notebook-5

October 7, 2024

1 Assignment 5: Clustering

1.1 Problem 1: Preprocessing the dataset

Read the dataset:

[45]:
```
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()
```

[45]:
```
    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:

[46]:
```
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()
```

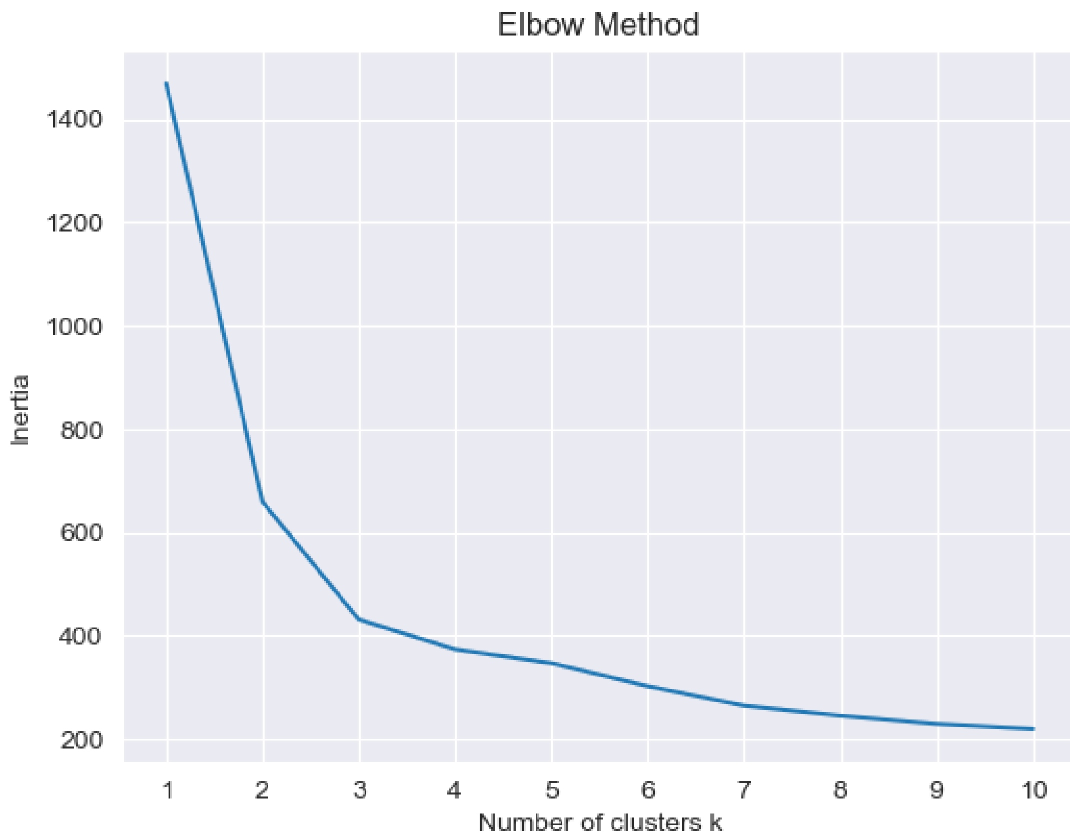
[46]:
```
       Area  Perimeter  Compactness  Length of kernel  Width of kernel  \
0  0.142098   0.215462     0.000061          0.304218         0.141702
1  0.011188   0.008224     0.428515         -0.168625         0.197432
2 -0.192067  -0.360201     1.442383         -0.763637         0.208048
3 -0.347091  -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:

[47]:
```
from sklearn.cluster import KMeans
import matplotlib.pyplot as plt

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

```python
                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")
```

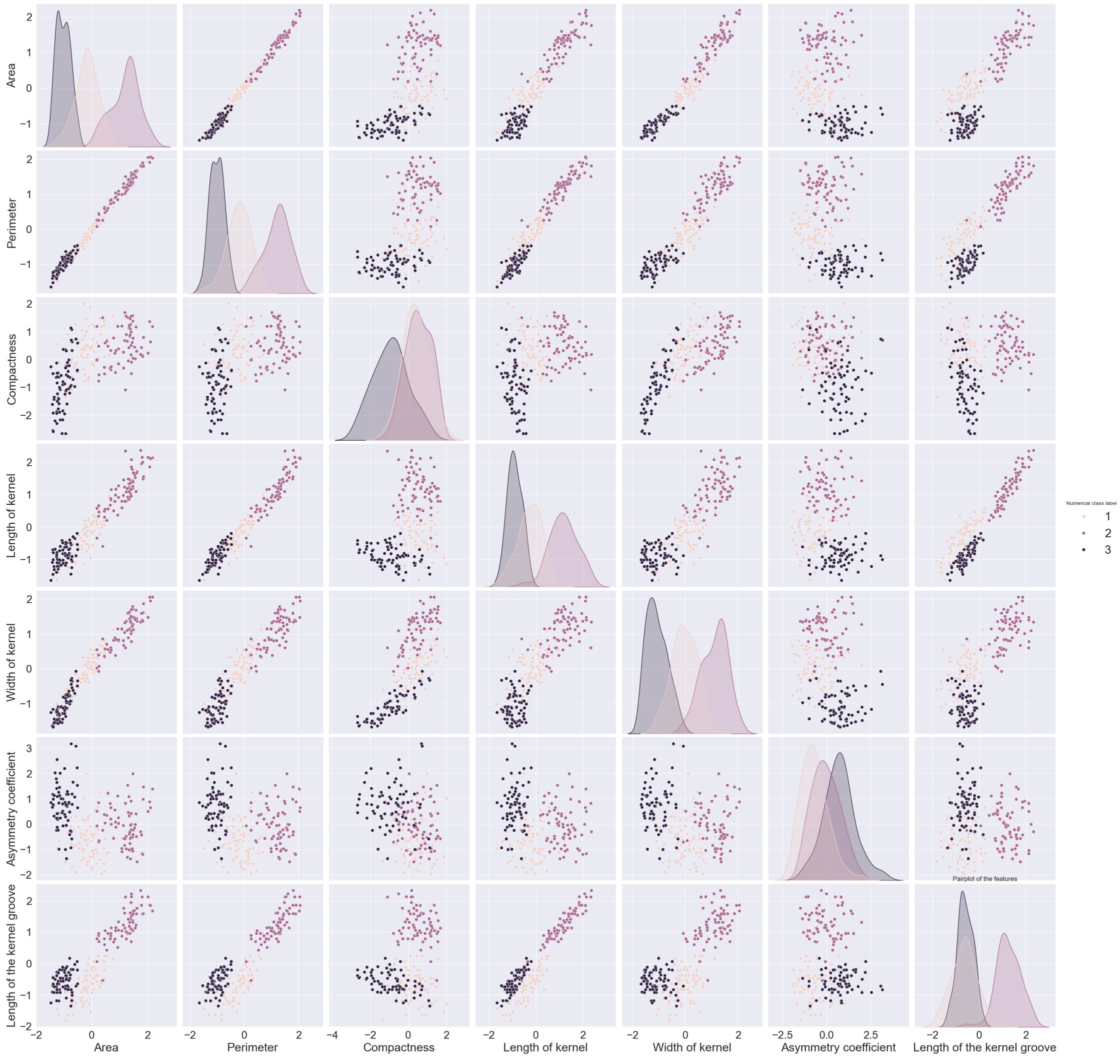


We can see that the optimal number of clusters is 3.

1.3 Problem 3: Visualizing the classes

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

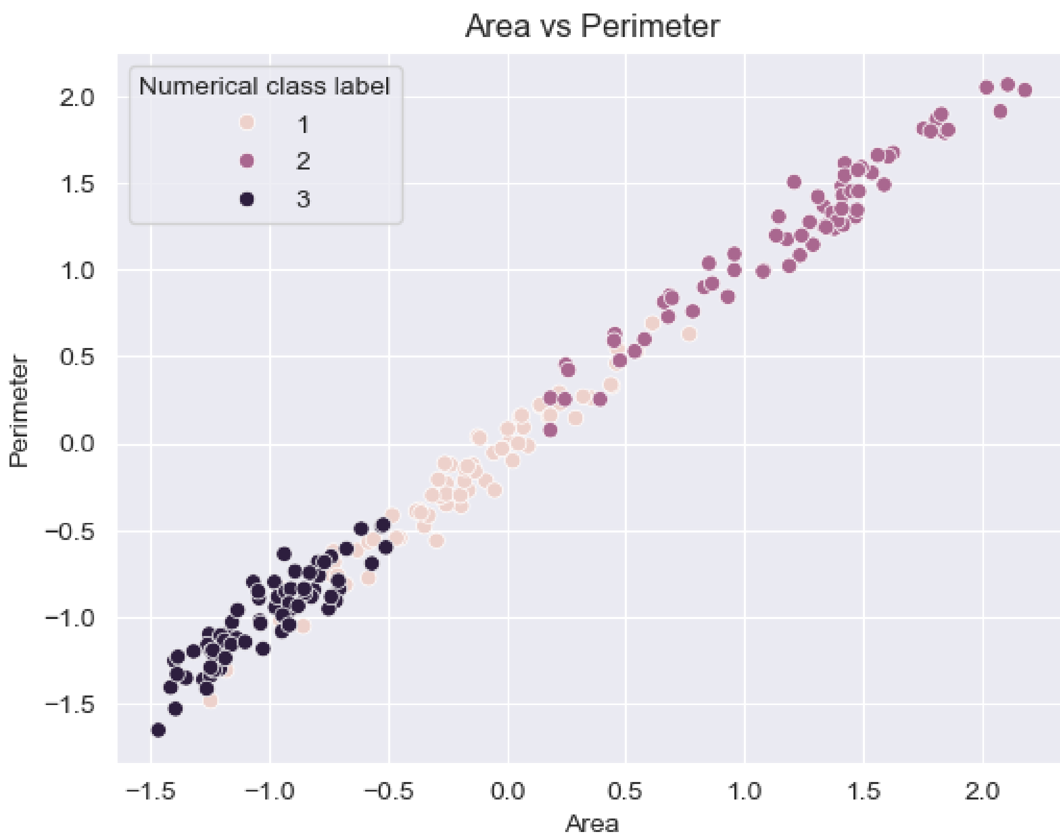
```
[76]: import seaborn as sns

sns.pairplot(
        scaled_df,
        hue="Numerical class label",
        height=4
)
plt.title("Pairplot of the features")
plt.savefig("figures/features_pairplot.png")
```



Scatterplot of one particular pair of features:

```
[49]: sns.scatterplot(
        x="Area",
        y="Perimeter",
```

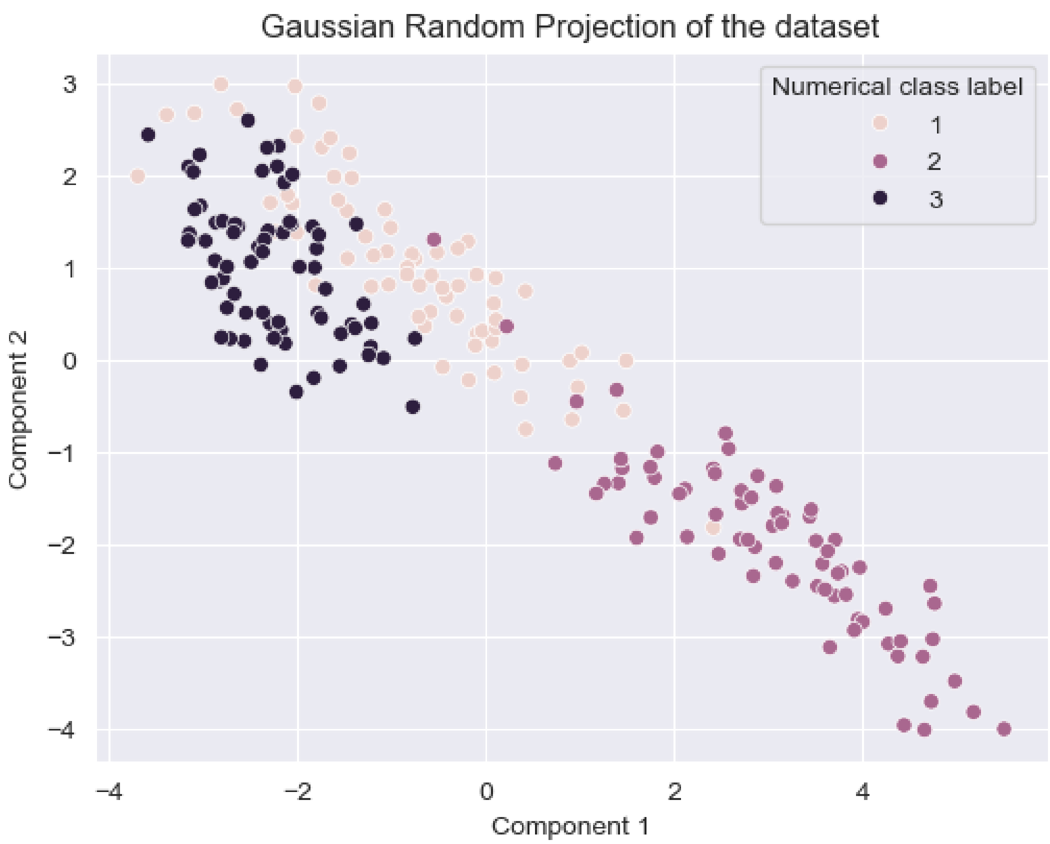
```
        data=scaled_df,
        hue="Numerical class label",
)
plt.title("Area vs Perimeter")
plt.savefig("figures/area_perimeter_scatterplot.png")
```



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

[50]:
```
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.title("Gaussian Random Projection of the dataset")
plt.xlabel("Component 1")
plt.ylabel("Component 2")
plt.savefig(
        "figures/gaussian_random_projection.png"
)
```

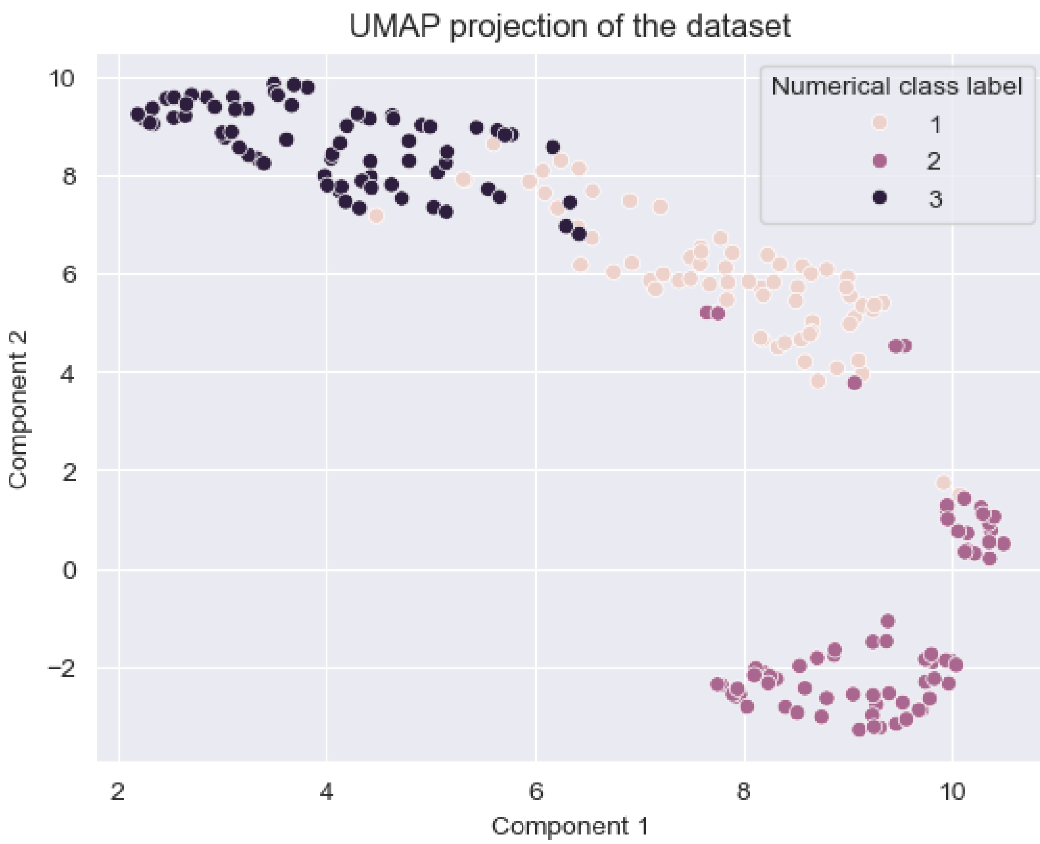


Scatterplot the UMAP projections of the dataset, coloring the points according to the cluster they belong to:

[51]:
```
from umap import UMAP

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

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

```python
        hue=df["Numerical class label"]
)
plt.title("UMAP projection of the dataset")
plt.xlabel("Component 1")
plt.ylabel("Component 2")
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:

[52]:
```python
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:

[53]:
```
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:.3f}")
```

```
Rand index: 0.900
```

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

[54]:
```
def compute_accuracy(y_true, y_pred):
        max_accuracy = float('-inf')
        combinations = list(
                itertools.permutations(range(1, k + 1))
        )
        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:.3f}")
```

```
Accuracy: 0.919
```

1.4.1 Problem 5: Agglomerative clustering

Hierarchically cluster the dataset with all the linkage methods:

[55]:
```
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:.3f}"
        )

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

```
Accuracy for linkage method ward: 0.929
Accuracy for linkage method complete: 0.876
Accuracy for linkage method average: 0.881
Accuracy for linkage method single: 0.348
Best linkage method: ward
```

Plot the dendrogram for the best linkage method:

[56]:
```
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.title("Dendrogram of the ward hierarchical clustering")
plt.savefig("figures/dendrogram.png")
```