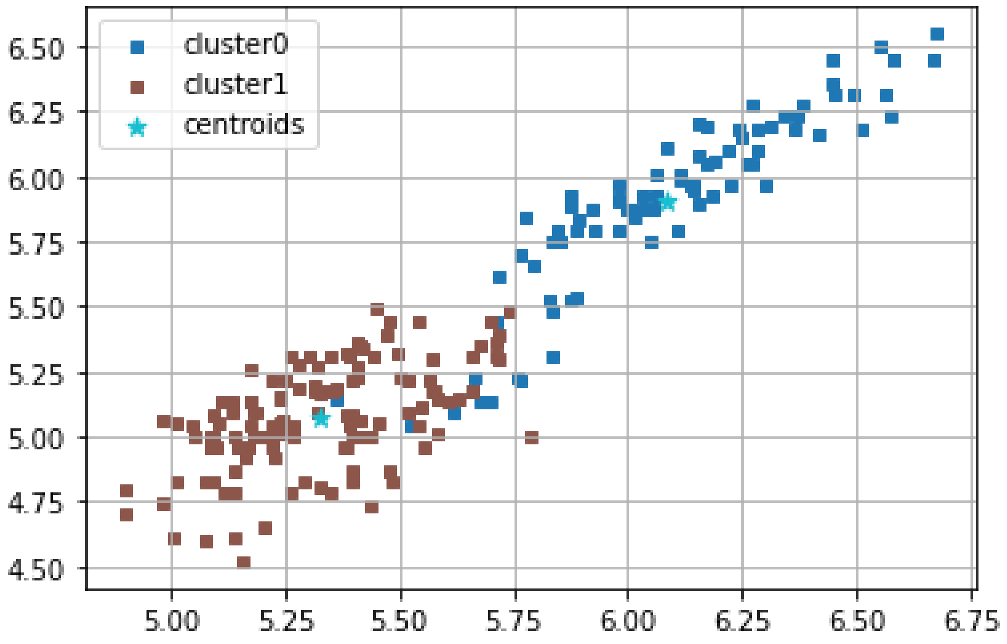
The silhouette scores plot tells us that we obtain the best result with 2 clusters

[52]:
```
silhouette_best_k = 2
```

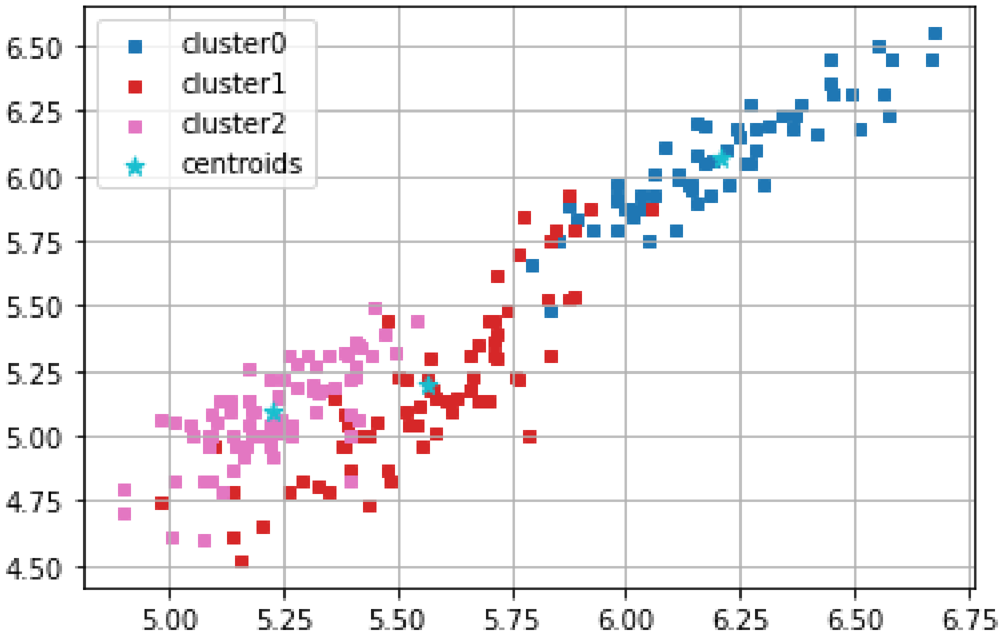
1.1.3 3. consider carefully the number of clusters, simple optimisation of the silhouette will not be enough, consider also the elbow plot and decide visually the best number of clusters

The elbow plot seems to suggest that there should be 3 clusters instead of 2. We will plot both clustering schemes and choose visually

[53]:
```
# First attempt with 2 clusters
km = KMeans(n_clusters = silhouette_best_k,
            init = 'k-means++',
            n_init = 10,
            max_iter = 300,
            tol = 1e-04,
            random_state = random_state)

y_km = km.fit_predict(X)
plot_clusters(X.to_numpy(), y_km, dim=(focus[0],focus[1]), points = km.
 ↪cluster_centers_)
```



[54]:
```
# Second attempt with 3 clusters
elbow_best_k = 3

km = KMeans(n_clusters = elbow_best_k,
            init = 'k-means++',
            n_init = 10,
            max_iter = 300,
            tol = 1e-04,
            random_state = random_state)

y_km = km.fit_predict(X)
plot_clusters(X.to_numpy(), y_km, dim=(focus[0],focus[1]), points = km.
 ↪cluster_centers_)
```



The clustering scheme with three clusters seems to indeed be the better one of the two

[64]:
```
best_k = 3
```

1.1.4 4. fit the clustering scheme to y_km, then produce the confusion matrix comparing y and y_km with sklearn.metrics.confusion_matrix, the resulting confusion matrix must be "sorted" using the function max_diag provided below, producing the final confusion matrix cm_km (5pt)

Let's start by fitting the clustering scheme to y_km and producing the confusion matrix

[65]:
```
km = KMeans(n_clusters = best_k,
            init = 'k-means++',
            n_init = 10,
            max_iter = 300,
            tol = 1e-04,
            random_state = random_state)
```

```
y_km = km.fit_predict(X)
km.fit(X, y = y_km)
```

[65]:
```
KMeans(n_clusters=3, random_state=42)
```

[72]:
```
cm = confusion_matrix(y, y_km)
print(cm)
```

```
[[ 1 60  9]
 [60 10  0]
 [ 0  2 68]]
```

We now have a look at the function max_diag

[58]:
```
help(max_diag)
```

```
Help on function max_diag in module max_diag:

max_diag(sq_arr)
    Given a square matrix produces another squared matrix with the same
contents,
    but the columns are re-orered in order to have the highest values in the
main diagonal
    Parameter: sq_arr - a squared matrix
    Example:
    In [1]: import numpy as np
            max_diag(np.array([[1,10],[20,2]]))
    Out[1]: array([[10.,  1.],
                   [ 2., 20.]])
    This function is useful to reorder a confusion matrix when the two label
vectors
    have different codings
```

We can now print the sorted confusion matrix

[71]:
```
cm_km = max_diag(cm)
print(cm_km)
```

```
[[60.  1.  9.]
 [10. 60.  0.]
 [ 2.  0. 68.]]
```

1.1.5 5. in a comment explain why function max_diag is useful (2pt)

As the help function says, **the function is useful to reorder a confusion matrix when the two label vectors have different codings**

1.1.6 6. compute the accuracy a_km of y_km versus y as the ratio the sum of the main diagonal of cm_km and the number of samples in X (2pt)

```
[74]: a_km = np.diagonal(cm_km).sum() / X.shape[0]
      print(f"The accuracy was {a_km * 100:.2f}%")
```

```
The accuracy was 89.52%
```

1.1.7 7. rescale X using sklearn.preprocessing.MinMaxScaler, producing the scaled dataset X_mms (3pt)

```
[77]: scaler = MinMaxScaler()
      X_mms = scaler.fit_transform(X)
      print(X_mms)
```

```
[[0.44098206 0.50206612 0.5707804  … 0.48610121 0.18930164 0.34515017]
 [0.40509915 0.44628099 0.66243194 … 0.50106914 0.03288302 0.21516494]
 [0.34938621 0.34710744 0.87931034 … 0.50392017 0.25145302 0.1506647 ]
 …
 [0.24645892 0.25826446 0.7277677  … 0.42908054 0.98166664 0.26440177]
 [0.11803588 0.16528926 0.39927405 … 0.14682823 0.36834441 0.25849335]
 [0.16147309 0.19214876 0.54718693 … 0.24518888 0.63346292 0.26784835]]
```

1.1.8 8. repeat point 3 and 5 above, fitting X_mms to y_km_mms and producing the confusion matrix cm_km_mms reordered with max_diag and the accuracy a_km_mms as above (3pt)

```
[78]: y_km_mms = km.fit_predict(X_mms)
      km.fit(X_mms, y = y_km_mms)

      cm_km_mms = max_diag(confusion_matrix(y, y_km_mms))
      a_km_mms = np.diagonal(cm_km).sum() / X.shape[0]
      print(f"The accuracy was {a_km_mms * 100:.2f}%")
```

```
The accuracy was 89.52%
```