Klion_Coding_HW2

March 3, 2022

0.1 Assignment 2: K-means and Hierarchical Clustering

[25]:
```
import numpy as np
import matplotlib.pyplot as plt
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler
from sklearn.datasets import make_circles, make_moons, make_blobs
from sklearn.cluster import KMeans
from itertools import cycle, islice
```

1 Question 1

1.1 Part A

[26]:
```
# Generate Datasets
n_samples = 100
random_state = 42

noisy_circles = make_circles(n_samples = n_samples, factor = 0.5, noise = 0.05)
noisy_moons = make_moons(n_samples = n_samples, noise = 0.05)
blobs = make_blobs(n_samples = n_samples, random_state = random_state)

# blobs with varied variances
varied = make_blobs(n_samples = n_samples, cluster_std=[1.0, 2.5, 0.5],␣
↪random_state = random_state)

# Anistropicly distributed data
X, y = make_blobs(n_samples=n_samples, random_state = random_state)
transformation = [[0.6, -0.6], [-0.4, 0.8]]
X_aniso = np.dot(X, transformation)
aniso = (X_aniso, y)
```

1.2 Part B

[27]:
```
def fit_kmeans(dataset, num_clusters):
    X, y = dataset
    #normalize dataset using standard scaler
    X = StandardScaler().fit_transform(X)
    y_pred = KMeans(n_clusters = num_clusters, init = "random").fit_predict(X)
    return y_pred
```

1.3 Part C

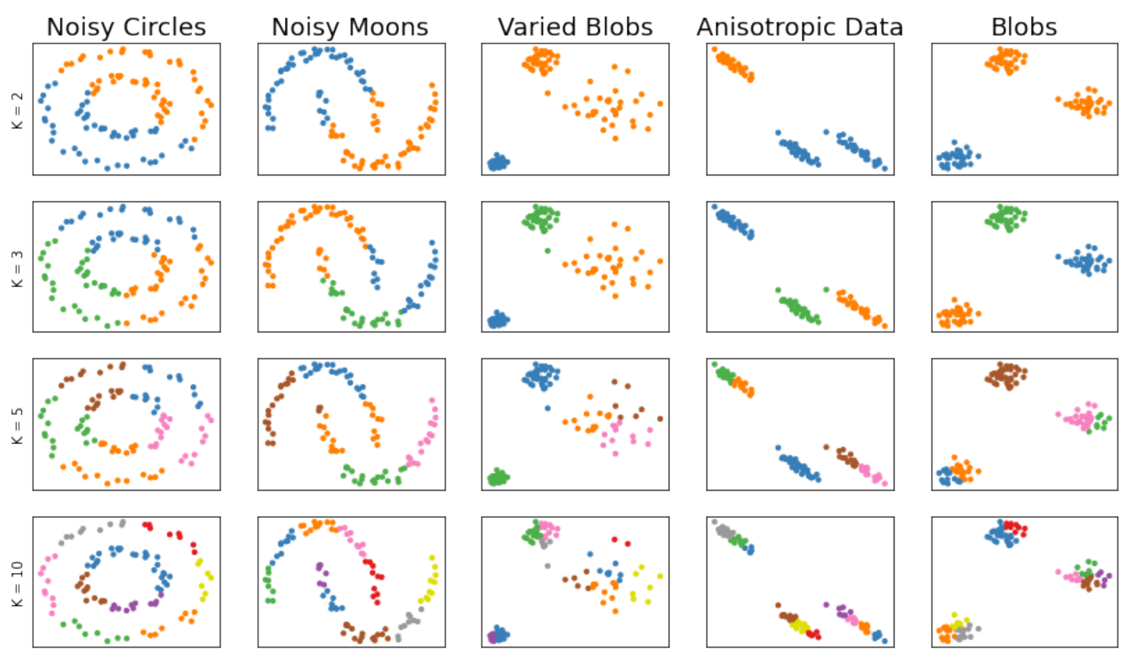
[28]:
```
clusters = [2, 3, 5, 10]
datasets = (
    ("Noisy Circles", noisy_circles),
    ("Noisy Moons", noisy_moons),
    ("Varied Blobs", varied),
    ("Anisotropic Data", aniso),
    ("Blobs", blobs),
)
plt.figure(figsize = (14, 8))
plot_num = 1

for i, k in enumerate(clusters):
    for ds_name, ds in datasets:
        X, y = ds
        y_pred = fit_kmeans(ds, k)
        #Create necessary subplot size (4 x 5)
        plt.subplot(len(clusters), len(datasets), plot_num)
        #Add titles to top row only
        if i == 0:
            plt.title(ds_name, size = 18)

        # Points colored by predicted label
        # FROM https://scikit-learn.org/stable/auto_examples/cluster/
↪plot_cluster_comparison.html
        colors = np.array(
            list(
                islice(
                    cycle(
                        [
                            "#377eb8",
                            "#ff7f00",
                            "#4daf4a",
                            "#f781bf",
                            "#a65628",
                            "#984ea3",
                            "#999999",
```

```
                            "#e41a1c",
                            "#dede00",
                        ]
                    ),
                    int(max(y_pred) + 1),
                )
            )
        )
        # add black color for outliers (if any)
        colors = np.append(colors, ["#000000"])
        plt.scatter(X[:, 0], X[:, 1], s=10, color=colors[y_pred])
        plt.xticks(())
        plt.yticks(())
        #Add y labels to
        if plot_num in [1, 6, 11, 16]:
                plt.ylabel("K = %d" % k)
        plot_num += 1

plt.show()
```



1.4 Part D

After repeating 1.C a few times, Noisy Circles and Noisy Moons are the most sensitive to the choice of initialization for the k = 2 or k = 3 cases.

2 Question 2

2.1 Part A

[5]:
```
blobs_2 = make_blobs(center_box = (-20, 20), n_samples = 20, centers = 5,␣
↪random_state = 12)
```

2.2 Part B

[6]:
```
def fit_kmeans(dataset, num_clusters):
    X, y = dataset
    #normalize dataset using standard scaler
    X = StandardScaler().fit_transform(X)
    kmeans = KMeans(n_clusters = num_clusters, init = "random").fit(X)

    #get the centroid of the cluster
    centroid = [X[kmeans.labels_ == i].mean(axis=0) for i in␣
↪range(num_clusters)]
    sse = np.zeros(num_clusters)
    for point, label in zip(X, kmeans.labels_):
        sse[label] += np.sqrt(np.sum((point - centroid[label]) ** 2))
    return sse.mean()
```

2.3 Part C

[7]:
```
sse_clusters = [1, 2, 3, 4, 5, 6, 7, 8]
sse = []
for k in sse_clusters:
    sse.append(fit_kmeans(blobs_2, k))
plt.plot(sse_clusters, sse)
plt.title("SSE vs. Number of Clusters")
plt.xlabel("Number of Clusters")
plt.ylabel("SSE")
plt.show()
```

```
C:\Users\klion\Anaconda3\lib\site-packages\sklearn\cluster\_kmeans.py:881:
UserWarning: KMeans is known to have a memory leak on Windows with MKL, when
there are less chunks than available threads. You can avoid it by setting the
environment variable OMP_NUM_THREADS=1.
  warnings.warn(
```

The optimal k is k = 2 based on the elbow method

2.4 Part D

[8]:
```
inertias = []
part2D_X, part2D_y = blobs_2
part2D_X = StandardScaler().fit_transform(part2D_X)
for k in sse_clusters:
    kmeans = KMeans(n_clusters = k, init = "random").fit(X)
    inertias.append(kmeans.inertia_)
plt.plot(sse_clusters, inertias)
plt.title("Inertia vs. Number of Clusters")
plt.xlabel("Number of Clusters")
plt.ylabel("Inertia")
plt.show()
```

```
C:\Users\klion\Anaconda3\lib\site-packages\sklearn\cluster\_kmeans.py:881:
UserWarning: KMeans is known to have a memory leak on Windows with MKL, when
there are less chunks than available threads. You can avoid it by setting the
environment variable OMP_NUM_THREADS=1.
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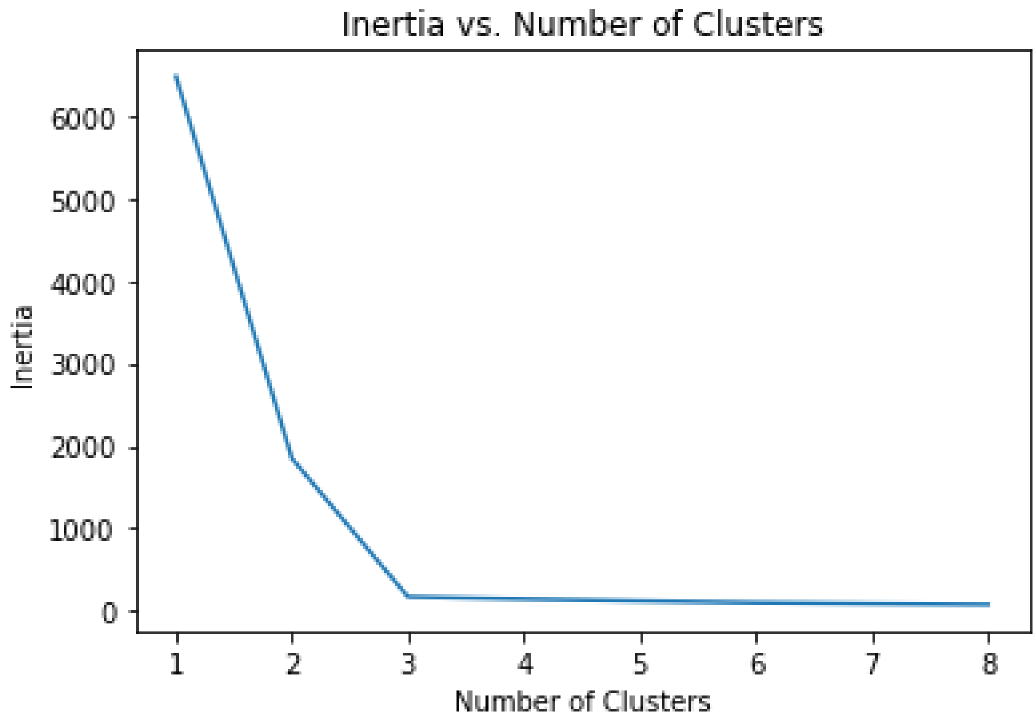


The optimal k from inertia is still k = 3 based on the elbow method, so the optimal k's agree.

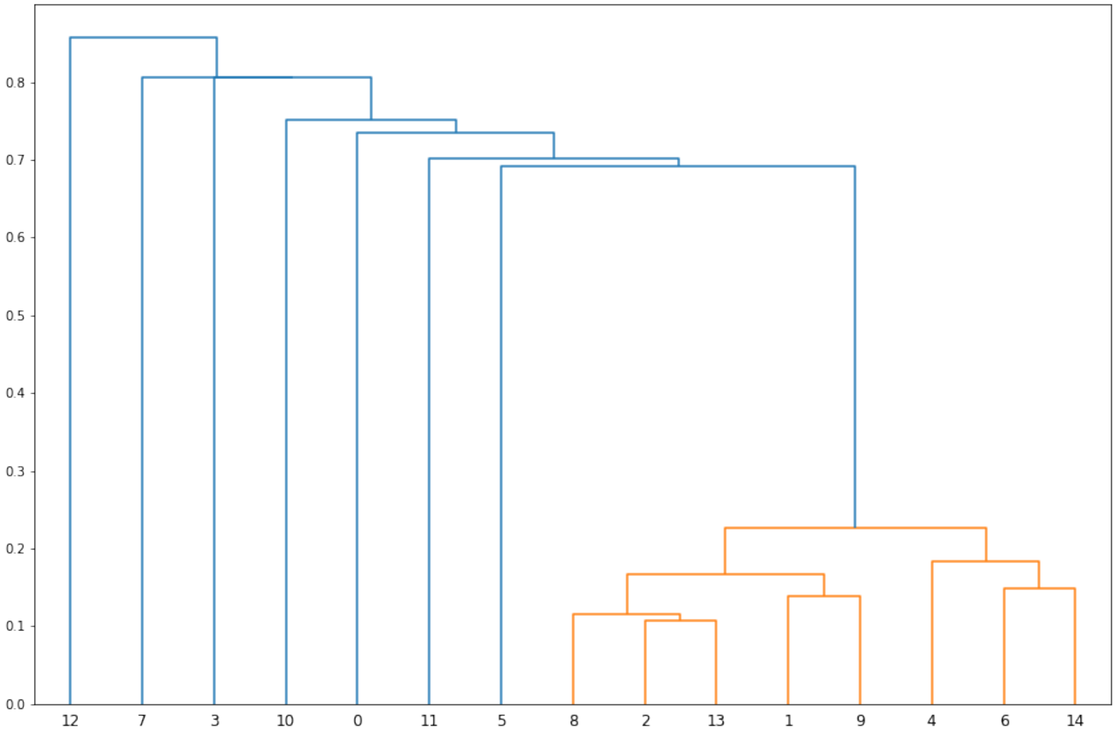
3 Problem 3

3.1 Part A

[29]:
```
#load the provided dataset
from scipy import io
toy_data = io.loadmat("hierarchical_toy_data.mat")
```

3.2 Part B

[38]:
```
#Create a linkage matrix Z with single linkage
from scipy.cluster import hierarchy
Z = hierarchy.linkage(toy_data['X'], method = 'single')
plt.figure(figsize=(15,10))
dendo = hierarchy.dendrogram(Z)
```



3.3 Part C

[31]:
```
# Find the iteration I = {8, 2, 13} and J = {1, 9} were merged
Z
```

[31]:
```
array([[ 2.        , 13.        ,  0.10777706,  2.        ],
       [ 8.        , 15.        ,  0.11566306,  3.        ],
       [ 1.        ,  9.        ,  0.13879878,  2.        ],
       [ 6.        , 14.        ,  0.14869505,  2.        ],
       [16.        , 17.        ,  0.16646191,  5.        ],
       [ 4.        , 18.        ,  0.18393601,  3.        ],
       [19.        , 20.        ,  0.22664301,  8.        ],
       [ 5.        , 21.        ,  0.69232603,  9.        ],
       [11.        , 22.        ,  0.70134235, 10.        ],
       [ 0.        , 23.        ,  0.73428364, 11.        ],
       [10.        , 24.        ,  0.75208442, 12.        ],
       [ 3.        , 25.        ,  0.80541514, 13.        ],
       [ 7.        , 26.        ,  0.80542732, 14.        ],
       [12.        , 27.        ,  0.85709025, 15.        ]])
```

Starting iterations at 0, clusters $\{8, 2, 13\}$ and $\{1, 9\}$ were merged at iteration 4.

3.4 Part D

[32]:
```
def dissimilarity(data, index_sets):
    X = data
    #Set the max dissimilarity to eventually chose the smallest one
    min_diss = 1
    #Check if both clusters are 1 element
    if np.size(index_sets[0]) == 1 and np.size(index_sets[1] == 1):
        i, j = index_sets
        diss = np.linalg.norm(X[i] - X[j])
        if diss < min_diss:
            min_diss = diss
    #Check if only the first cluster is 1 element
    elif np.size(index_sets[0]) == 1 and np.size(index_sets[1] != 1):
        i = index_sets[0]
        for j in index_sets[1]:
            diss = np.linalg.norm(X[i] - X[j])
            if diss < min_diss:
                min_diss = diss
    #Check if the second cluster is 1 element and the other one isn't
    elif np.size(index_sets[1]) == 1 and np.size(index_sets[0] != 1):
        j = index_sets[1]
        for i in index_sets[0]:
            diss = np.linalg.norm(X[i] - X[j])
            if diss < min_diss:
                min_diss = diss
    #All other variations
    else:
        for i in index_sets[0]:
            for j in index_sets[1]:
                diss = np.linalg.norm(X[i] - X[j])
                if diss < min_diss:
                    min_diss = diss
    print("The dissimilarity given by single link clustering for clusters {}␣
↪and {} is: {}".format(index_sets[0], index_sets[1], min_diss))
    return min_diss
```

[33]:
```
part3D = dissimilarity(toy_data['X'], ((2, 13, 8), (1, 9)))
```

```
The dissimilarity given by single link clustering for clusters (2, 13, 8) and
(1, 9) is: 0.16646190977808642
```

3.5 Part E

All available clusters when Part D was merged:
{{8, 2, 13}, {1, 9}, {6, 14}, {0}, {3}, {4}, {5}, {7}, {10}, {11}, {12}}

3.6 Part F

No, the algorithm does not ever produce two rings

3.7 Part G

The dendogram does illustrate one cluster that is continuously merging with all available points

4 Question 4

4.1 Part A

[34]:
```
from sklearn.cluster import AgglomerativeClustering
def fit_hier_cluster(dataset, linkage, num_clusters):
    data = StandardScaler().fit_transform(dataset)
    y_pred = AgglomerativeClustering(n_clusters = num_clusters, linkage =␣
 ↪linkage).fit_predict(data)
    return y_pred
```

4.2 Part B

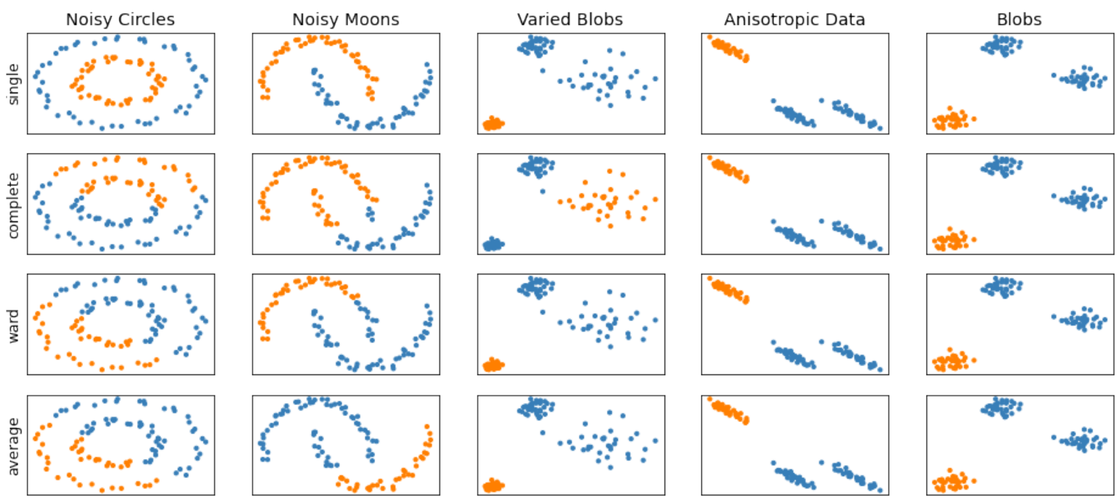
[170]:
```
linkage_types = ["single", "complete", "ward", "average"]
plt.figure(figsize = (16, 7))
plot_num = 1

for i, k in enumerate(linkage_types):
    for ds_name, ds in datasets:
        X, y = ds
        y_pred = fit_hier_cluster(X, k, 2)
        #Create necessary subplot size (4 x 5)
        plt.subplot(len(linkage_types), len(datasets), plot_num)
        #Add titles to top row only
        if i == 0:
            plt.title(ds_name, size = 14)

        # Points colored by predicted label
        # FROM https://scikit-learn.org/stable/auto_examples/cluster/
 ↪plot_cluster_comparison.html
        colors = np.array(
            list(
                islice(
                    cycle(
                        [
                            "#377eb8",
                            "#ff7f00",
                        ]
                    ),
                    int(max(y_pred) + 1),
```

```
                )
            )
        )
        # add black color for outliers (if any)
        colors = np.append(colors, ["#000000"])
        plt.scatter(X[:, 0], X[:, 1], s=10, color=colors[y_pred])
        plt.xticks(())
        plt.yticks(())
        #Add y labels to
        if plot_num in [1, 6, 11, 16]:
                plt.ylabel("%s" % k, size = 12)
        plot_num += 1

plt.show()
```



For single linkage, it appears noisy circles and noisy moons are now correctly clustered where they were not with k-means.

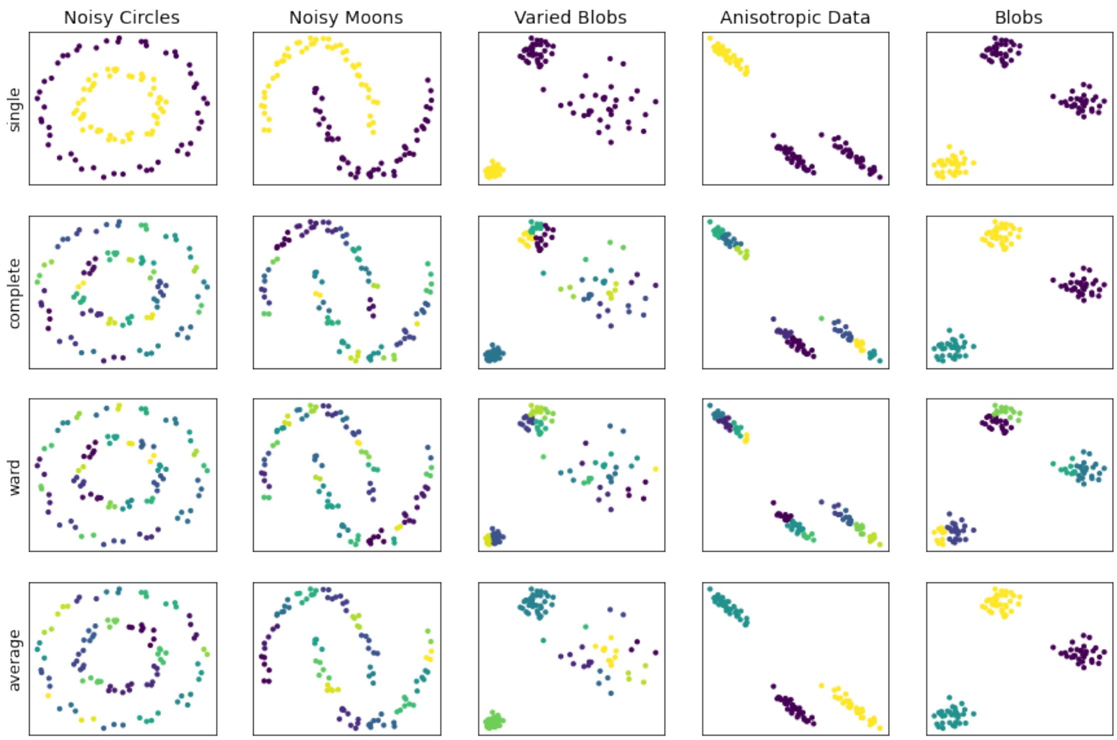
4.3 Part C

[161]:
```
def fit_hier_cluster_distance(X, linkage, eps = 1e-5):
    X = StandardScaler().fit_transform(X)
    Z = hierarchy.linkage(X)
    diff = np.diff(Z[:,2])
    idx = np.argmax(diff)
    threshold = Z[idx, 2]
    model = AgglomerativeClustering(n_clusters=None, linkage = linkage,␣
↪distance_threshold = threshold + eps, compute_distances=True).fit(X)
    y_pred = model.fit_predict(X)
    return y_pred
```

[171]:
```
linkage_types = ["single", "complete", "ward", "average"]
plt.figure(figsize = (15,10))
plot_num = 1
for i, k in enumerate(linkage_types):
    for ds_name, ds in datasets:
        X, y = ds
        y_pred = fit_hier_cluster_distance(X, k)
        #Create necessary subplot size (4 x 5)
        plt.subplot(4, 5, plot_num)
        #Add titles to top row only
        if (i == 0):
            plt.title(ds_name, size = 14)

        # Points colored by predicted label
        # FROM https://scikit-learn.org/stable/auto_examples/cluster/
 ↪plot_cluster_comparison.html
        # add black color for outliers (if any)
        colors = np.append(colors, ["#000000"])
        plt.scatter(X[:, 0], X[:, 1], s=10, c=y_pred)
        plt.xticks(())
        plt.yticks(())
        #Add y labels to
        if plot_num in [1, 6, 11, 16]:
                plt.ylabel("%s" % k, size = 12)
        plot_num += 1

plt.show()
```


Noisy Circles
Noisy Moons
Varied Blobs
Anisotropic Data
Blobs
single
complete
ward
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