workshop04tasks

March 21, 2021

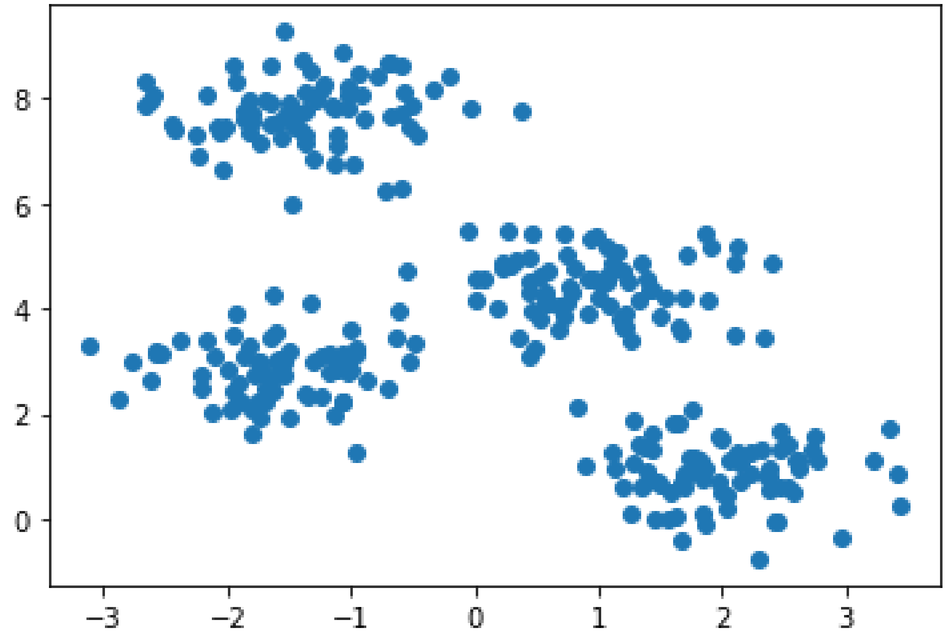
1 Welcome to Week 4: 1. Clustering

- ### 1.1 Task to be discussed in this Workshop are:
- ### 1.2 Demo for K-means clustering
- ### 1.3 Task 1.1 Perform K-means on a real dataset
- ### 1.4 Task 1.2 (Optional) Try PCA for dimensionality reduction.
- ### 1.5 Task 1.3: Perform agglomerative clustering on this data set

[1]:
```
import math
import numpy as np
import pandas as pd
from matplotlib import pyplot as plt

#from sklearn.datasets.samples_generator import make_blobs
from sklearn.datasets import make_blobs

from sklearn.cluster import KMeans
from sklearn.metrics import davies_bouldin_score, adjusted_rand_score

from sklearn.metrics import pairwise_distances
from scipy.cluster.hierarchy import linkage, dendrogram, cut_tree
from scipy.spatial.distance import pdist
```

[ ]:
```
```

[2]:
```
# Generate an exmaple 2-dimensional datasets containing 4 clusters for a demo
X, y = make_blobs(n_samples=300, centers=4, cluster_std=0.60, random_state=0)

# Visualize the data
plt.scatter(X[:,0], X[:,1])
plt.show()
```

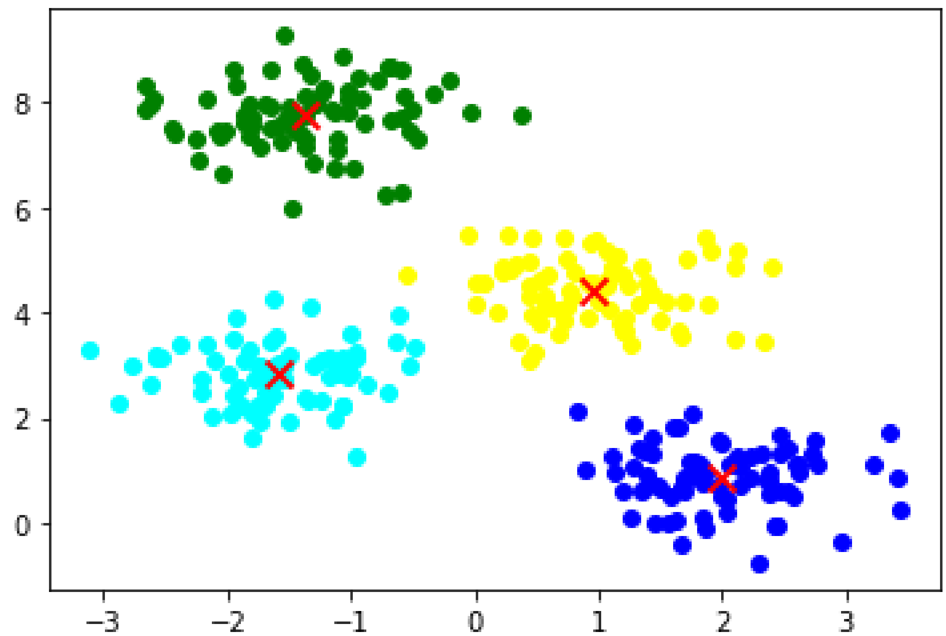


[3]:
```
# Create a K-means clustering model with k=4, and k-means++ as the␣
↪intialization strategy
kmeans = KMeans(n_clusters=4, init='k-means++', max_iter=300, random_state=0)

# Perform clustering by fitting the model with the data
kmeans.fit(X)

# We can explore the parameters learned from the data.
# What's the cluster center?
print('\n Cluter center: \n', kmeans.cluster_centers_)

# What's is overall distorion (inertia)?
print('\n Overall distortion: \n', kmeans.inertia_)
# Average standard distortion
print('\n Average distortion: \n', math.sqrt(kmeans.inertia_/X.shape[0]))
```

```
Cluter center:
[[ 1.98258281  0.86771314]
```

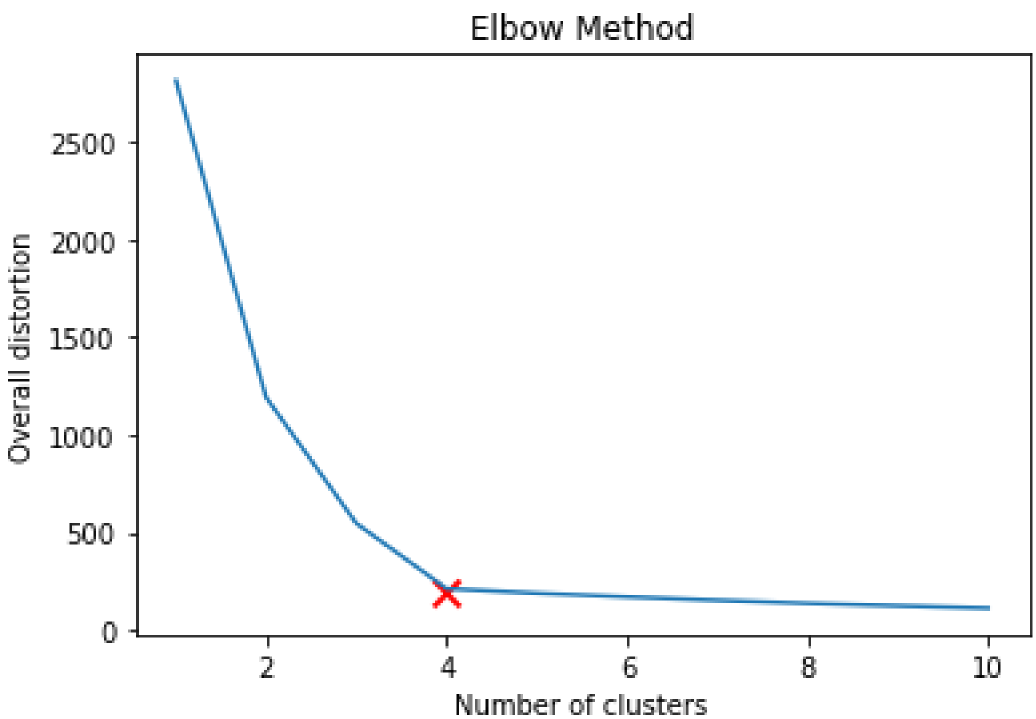
```
[ 0.94973532  4.41906906]
[-1.37324398  7.75368871]
[-1.58438467  2.83081263]]

Overall distortion:
212.00599621083472

Average distortion:
0.8406465690384489
```

[4]:
```python
# Predict the cluster for each data instance. This step can be combined with
↪the last one by using kmeans.fit_predict(X)
y_pred = kmeans.predict(X)

# Visualize the cluster centers to explore how the clustering result looks like
colors = ['blue', 'yellow', 'green', 'cyan']
for i, color in enumerate(colors):
    plt.scatter(X[y_pred == i, 0], X[y_pred == i, 1], c=color)

plt.scatter(kmeans.cluster_centers_[:, 0], kmeans.cluster_centers_[:, 1],
↪marker='x', lw=2, c='red', s=100)
plt.show()
```



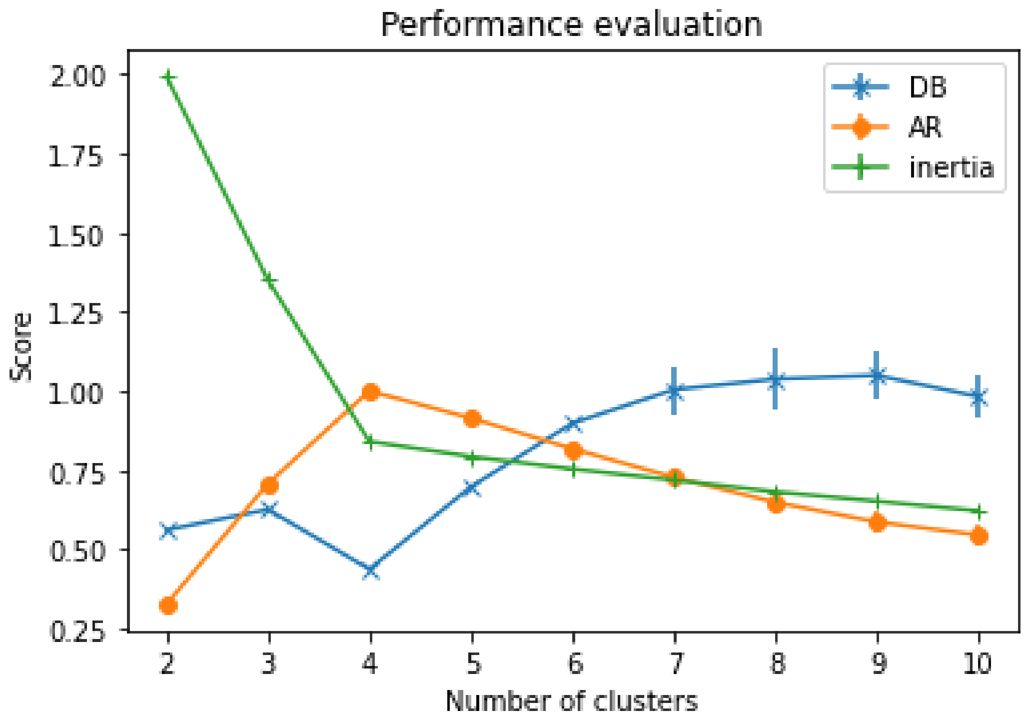
[5]:
```python
# How about other k values? Which k value should we choose to get the optimal
↪clustering? Let's vary k from 1 to 10 and see how the distortion changes.
distortions = []
```

```
for i in range(1, 11):
    kmeans = KMeans(n_clusters=i, init='k-means++', max_iter=300,␣
 ↪random_state=0)
    kmeans.fit(X)
    distortions.append(kmeans.inertia_)

# Plot the relationship between the distortion and k. Then, we can have the␣
 ↪Elbow method to help identify a good value for k.
plt.plot(range(1, 11), distortions)
plt.title('Elbow Method')
plt.xlabel('Number of clusters')
plt.ylabel('Overall distortion')
plt.scatter(4, distortions[4], marker='x', lw=2, c='red', s=100)
plt.show()

# It can be seen that k=4 is reasonably good
```

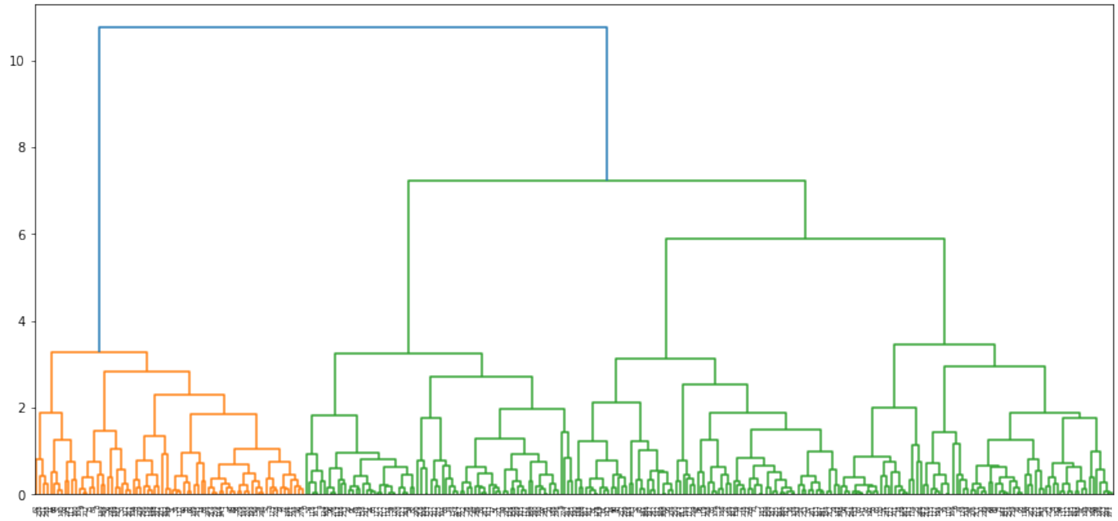


[6]:
```
# Let's evaluate the learned model with other quality criteria

# Internal evaluation, davies bouldin score (the lower, the better)
db_scores = []
db_scores_std = []
```

```python
# External evaluation, adjusted rand index (the higher, the better)
ar_scores = []
ar_scores_std = []

# Inertia (average standardized)
inertia = []
inertia_std = []

for i in range(2, 11):
    # Multiple runs for stable indicators
    db_scores_tmp = []
    ar_scores_tmp = []
    inertias_tmp = []

    n_iteration=5
    for j in range(0, n_iteration):
        # Note: 'random_state' parameter should be set as default or None
        #kmeans = KMeans(n_clusters=i, init='k-means++', max_iter=300,␣
 ↪n_init=10)
        kmeans = KMeans(n_clusters=i, init='random', max_iter=300)
        kmeans.fit(X)
        labels = kmeans.labels_
        db_scores_tmp.append(davies_bouldin_score(X, labels))
        ar_scores_tmp.append(adjusted_rand_score(labels, y_pred))
        inertias_tmp.append(math.sqrt(kmeans.inertia_/X.shape[0]))

    db_scores.append(np.mean(db_scores_tmp))
    db_scores_std.append(np.std(db_scores_tmp))
    ar_scores.append(np.mean(ar_scores_tmp))
    ar_scores_std.append(np.std(ar_scores_tmp))
    inertia.append(np.mean(inertias_tmp))
    inertia_std.append(np.std(inertias_tmp))

# Plot the relationship between the davies bouldin score and k
plt.errorbar(range(2, 11), db_scores, yerr=db_scores_std, marker='x',␣
 ↪label='DB')
plt.errorbar(range(2, 11), ar_scores, yerr=ar_scores_std, marker='o',␣
 ↪label='AR')
plt.errorbar(range(2, 11), inertia, yerr=inertia_std, marker='+',␣
 ↪label='inertia')
plt.title('Performance evaluation')
plt.xlabel('Number of clusters')
plt.ylabel('Score')
plt.legend(loc='best')
plt.show()
```



[7]:
```
# Try agglomerative clustering on this dataset, and visualise the hierarchy.

dist = pdist(X, 'euclidean')
linkage_matrix = linkage(dist, method = 'complete')

plt.figure(figsize=(15,7))
dendrogram(linkage_matrix)
plt.show()

# It can be seen that the clustering structure contains four main clusters,␣
 ↪complying with the data.
```



1.6 Task Clustering on the MNIST data set

[8]:
```
# Now, let's work on a real dataset. See detailed information for the dataset:␣
↪https://en.wikipedia.org/wiki/MNIST_database.

#Load the data. Orignal data set has been processed (downsampled) to facilitate␣
↪your data analysis
raw_data = pd.read_csv("/home/dalia/Master of Information Technology in␣
↪Cybersecurity/Session 3/COMP8325 Artificial Intelligence/week_4/Week 4␣
↪Workshop -20210321/data/mnist-0.1.csv")
print('\n data size: (%d, %d)\n' % raw_data.shape)

# Specifying features and target attribute
X = raw_data.drop(['Label'], axis='columns')

# Pre-processing with standardization
from sklearn import preprocessing
scaler = preprocessing.MinMaxScaler()
X_data = X.values
X_scaled = scaler.fit_transform(X_data)
X = X_scaled

y = raw_data['Label'].values
```

```
data size: (5243, 785)
```

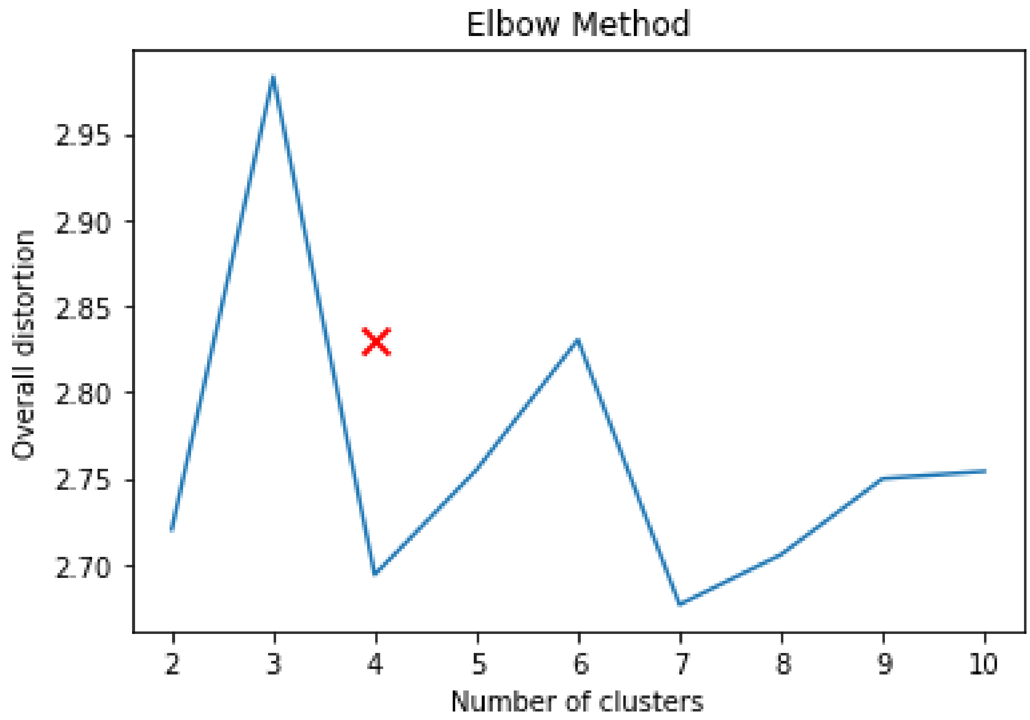
[9]:
```
# K-means clustering model
model = KMeans(n_clusters=2)
model.fit(X)
print('\n cluster means: \n', model.cluster_centers_)
print('\n inertia: %f'% model.inertia_)
print('\n average inertia: %f\n' % math.sqrt(model.inertia_/y.size))
```

```
cluster means:
[[0. 0. 0. … 0. 0. 0.]
[0. 0. 0. … 0. 0. 0.]]

inertia: 214710.126187

average inertia: 6.399357
```

[10]:
```
# Evaluation (internal)
labels = model.labels_
scores=davies_bouldin_score(X, labels)
print('\n davies_bouldin_score: %f\n' % scores)
```

```
davies_bouldin_score: 2.722454
```

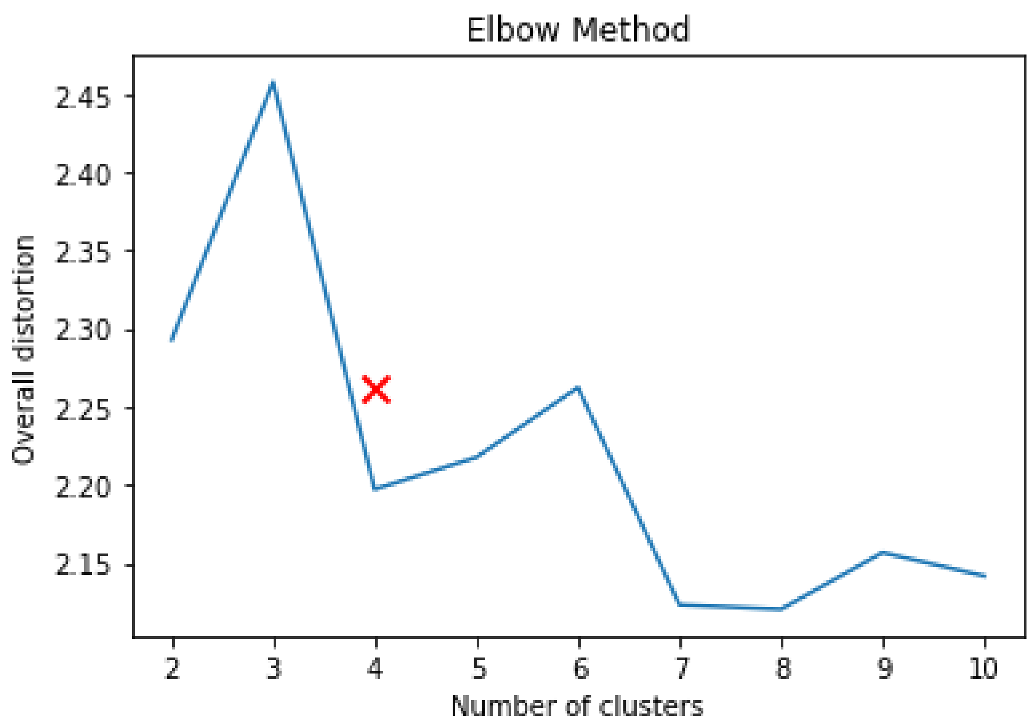
[11]:
```
# Task 1.1 Try k from 2 to 10 to determine which is the best value w.r.t.␣
↪davies_bouldin_score, plot the relationship between the davies_bouldin_score␣
↪and k

# Compute davies bouldin score

distortions = []
for i in range(2, 11):
    kmeans = KMeans(n_clusters=i)
    kmeans.fit(X)
    labels = kmeans.labels_
    distortions.append(davies_bouldin_score(X, labels))

# Plot the relationship between the distortion and k

plt.plot(range(2, 11), distortions)
plt.title('Elbow Method')
plt.xlabel('Number of clusters')
plt.ylabel('Overall distortion')
plt.scatter(4, distortions[4], marker='x', lw=2, c='red', s=100)
plt.show()
```



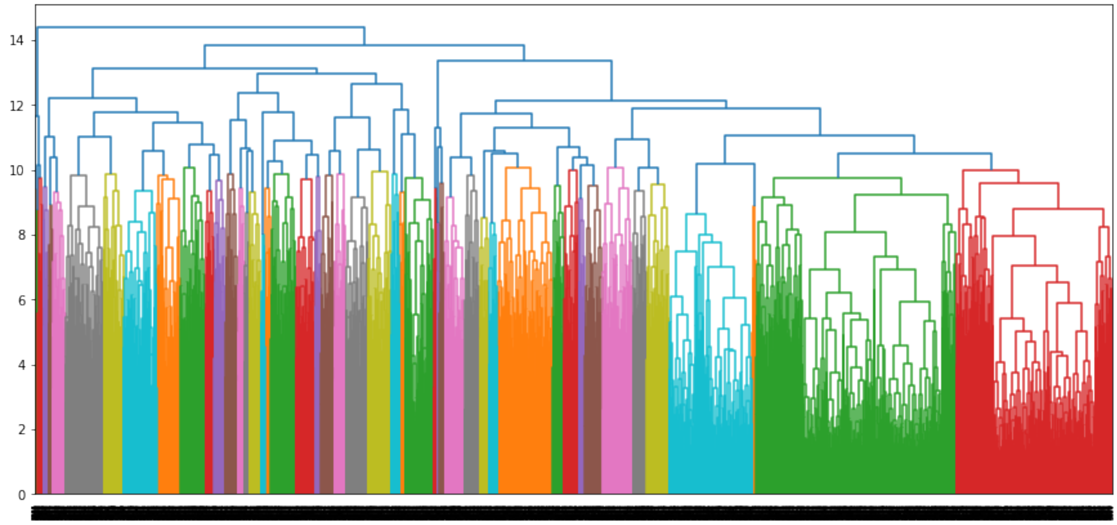
[12]:
```
# Task 1.2 (Optional) Given that this is a high dimensional data. It might be␣
↪good to reduce the dimension first.
# PCA can be used for this purpose. Try some reduced dimensionality, e.g., math.
↪sqrt(X.shape[1]). Try this for different k values with plotting.

# dimenion redcution
from sklearn.decomposition import PCA
pca = PCA(n_components=int(math.sqrt(X.shape[1])))

# Compute davies bouldin score

X_reduced = pca.fit(X).transform(X)
X = X_reduced
print('\n After dimension reduction: (%d, %d)\n' % X.shape)

distortions = []
for i in range(2, 11):
    kmeans = KMeans(n_clusters=i, init='k-means++', max_iter=300, n_init=10,␣
↪random_state=0)
    kmeans.fit(X)
    labels = kmeans.labels_
    distortions.append(davies_bouldin_score(X, labels))
```

```
# Plot the relationship between the score and k

plt.plot(range(2, 11), distortions)
plt.title('Elbow Method')
plt.xlabel('Number of clusters')
plt.ylabel('Overall distortion')
plt.scatter(4, distortions[4], marker='x', lw=2, c='red', s=100)
plt.show()
```

```
After dimension reduction: (5243, 28)
```



[15]:
```
# Task 1.3 Try to perform agglomerative clustering on the dataset, and␣
↪visualise the hierarchy.



dist = pdist(X, 'euclidean')
linkage_matrix = linkage(dist, method = 'complete')

plt.figure(figsize=(15,7))
dendrogram(linkage_matrix)
plt.show()
```


14
12
10
8
6
4
2
0

[ ]: