notebook-5

October 5, 2024

1 Assignment 5: Clustering

1.1 Problem 1: Preprocessing the dataset

Read the dataset:

[73]:
```
import itertools

import numpy as np
import pandas as pd
from sklearn.preprocessing import StandardScaler

column_labels = [
        'Area',
        'Perimeter',
        'Compactness',
        'Length of kernel',
        'Width of kernel',
        'Asymmetry coefficient',
        'Length of the kernel groove',
        'Numerical class label',
]
df = pd.read_csv(
        'data/seeds.tsv',
        sep='\t',
        header=None,
        names=column_labels
)
df.head()
```

[73]:
```
    Area  Perimeter  Compactness  Length of kernel  Width of kernel  \
0  15.26      14.84       0.8710             5.763            3.312
1  14.88      14.57       0.8811             5.554            3.333
2  14.29      14.09       0.9050             5.291            3.337
3  13.84      13.94       0.8955             5.324            3.379
4  16.14      14.99       0.9034             5.658            3.562

   Asymmetry coefficient  Length of the kernel groove  Numerical class label
```

0	2.221	5.220	1
1	1.018	4.956	1
2	2.699	4.825	1
3	2.259	4.805	1
4	1.355	5.175	1

Scale the dataset using a normalizer:

[74]:
```
scaler = StandardScaler()

scaled_data = pd.DataFrame(
        scaler.fit_transform(
                df.drop(columns="Numerical class label")
        ),
        columns=column_labels[:-1]
)
scaled_df = pd.concat(
        [scaled_data, df["Numerical class label"]],
        axis=1
)
scaled_df.head()
```

[74]:

	Area	Perimeter	Compactness	Length of kernel	Width of kernel	\
0	0.142098	0.215462	0.000061	0.304218	0.141702	
1	0.011188	0.008224	0.428515	-0.168625	0.197432	
2	-0.192067	-0.360201	1.442383	-0.763637	0.208048	
3	-0.347091	-0.475333	1.039381	-0.688978	0.319508	
4	0.445257	0.330595	1.374509	0.066666	0.805159	

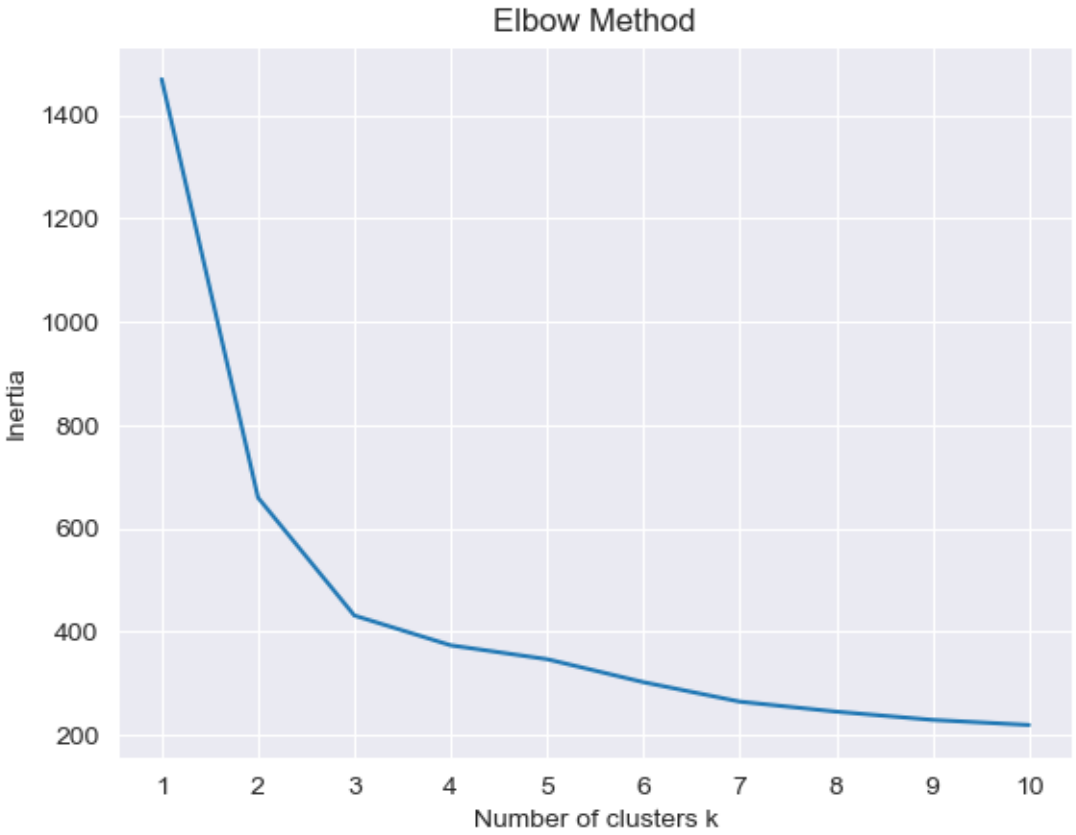
	Asymmetry coefficient	Length of the kernel groove	Numerical class label
0	-0.986152	-0.383577	1
1	-1.788166	-0.922013	1
2	-0.667479	-1.189192	1
3	-0.960818	-1.229983	1
4	-1.563495	-0.475356	1

1.2 Problem 2: Determining the appropriate number of clusters

Iterating over a range of cluster numbers, determine the optimal number of clusters using the elbow method:

[75]:
```
from sklearn.cluster import KMeans
import matplotlib.pyplot as plt

k = range(1, 11)
inertia = []
for i in k:
        kmeans = KMeans(
```

```
                n_clusters=i,
                random_state=0,
                n_init="auto"
        ).fit(scaled_data)
        inertia.append(kmeans.inertia_)

plt.plot(k, inertia)
plt.title('Elbow Method')
plt.xlabel('Number of clusters k')
plt.ylabel('Inertia')
plt.xticks(k)
plt.savefig("figures/elbow_method.png")
```

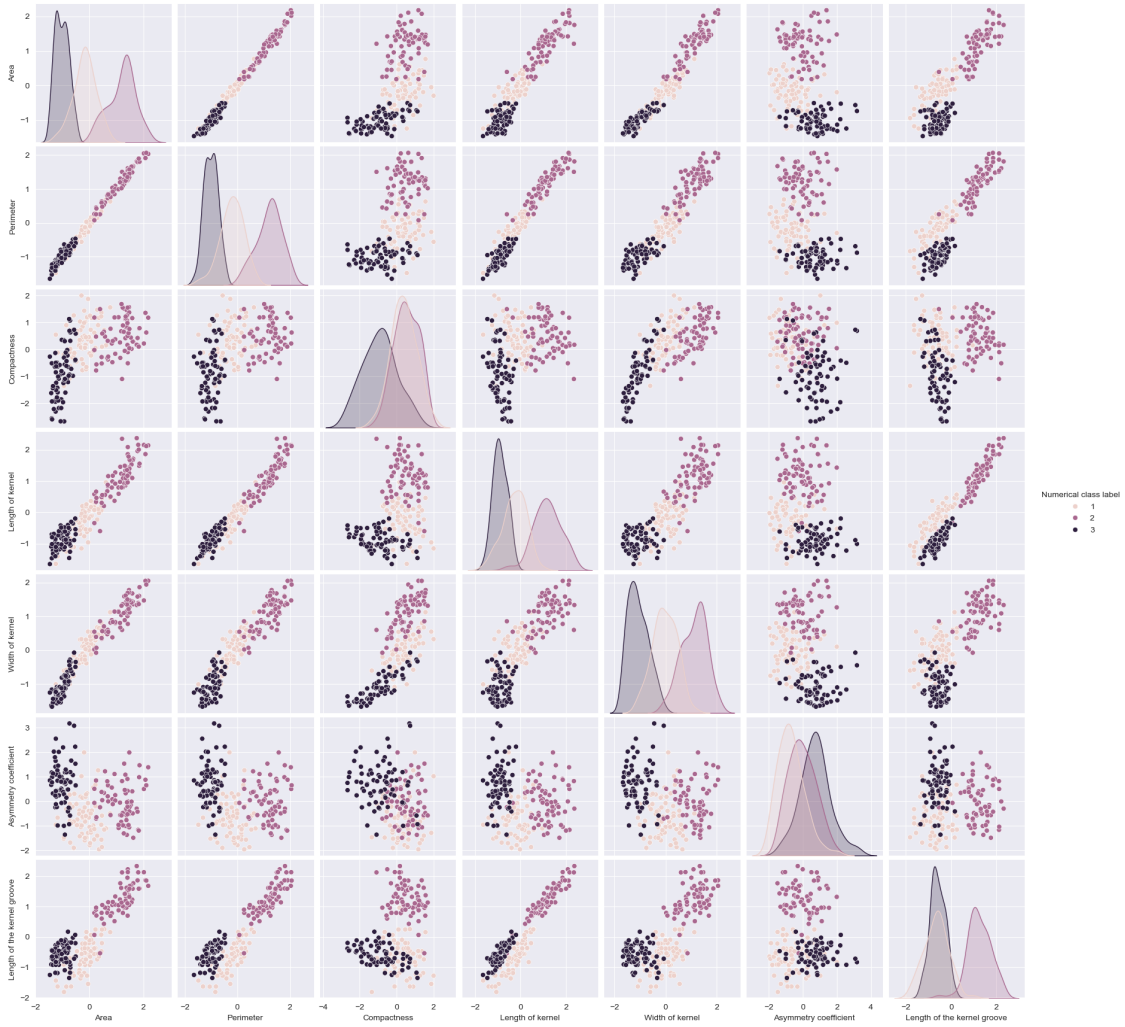


We can see that the optimal number of clusters is 3.

1.3 Problem 3: Visualizing the classes

Scatterplot the pairs of features, coloring the points according to the cluster they belong to:

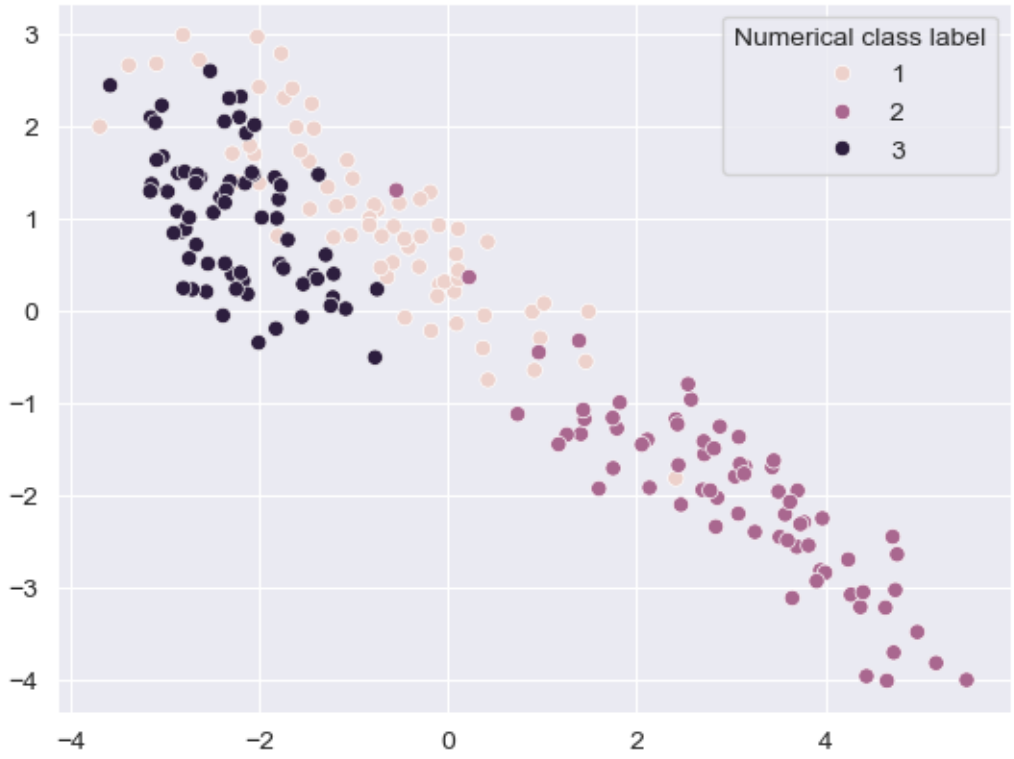
[76]:
```
import seaborn as sns

sns.pairplot(
        scaled_df,
        hue="Numerical class label"
)
plt.savefig("figures/features_pairplot.png")
```



Scatterplot the Gaussian random projections of the dataset, coloring the points according to the cluster they belong to:

[77]:
```
from sklearn.random_projection import \
        GaussianRandomProjection

embedding = GaussianRandomProjection(
        random_state=42, n_components=2
```

```
).fit_transform(scaled_data)

sns.scatterplot(
        x=embedding[:, 0],
        y=embedding[:, 1],
        hue=df["Numerical class label"]
)
plt.savefig(
        "figures/gaussian_random_projection.png")
```

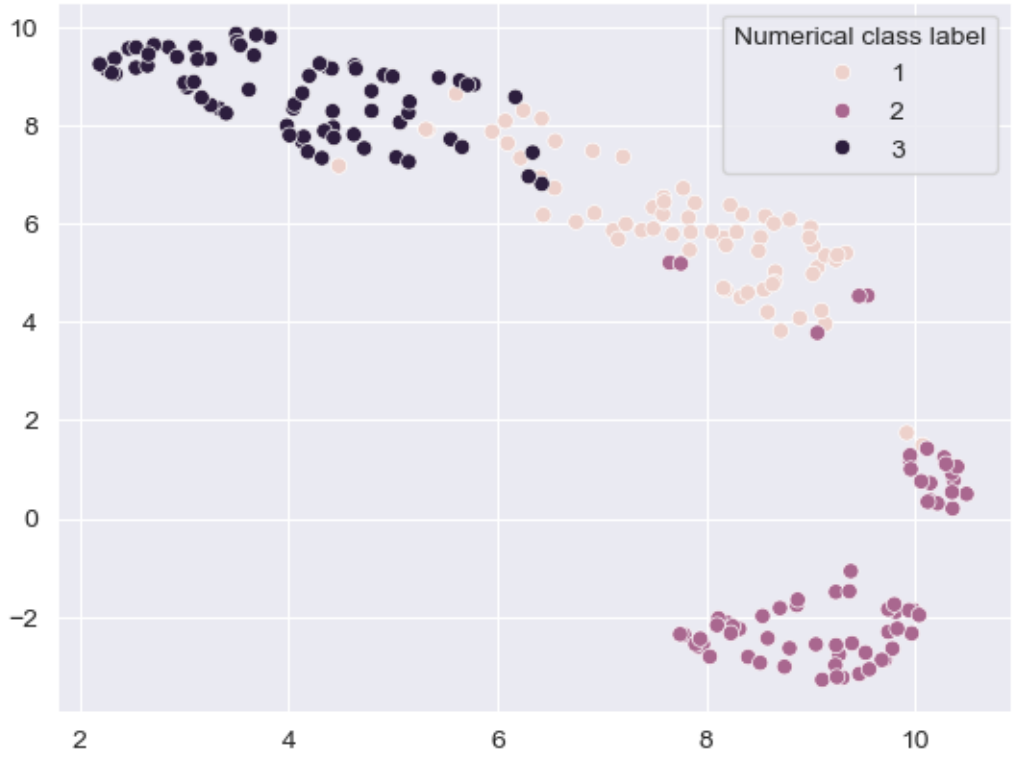


Scatterplot the UMAP projections of the dataset, coloring the points according to the cluster they belong to:

[78]:
```
from umap import UMAP

embedding = UMAP(
        random_state=42, n_components=2
).fit_transform(scaled_data)

sns.scatterplot(
        x=embedding[:, 0],
        y=embedding[:, 1],
```

```
        hue=df["Numerical class label"]
)
plt.savefig("figures/umap_projection.png")
```

```
/Users/giacomo/.miniforge/envs/ds/lib/python3.11/site-
packages/umap/umap_.py:1945: UserWarning: n_jobs value 1 overridden to 1 by
setting random_state. Use no seed for parallelism.
  warn(f"n_jobs value {self.n_jobs} overridden to 1 by setting random_state. Use
no seed for parallelism.")
```



1.4 Problem 4: Evaluating clustering

Cluster the dataset using the optimal number of clusters:

[79]:
```
k = scaled_df["Numerical class label"].nunique()

kmeans = KMeans(
        n_clusters=k,
        random_state=0,
        n_init="auto"
).fit(scaled_data)
```

Compute the rand index:

[80]:
```
from sklearn.metrics import rand_score, \
        accuracy_score

rand_index = rand_score(
        scaled_df["Numerical class label"],
        kmeans.labels_
)
print(f"Rand index: {rand_index}")
```

```
Rand index: 0.8997038049669629
```

Compute the accuracy by finding the maximum accuracy on all the cluster labels permutations:

[81]:
```
def compute_accuracy(y_true, y_pred):
        max_accuracy = float('-inf')
        combinations = list(
                itertools.permutations(range(0, k))
        )
        for combination in combinations:
                transformed_labels = np.array(
                        [combination[label] for label in y_pred]
                )
                max_accuracy = max(
                        max_accuracy,
                        accuracy_score(y_true, transformed_labels)
                )
        return max_accuracy


accuracy = compute_accuracy(
        scaled_df["Numerical class label"],
        kmeans.labels_
)
print(f"Accuracy: {accuracy}")
```

```
Accuracy: 0.6047619047619047
```

1.4.1 Problem 5: Agglomerative clustering

Hierarchically cluster the dataset with all the linkage methods:

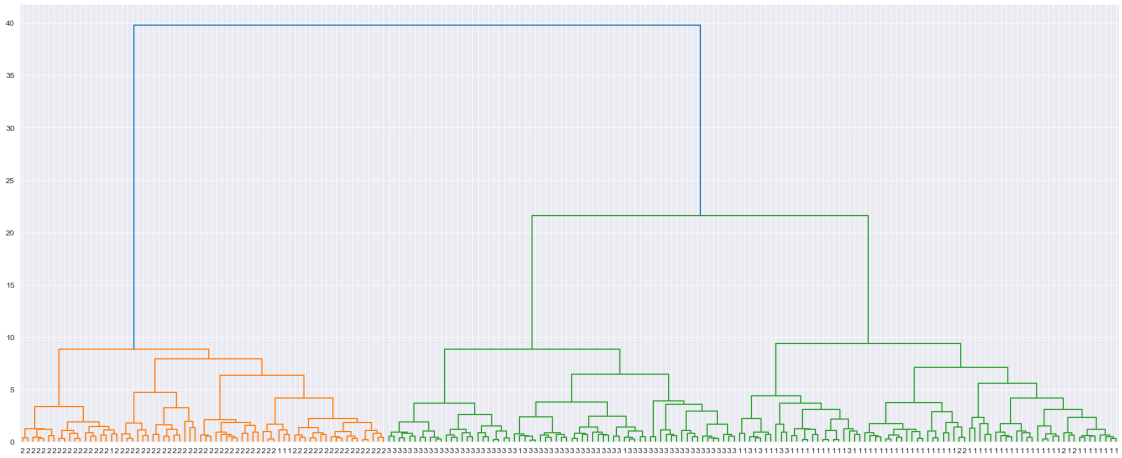
[82]:
```
from sklearn.cluster import \
        AgglomerativeClustering

best_method = None
best_accuracy = float('-inf')
linkage_methods = [
        "ward",
        "complete",
```

```
        "average",
        "single"
]
for method in linkage_methods:
        cluster = AgglomerativeClustering(
                n_clusters=k,
                linkage=method
        ).fit(scaled_data)
        accuracy = compute_accuracy(
                scaled_df["Numerical class label"],
                cluster.labels_
        )

        if accuracy > best_accuracy:
                best_accuracy = accuracy
                best_method = method

        print(
                f"Accuracy for linkage method {method}: {accuracy}"
        )

print(f"Best linkage method: {best_method}")
```

```
Accuracy for linkage method ward: 0.6190476190476191
Accuracy for linkage method complete: 0.5428571428571428
Accuracy for linkage method average: 0.5857142857142857
Accuracy for linkage method single: 0.3380952380952381
Best linkage method: ward
```

Plot the dendrogram for the best linkage method:

[83]:
```
from scipy.cluster.hierarchy import dendrogram, \
        linkage

plt.figure(figsize=(25, 10))
dendrogram(
        linkage(scaled_data, method=best_method),
        labels=scaled_df[
                "Numerical class label"
        ].values,
        leaf_font_size=10,
        leaf_rotation=0
)
plt.savefig("figures/dendrogram.png")
```


40
35
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