Hands-on Practice for CLUS Module

0. Setting up necessary packages

Upgrade scikit-learn package.

In [1]:
```
!pip install --user scikit-learn --upgrade
```

...

Import necessary packages

In [2]:
```
import numpy as np
import matplotlib.pyplot as plt
import matplotlib.cm as cm
import seaborn as sns

from sklearn import datasets

# importing clustering algorithms
from sklearn.cluster import KMeans
from sklearn.mixture import GaussianMixture
from sklearn.cluster import AgglomerativeClustering
from sklearn.cluster import DBSCAN
from sklearn.cluster import SpectralClustering

from sklearn.metrics import silhouette_samples
```

1. Generating and visualizing data

Create seven datasets using functions from the datasets package:

1. **Blobs1**: three well separated clusters
2. **Blobs2**: three well separated clusters with high standard deviation
3. **Moons1**: two half-moon like separated clusters
4. **Moons2**: two half-moon like separated clusters with high standard deviation
5. **Circles1**: two concentric, but separated clusters
6. **Circles2**: two concentric, but separated clusters with high standard deviation
7. **Rand**: Random set of points

Total number of datapoints in each dataset: 1500.

Number of attributes: 2

In [3]:
```
n_samples = 1500
random_state = 10

Blobs1_X, Blobs1_y = datasets.make_blobs(n_samples=n_samples,
                                         random_state=random_state)
Blobs2_X, Blobs2_y = datasets.make_blobs(n_samples=n_samples,
                                         cluster_std=[2.5, 2.5, 2.5],
                                         random_state=random_state)
Moons1_X, Moons1_y = datasets.make_moons(n_samples=n_samples, noise=0.05,
                                         random_state=random_state)
Moons2_X, Moons2_y = datasets.make_moons(n_samples=n_samples, noise=0.1,
                                         random_state=random_state)
Circles1_X, Circles1_y = datasets.make_circles(n_samples=n_samples, factor=.5,
                                               noise=.05, random_state=random_state)
Circles2_X, Circles2_y = datasets.make_circles(n_samples=n_samples, factor=.5,
                                               noise=0.1, random_state=random_state)
Rand_X = np.random.rand(n_samples, 2);
```

Printing the dimensions of the Blobs1 data...

In [4]:
```
Blobs1_X.shape
```

Out[4]:
```
(1500, 2)
```

Printing Blobs1 data...

In [5]:
```
Blobs1_X
```

Out[5]:
```
array([[ 0.15042904, -5.5490135 ],
       [ 4.84805107,  5.4847015 ],
       [ 3.82847698,  5.6755923 ],
       ...,
       [ 2.80778483,  5.72054107],
       [ 1.60111675,  5.71447101],
       [ 3.59907164,  4.92802023]])
```

Printing 'ground truth' clusters for Blobs1 data...

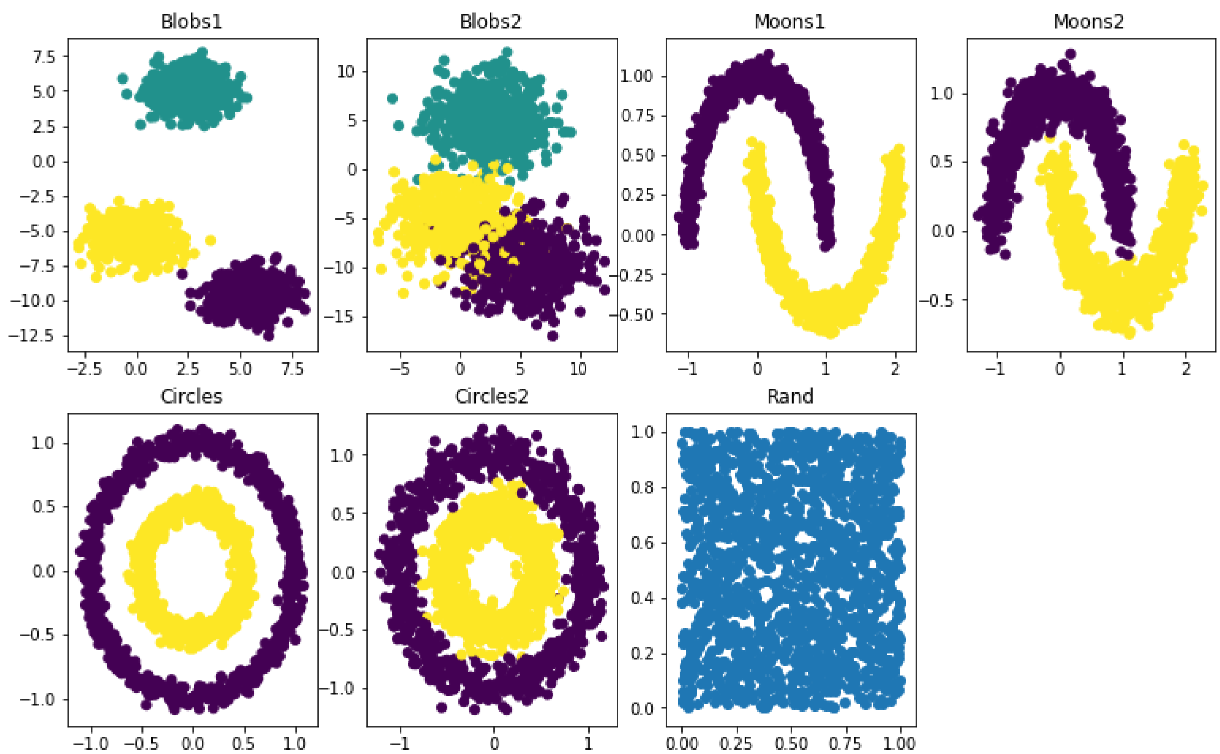
In [6]:
```
Blobs1_y
```

Out[6]:
```
array([2, 1, 1, ..., 1, 1, 1])
```

Notice that the ground truth clustering is a vector of length n where n is the number of data points. Each element of the vector is the cluster number assigned for the corresponding data point.

Question: Plot the five datasets using scatter function from the matplotlib package. Use the ground truth labels to color the data points.

In [7]:
```
plt.figure(figsize=(13,8))

plt.subplot(2,4,1)
plt.scatter(Blobs1_X[:, 0], Blobs1_X[:, 1], c= Blobs1_y)
plt.title('Blobs1')

plt.subplot(2,4,2)
plt.scatter(Blobs2_X[:, 0], Blobs2_X[:, 1], c= Blobs2_y)
plt.title('Blobs2')

plt.subplot(2,4,3)
plt.scatter(Moons1_X[:, 0], Moons1_X[:, 1], c= Moons1_y)
plt.title('Moons1')

plt.subplot(2,4,4)
plt.scatter(Moons2_X[:, 0], Moons2_X[:, 1], c= Moons2_y)
plt.title('Moons2')

plt.subplot(2,4,5)
plt.scatter(Circles1_X[:, 0], Circles1_X[:, 1], c= Circles1_y)
plt.title('Circles')

plt.subplot(2,4,6)
plt.scatter(Circles2_X[:, 0], Circles2_X[:, 1], c= Circles2_y)
plt.title('Circles2')

plt.subplot(2,4,7)
plt.scatter(Rand_X[:, 0], Rand_X[:, 1])
plt.title('Rand')
plt.show()
```



2. Clustering the data using K-Means, EM, Agglomerative, DBSCAN, and Spectral clustering algorithms

a. K-Means clustering

Question: Discover 3 clusters in Blobs1_X data using k-Means clustering. Compute SSE score for this clustering.

Initializing the KMeans object with n_clusters = 3

In [8]:
```
n_clusters = 3
kmeans = KMeans(n_clusters=n_clusters, random_state=random_state);
```

Using *fit_predict()* function in KMeans object to find cluster labels for Blobs1 data.

In [9]:
```
y_pred = kmeans.fit_predict(Blobs1_X)
```

Printing *y_pred* that captures the result of k-means clustering.

In [10]:
```
y_pred
```

Out[10]:
```
array([2, 1, 1, ..., 1, 1, 1], dtype=int32)
```

This is a vector whose length is the same as the number of data points. Each value indicates the cluster to which the point is assigned by k-means algorithm.

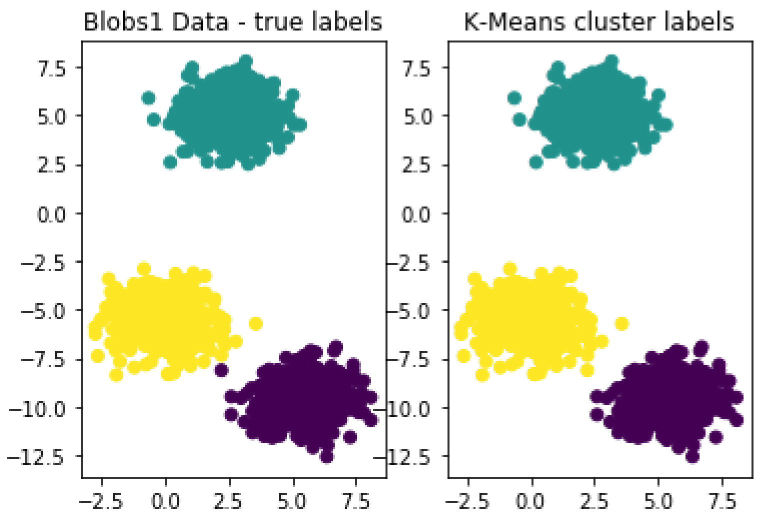
Using *score()* function in KMeans object to find SSE score for the above clustering. The '-' sign is to flip the -SSE returned by score function.

In [11]:
```
score = -kmeans.score(Blobs1_X)
print(score)
```

```
2875.575460810548
```

Question: Plot the data with colors based on true cluster memberships and with cluster memberships discovered using KMeans.

In [12]:
```
fig, ax = plt.subplots()
plt.subplot(1,2,1)
plt.scatter(Blobs1_X[:, 0], Blobs1_X[:, 1], c=Blobs1_y) # true clusters
plt.title('Blobs1 Data - true labels')
plt.subplot(1,2,2)
plt.scatter(Blobs1_X[:, 0], Blobs1_X[:, 1], c=y_pred)  # KMeans clusters
plt.title('K-Means cluster labels')
plt.show()
```



Question: Is KMeans able to find the original clusters in the Blobs1 data?

Answer: Yes, KMeans is able to find the original clusters in the Blobs1 data.

b. EM approach for clustering

Question: Discover 3 clusters in Blobs1_X data using EM/Gaussian Mixture Model approach.

Initializing the GaussianMixture object with n_clusters = 3

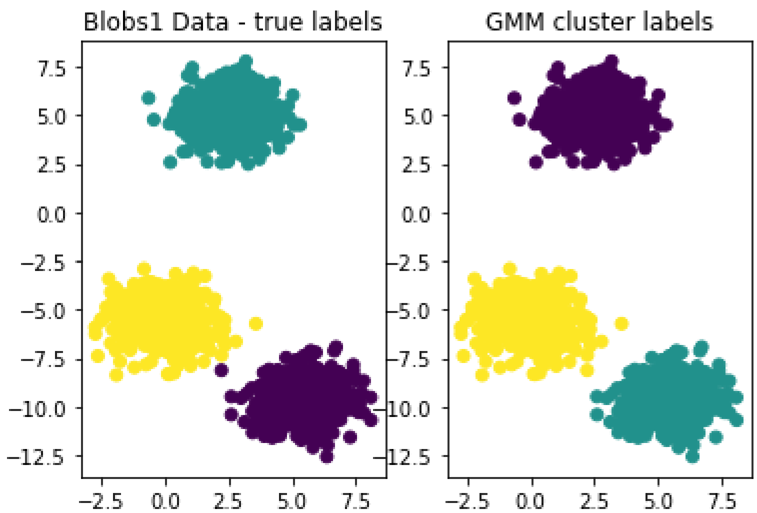
In [13]:
```
n_clusters = 3;
gmm = GaussianMixture(n_components=n_clusters, covariance_type='full')
```

Using *fit_predict()* function in GaussianMixture object to find cluster labels for Blobs1 data.

In [14]:
```
y_pred = gmm.fit_predict(Blobs1_X)
```

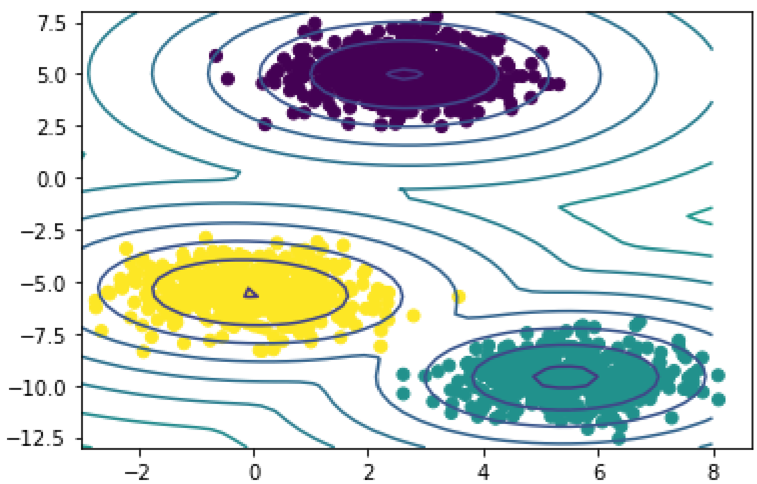
Question: Plot the data with colors based on true cluster memberships and with cluster memberships discovered using EM approach.

In [15]:
```
plt.subplot(1,2,1)
plt.scatter(Blobs1_X[:, 0], Blobs1_X[:, 1], c=Blobs1_y) # true clusters
plt.title('Blobs1 Data - true labels')
plt.subplot(1,2,2)
plt.scatter(Blobs1_X[:, 0], Blobs1_X[:, 1], c=y_pred)  # EM clusters
plt.title('GMM cluster labels')
plt.show()
```



Question: Plot the Gaussian distribution contours for each cluster.

In [16]:
```
from matplotlib.colors import LogNorm

x = np.linspace(-3, 8) #x-axis
y = np.linspace(-13, 8) #y-axis
X, Y = np.meshgrid(x, y) #grid
XX = np.array([X.ravel(), Y.ravel()]).T
Z = -gmm.score_samples(XX) #probability at each point
Z = Z.reshape(X.shape)

plt.scatter(Blobs1_X[:, 0], Blobs1_X[:, 1], c=y_pred)  #plot data
plt.contour(X, Y, Z, norm=LogNorm(vmin=1.0, vmax=1000.0),
                 levels=np.logspace(0, 3, 20)) #plot prob. density
plt.show()
```



Question: What do the above contours represent?

Answer: These contours depict the probability for a data point to belong to each of the clusters.

c. Agglomerative Clustering

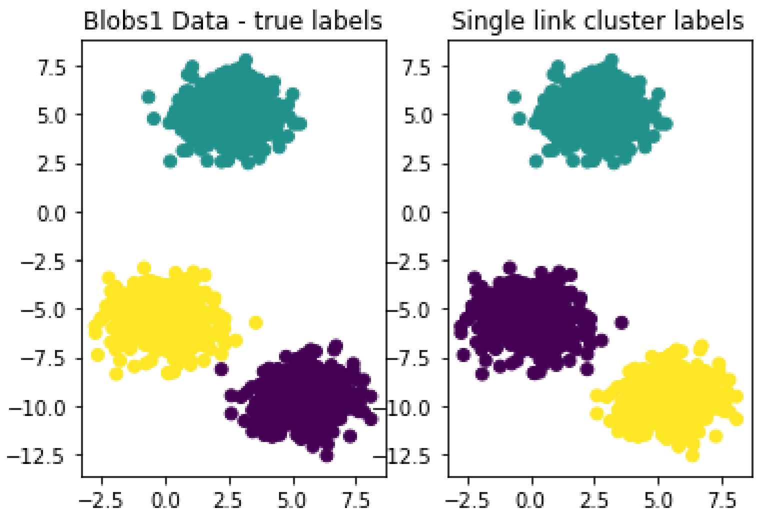
Question: Discover 3 clusters in Blobs1_X data using **single-link agglomerative clustering**.

Initializing the Agglomerative clustering object with single-link and n_clusters = 3. Finding cluster assignments on Blobs1 dataset using *fit_predict()*.

In [17]:
```
n_clusters = 3
single_linkage = AgglomerativeClustering(linkage="single", n_clusters=n_clusters)
y_pred = single_linkage.fit_predict(Blobs1_X)
```

Question: Plot the cluster assignments and compare with true labels.

In [18]:
```
plt.subplot(1,2,1)
plt.scatter(Blobs1_X[:, 0], Blobs1_X[:, 1], c=Blobs1_y)
plt.title('Blobs1 Data - true labels')
plt.subplot(1,2,2)
plt.scatter(Blobs1_X[:, 0], Blobs1_X[:, 1], c=y_pred)
plt.title('Single link cluster labels')
plt.show()
```



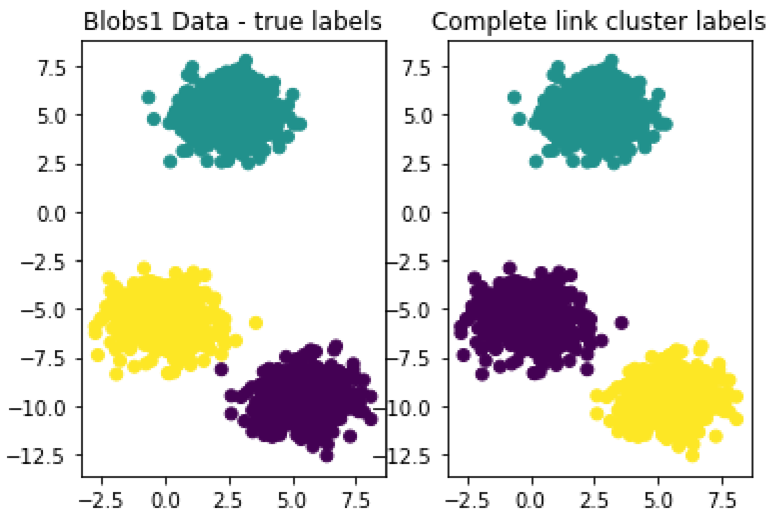
Question: Discover 3 clusters in Blobs1_X data using **complete-link agglomerative clustering**.

Initializing the Agglomerative clustering object with complete-link and n_clusters = 3. Finding cluster assignments on Blobs1 dataset using *fit_predict()*.

In [19]:
```
n_clusters = 3
complete_linkage = AgglomerativeClustering(linkage="complete", n_clusters=n_clust
y_pred = complete_linkage.fit_predict(Blobs1_X)
```

Question: Plot cluster assignments and compare with true labels.

In [20]:
```
plt.subplot(1,2,1)
plt.scatter(Blobs1_X[:, 0], Blobs1_X[:, 1], c=Blobs1_y)
plt.title('Blobs1 Data - true labels')
plt.subplot(1,2,2)
plt.scatter(Blobs1_X[:, 0], Blobs1_X[:, 1], c=y_pred)
plt.title('Complete link cluster labels')
plt.show()
```



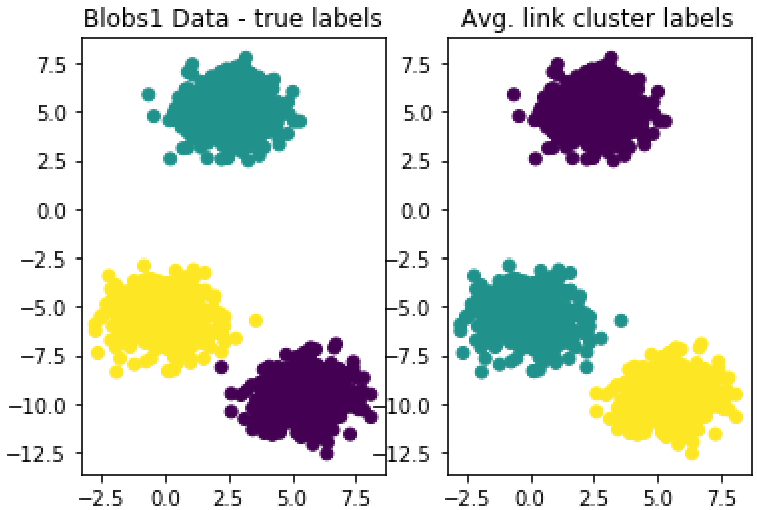
Question: Discover 3 clusters in Blobs1_X data using **average-link agglomerative clustering**.

Initializing the Agglomerative clustering object with average-link and n_clusters = 3. Finding cluster assignments on Blobs1 dataset using *fit_predict()*.

In [21]:
```
n_clusters = 3
average_linkage = AgglomerativeClustering(linkage="average", n_clusters=n_cluster
y_pred = average_linkage.fit_predict(Blobs1_X)
```

Question: Plot cluster assignments and compare with true labels.

In [22]:
```
plt.subplot(1,2,1)
plt.scatter(Blobs1_X[:, 0], Blobs1_X[:, 1], c=Blobs1_y)
plt.title('Blobs1 Data - true labels')
plt.subplot(1,2,2)
plt.scatter(Blobs1_X[:, 0], Blobs1_X[:, 1], c=y_pred)
plt.title('Avg. link cluster labels')
plt.show()
```



d. DBSCAN Algorithm

Question: Discover 3 clusters in Blobs1_X data using **DBSCAN** approach.

Initializing DBSCAN object with eps=1 and min_samples=10. Note that DBSCAN does not take n_clusters as input. Finding clusters on Blobs1 dataset using *fit_predict()*

In [23]:
```
dbscan = DBSCAN(eps=1, min_samples=10)
y_pred = dbscan.fit_predict(Blobs1_X)
```

Question: How many noise points did **DBSCAN** approach find.

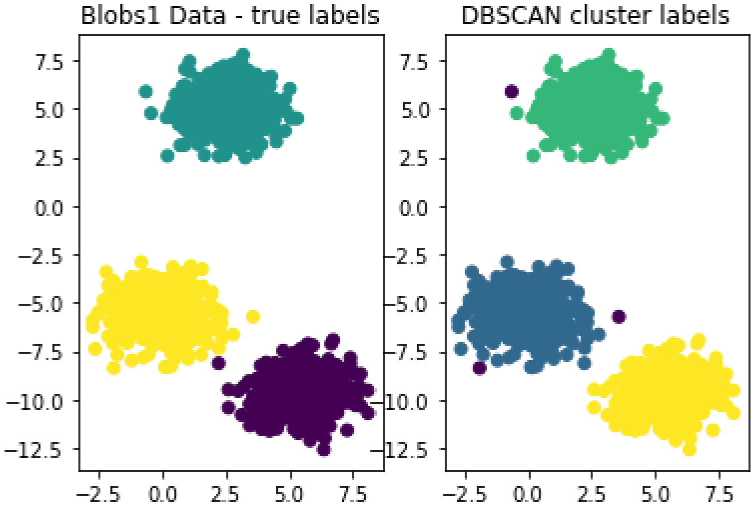
DBSCAN assigns noise points a value of '-1'

In [24]:
```
np.sum(y_pred==-1)
```

Out[24]: 3

Question: Plot cluster assignments and compare with true labels.

In [25]:
```
plt.subplot(1,2,1)
plt.scatter(Blobs1_X[:, 0], Blobs1_X[:, 1], c=Blobs1_y)
plt.title('Blobs1 Data - true labels')
plt.subplot(1,2,2)
plt.scatter(Blobs1_X[:, 0], Blobs1_X[:, 1], c=y_pred)
plt.title('DBSCAN cluster labels')
plt.show()
```



e. SpectralClustering Algorithm

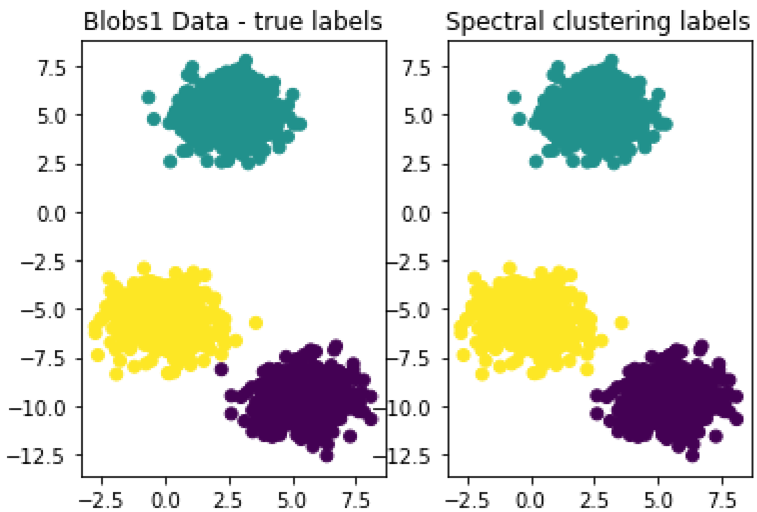
Question: Discover 3 clusters in Blobs1_X data using **Spectral clustering** approach.

Initializing SpectralClustering object with n_clusters = 3. Finding cluster assignments on Blobs1 dataset using fit_predict().

In [26]:
```
n_clusters = 3
spectral = SpectralClustering(n_clusters=n_clusters, random_state=random_state)
y_pred = spectral.fit_predict(Blobs1_X)
```

Question: Plot cluster assignments and compare with true labels.

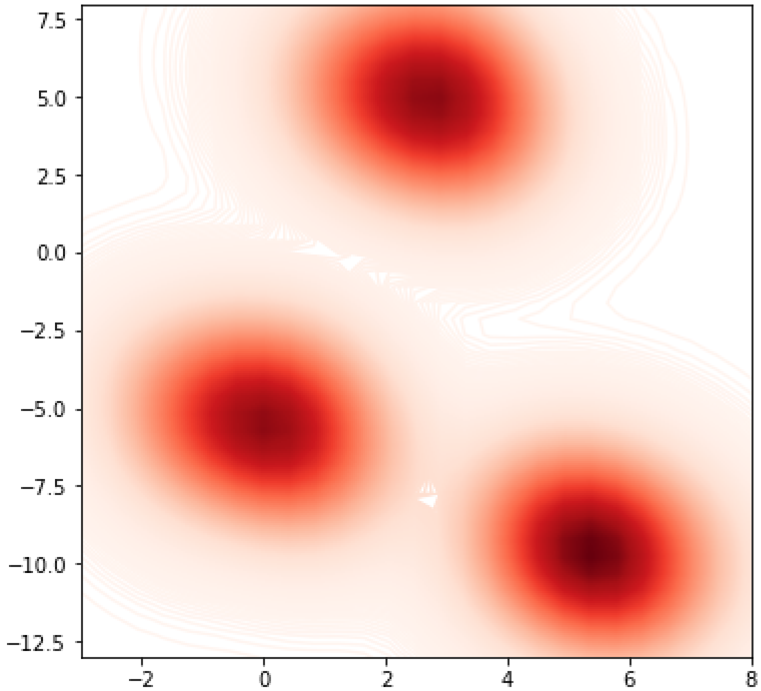
In [27]:
```
plt.subplot(1,2,1)
plt.scatter(Blobs1_X[:, 0], Blobs1_X[:, 1], c=Blobs1_y)
plt.title('Blobs1 Data - true labels')
plt.subplot(1,2,2)
plt.scatter(Blobs1_X[:, 0], Blobs1_X[:, 1], c=y_pred)
plt.title('Spectral clustering labels')
plt.show()
```



3. Kernel Density Estimation

Question: Compute and plot kernel density using a Gaussian kernel with a bandwidth of 5.

In [28]:
```
plt.figure(figsize=(6,6))
sns.kdeplot(Blobs1_X[:, 0], Blobs1_X[:, 1], kernel = 'guassian', bw = 5, cmap="Re
plt.xlim(-3,8)
plt.ylim(-13,8)
plt.show()
```



4. Clustering Evaluation

Question: Determine the choice of k using SSE

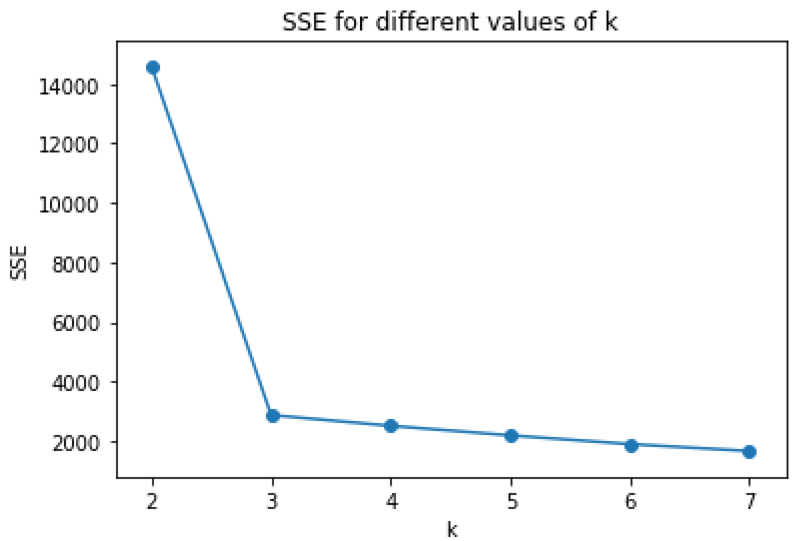
We first compute SSE for different values of k = {2,3,4,5,6,7}

In [29]:
```
score = np.zeros(8);
for i in range(2,8):
    kmeans = KMeans(n_clusters=i, random_state=random_state); #Initializing KMean
    kmeans.fit_predict(Blobs1_X)  #Clustering using KMeans
    score[i] = -kmeans.score(Blobs1_X)  #Computing SSE
    print("SSE for k=",i,":", round(score[i],2)) #Printing SSE
```

```
SSE for k= 2 : 14581.78
SSE for k= 3 : 2875.58
SSE for k= 4 : 2511.66
SSE for k= 5 : 2190.15
SSE for k= 6 : 1897.27
SSE for k= 7 : 1664.27
```

Plotting SSE for different values of k.

In [30]:
```
plt.plot(range(2,8),score[2:8])
plt.scatter(range(2,8),score[2:8])
plt.xlabel('k')
plt.ylabel('SSE')
plt.title('SSE for different values of k')
plt.show()
```



Answer: Based on this plot, we see that beyond k=3 there is no significant reduction in SSE. So we choose k=3.

b. Silhouette Coefficient

Question: Compute Silhouette coefficient for each data point using the K-Means clustering with k=2 on Blobs1 data.

We first cluster Blobs1 dataset into two clusters using KMeans.

In [31]:
```
n_clusters = 2;
kmeans = KMeans(n_clusters=n_clusters, random_state=random_state);
y_pred = kmeans.fit_predict(Blobs1_X)
```

We now compute silhouette coefficient for this clustering.

In [32]:
```
sample_silhouette_values = silhouette_samples(Blobs1_X, y_pred)
```

In [33]:
```
sample_silhouette_values.shape
```

Out[33]:
```
(1500,)
```

Question: Compute the mean of silhouette values of all the data points.

In [34]:
```
np.mean(sample_silhouette_values)
```

Out[34]:
```
0.7226129828708546
```

Question: What does this mean value indicate?

Answer: It is indicative of the overall quality of the clustering. As the best possible value is 1, the value of 0.722 indicates that there is good cohesion and separation between the clusters.

Question: Can the above result give any information about the individual clusters?

Answer: It does not inform which clusters have better silhouette values. To capture this, we have to compute silhouette values for each cluster separately.

Question: Compute the silhoutte values of each cluster separately.

In [35]:
```
for i in range(0,n_clusters):
    print(np.mean(sample_silhouette_values[y_pred==i]))
```

```
0.652856790077307
0.8621253684579501
```

Question: What do you observe from the above silhoutte values?

Answer: This indicates that cluster 1 has relatively low cohesion/separation compared to cluster 2.

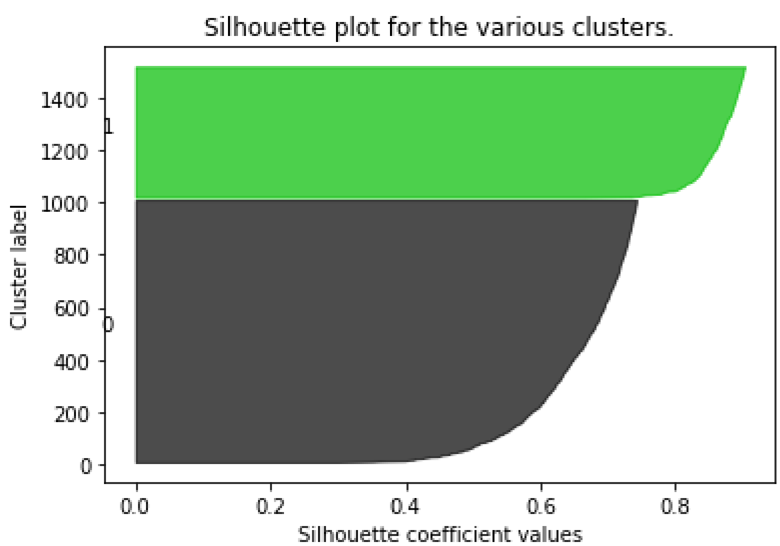
Question: Write a function to plot silhouette values for points in each cluster separately.

This function takes two input arguments: datamatrix X and cluster labels

In [36]:
```
def silhouette(X,labels):
    n_clusters = np.size(np.unique(labels));
    sample_silhouette_values = silhouette_samples(X, labels)
    y_lower = 10
    for i in range(n_clusters):
        ith_cluster_silhouette_values = sample_silhouette_values[labels == i]
        ith_cluster_silhouette_values.sort()
        size_cluster_i = ith_cluster_silhouette_values.shape[0]
        y_upper = y_lower + size_cluster_i

        color = cm.nipy_spectral(float(i) / n_clusters)
        plt.fill_betweenx(np.arange(y_lower, y_upper),
                          0, ith_cluster_silhouette_values,
                          facecolor=color, edgecolor=color, alpha=0.7)

        # Label the silhouette plots with their cluster numbers at the middle
        plt.text(-0.05, y_lower + 0.5 * size_cluster_i, str(i))
        #Compute the new y_lower for next cluster
        y_lower = y_upper + 10  # 10 for the 0 samples
    plt.title("Silhouette plot for the various clusters.")
    plt.xlabel("Silhouette coefficient values")
    plt.ylabel("Cluster label")
    plt.show()
```

Question: Use "silhouette" function to plot per-cluster silhouette values from each cluster in separate colors.

In [37]:
```
silhouette(Blobs1_X,y_pred)
```

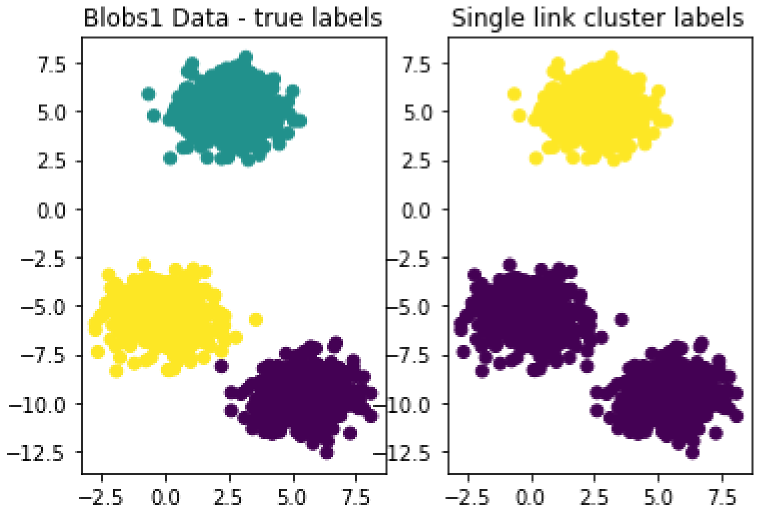


Question: How do you interpret this plot?

Answer: This plots indicates that most points in 'cluster 1' exhibit very strong cohesion and separation, while points in 'cluster 2' do not. This can be explained by the following plot that shows that the bottom two sets of points are merged into 1 cluster, as we are forcing the algorithm to find only 2 clusters (n_clusters = 2) while there are 3 clusters.

In [38]:

```
plt.subplot(1,2,1)
plt.scatter(Blobs1_X[:, 0], Blobs1_X[:, 1], c=Blobs1_y)
plt.title('Blobs1 Data - true labels')
plt.subplot(1,2,2)
plt.scatter(Blobs1_X[:, 0], Blobs1_X[:, 1], c=y_pred)
plt.title('Single link cluster labels')
plt.show()
```



c. Hopkins Statistic

Hopkins Statistic samples p 'real' data points from the data matrix and p 'random' data points in the R^d space. For each of the real data points, nearest neighbor distances to other real data points w_i and to random data points u_i are computed.

Finally, Hopkins statistic is computed as

$$H = \frac{\sum_{i=1}^{p} w_i}{\sum_{i=1}^{p} u_i + \sum_{i=1}^{p} w_i}$$

A value close to 1 indicates that there is strong cluster structure in the data. A value close to 0 indicates that data is regularly distributed in the R^d space.

Question: Write a function hopkins(X) to compute Hopkins statistic described above.

In [39]:
```
from sklearn.neighbors import NearestNeighbors
from random import sample
from numpy.random import uniform
from math import isnan

def hopkins(X):
    n = X.shape[0] #rows
    d = X.shape[1] #cols
    p = int(0.1 * n) #considering 10% of points
    nbrs = NearestNeighbors(n_neighbors=1).fit(X)

    rand_X = sample(range(0, n), p)

    uj = []
    wj = []
    for j in range(0, p):
        u_dist, _ = nbrs.kneighbors(uniform(np.amin(X,axis=0),np.amax(X,axis=0),d
        uj.append(u_dist[0][1]) #distances to nearest neighbors in random data
        w_dist, _ = nbrs.kneighbors(X[rand_X[j]].reshape(1, -1), 2, return_distan
        wj.append(w_dist[0][1]) #distances to nearest neighbors in real data

    H = sum(uj) / (sum(uj) + sum(wj))
    if isnan(H):
        print(uj, wj)
        H = 0

    return H
```

This function takes only the dataset X as input.

Question: Using the same function determine the clustering tendency in Blobs1 dataset.

In [40]:
```
hopkins(Blobs1_X)
```

Out[40]:
```
0.9395043726056117
```

Question: What does the above value say about the clustering tendency?

Answer: Because the value is close to 1, we conclude that the Blobs1 dataset has good clustering tendency.

d. Rand index

Rand index measures the similarity between two clusterings.

For two clusterings S and T, we first compute the following:

- f_{11} is the number of pairs of elements that are in the same cluster in S and in the same cluster in T.
- f_{00} is the number of pairs of elements that are in different clusters in S and in different clusters in T.

- f_{01} is the number of pairs of elements that are in different clusters in S but in same cluster in T.
- f_{10} is the number of pairs of elements that are in same cluster in S but in different clusters in T.

Rand index is computed as

$$\text{Rand Index} = \frac{f_{00} + f_{11}}{f_{00} + f_{01} + f_{10} + f_{11}}$$

A value of 1 indicates that the two clusterings S and T are identical.

Question: Write a function rand_index(S,T) to compare two clusterings S and T.

In [41]:
```
from scipy.special import comb
def rand_index(S, T):

    Spairs = comb(np.bincount(S), 2).sum()
    Tpairs = comb(np.bincount(T), 2).sum()

    A = np.c_[(S, T)]

    f_11 = sum(comb(np.bincount(A[A[:, 0] == i, 1]), 2).sum()
             for i in set(S))

    f_10 = Spairs - f_11
    f_01 = Tpairs - f_11
    f_00 = comb(len(A), 2) - f_11 - f_10 - f_01
    return (f_00 + f_11) / (f_00 + f_01 + f_10 + f_11)
```

Question: First compute K-Means clustering and Avg. link clustering on Blobs1 dataset using n_clusters = 2. Then compute the rand index between the two.

In [42]:
```
n_clusters = 2;
kmeans = KMeans(n_clusters=n_clusters, random_state=random_state);
y_pred_kmeans = kmeans.fit_predict(Blobs1_X)

average_linkage = AgglomerativeClustering(linkage="average", n_clusters=n_cluster
y_pred_avg = average_linkage.fit_predict(Blobs1_X)
```

In [43]:
```
print(rand_index(y_pred_kmeans, y_pred_avg))
```

```
1.0
```

Question: What does this rand_index value of 1.0 indicate?

Answer: As the value of rand index is 1, we can say that the above clusterings from K-Means and Avg. link are identical.

Question: Also, use this metric to determine how similar the cluster assigments are to the ground truth.

In [44]:
```python
print(rand_index(y_pred_kmeans, Blobs1_y))
print(rand_index(y_pred_avg, Blobs1_y))
```

```
0.77762953079831
0.77762953079831
```

Question: What do the above values indicate

Answer: As the values are ~0.77, we can say that the clusterings are similar to the ground truth to an extent, but not entirely similar to it.

In [ ]:
```python

```