demo_notebook_Summer18-Copy1

June 10, 2018

Below is a demo of jhu_primitives. The data set we use is DS01876 = datasetID (as defined by d3m). In particular, for visualization purposes, we use the induced subgraph of the first 50 vertices, as defined by their node ID.

```
In [1]: %pylab inline
```

```
Populating the interactive namespace from numpy and matplotlib
```

```
In [2]: import d3m
        from d3m.container import pandas as pd
        from d3m.container import dataset as ds
        from d3m.metadata import hyperparams

        import jhu_primitives

        import os
        from urllib import parse as url_parse
        import numpy as np
        import networkx as nx

        from rpy2.robjects import r
        import rpy2.robjects.numpy2ri
        import rpy2.robjects as ro
```

```
In [6]: def data_file_path_conversion(abs_file_path, uri= "", datasetDoc = False):
            local_drive, file_path = abs_file_path.split(':')[0], abs_file_path.split(':')[1]
            path_sep = file_path[0]
            file_path = file_path[1:]  # Remove initial separator
            if len(file_path) == 0:
                print("Invalid file path: len(file_path) == 0")
                return

            valid_type = False
            while not valid_type:
                type_ = input("Enter \n 0: exit \n 1: seed_datasets_current \n 2: training_data
                              + " 3: if already in the data folder \n")
                if type_ == '0':
```

```
        return
    elif type_ == '1':
        data_dir = "datasets/seed_datasets_current"
        valid_type = True
    elif type_ == '2':
        data_dir = "datasets/training_datasets"
        valid_type = True
    elif type_ == '3':
        data_dir = ""
        valid_type = True
    else:
        print("Please enter 0, 1 or 2")

valid_folder = False
while not valid_folder:
    folder = input("Enter \n 0: exit \n Name of the data folder (case sensitive; mu
    if folder == "0":
        return
    if type_ == '3':
        if os.path.isdir(folder):
            data_dir += folder
            valid_folder= True
    else:
        if os.path.isdir(data_dir  + "/" + folder):
            data_dir += "/" + folder
            valid_folder = True

s = ""
if path_sep == "/":
    splits = file_path.split("/")
    #data_folder = splits[-1]

elif path_sep == "\\":
    splits = file_path.split("\\")
    #data_folder = splits[-1]
    for i in splits:
        if i != "":
            s += "/" + i
else:
    print("Unsupported path separator!")
    return

if datasetDoc:
    s = s + "/" + data_dir + "/" + "datasetDoc.json"#+ folder + "_dataset/datasetD

if uri == "file":
    return "file://localhost" + s
else:
```

```
                return local_drive + ":" + s
```

```
In [7]: abs_file_path = os.path.abspath(os.getcwd())
        dataset_uri = data_file_path_conversion(abs_file_path, uri = "file", datasetDoc = True)
```

```
Enter
 0: exit
 1: seed_datasets_current
 2: training_datasets
 3: if already in the data folder
3
Enter
 0: exit
 Name of the data folder (case sensitive; must be in )
DS01876_datset
Enter
 0: exit
 Name of the data folder (case sensitive; must be in )
DS01876_dataset
```

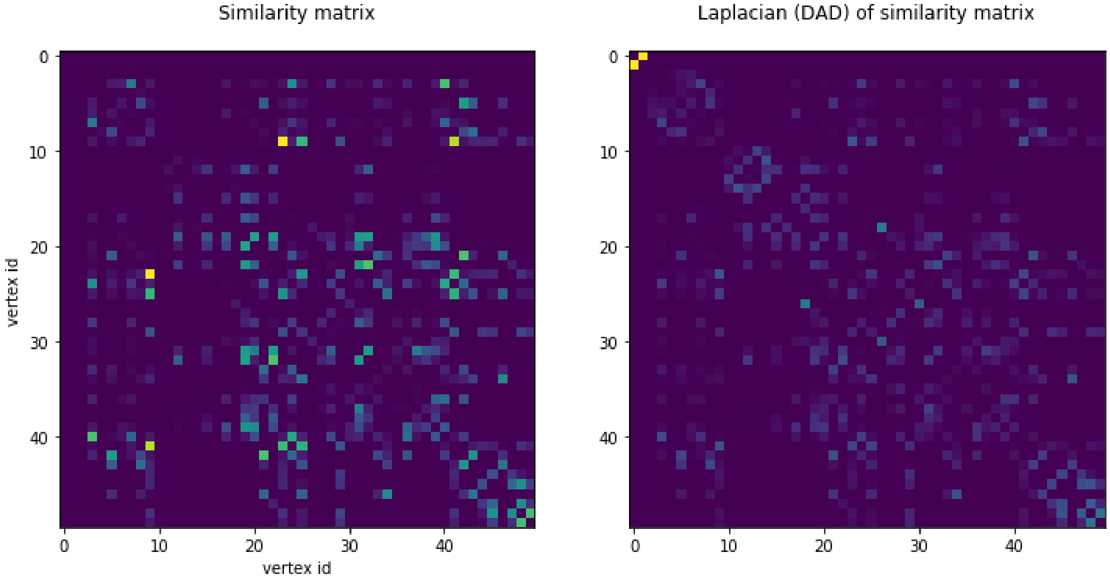
```
In [8]: data = ds.D3MDatasetLoader().load(dataset_uri = dataset_uri)
```

```
In [57]: G = data['0'] # Load the first data object
         G = G.subgraph(np.arange(50)).copy() # Induced subgraph on the first 50 vertices (for

         A = nx.to_numpy_array(G)

         n = A.shape[0] # Find the number of vertices/nodes

         D = np.linalg.pinv(np.diag(A.sum(axis=1))**(1/2))

         L = D @ A @ D

         n, A.shape, D.shape, L.shape
```

```
Out[57]: (50, (50, 50), (50, 50), (50, 50))
```

```
In [58]: fig, (ax1, ax2) = subplots(1, 2, figsize = (12,8))
         ax1.matshow(A)
         ax1.set_ylabel('vertex id')
         ax1.set_xlabel('vertex id')
         ax1.set_title('Similarity matrix')
         ax1.xaxis.tick_bottom()
         plt.colorbar

         ax2.matshow(L)
         ax2.set_title('Laplacian (DAD) of similarity matrix')
         ax2.xaxis.tick_bottom()
         plt.colorbar
```

Out[58]:
```
<function matplotlib.pyplot.colorbar>
```



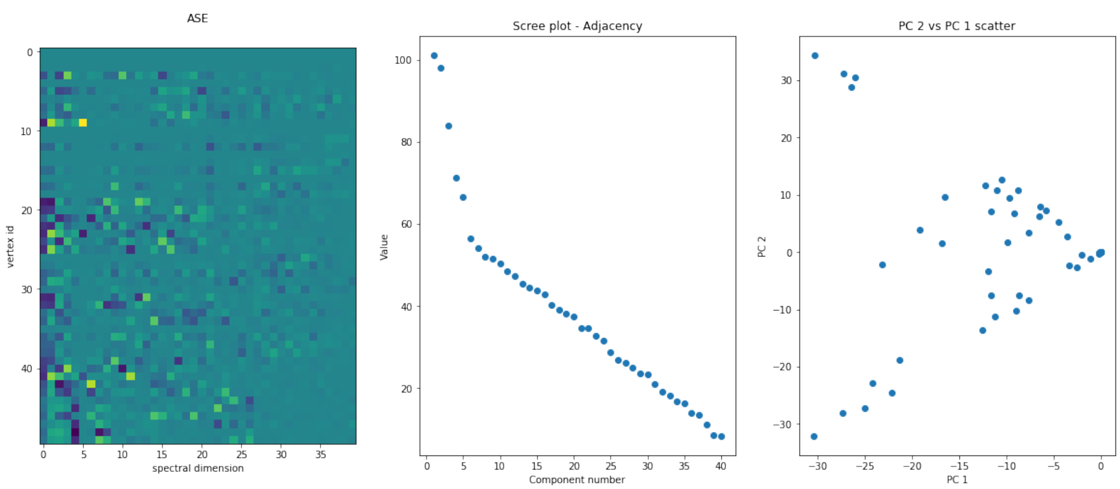
In [8]:
```
A = ro.Matrix(A)
ro.r.assign("A", A)

L = ro.Matrix(L)
ro.r.assign("L", L)
```

Out[8]:
```
R object with classes: ('matrix',) mapped to:
<Matrix - Python:0x0000026D7B6F4C08 / R:0x0000026D7B3D0010>
[0.000000, 1.000000, 0.000000, 0.000000, ..., 0.000000, 0.099684, 0.376517, 0.000000]
```

In [67]:
```
# ASE
d_max = 40

hp = jhu_primitives.ase.ase.Hyperparams
hp = hp({'max_dimension' : d_max})  # ASE hyperparameter(s) are:
                                    # 'max_dimension' = maximum embedding dimension (

ASE = jhu_primitives.AdjacencySpectralEmbedding(hyperparams = hp)
SVD = ASE.produce(inputs=A)
V = SVD.value[0]
U = SVD.value[1]

fig, (ax1, ax2, ax3) = plt.subplots(1, 3, figsize = (20, 8))
ax1.matshow(V)
ax1.set_xlabel('spectral dimension')
ax1.set_ylabel('vertex id')
```

```
ax1.set_title('ASE')
ax1.xaxis.tick_bottom()

#fig, ax2 = plt.subplots(1, 1, figsize = (8, 6))
ax2.scatter(arange(1,len(U) + 1), U**(1/2))
ax2.set_xlabel('Component number')
ax2.set_ylabel('Value')
ax2.set_title('Scree plot - Adjacency')
ax1.xaxis.tick_bottom()

#fig, ax3 = plt.subplots(1, 1, figsize = (8, 6))
ax3.scatter(V[:,0], V[:,1])
ax3.set_xlabel('PC 1')
ax3.set_ylabel('PC 2')
ax3.set_title('PC 2 vs PC 1 scatter')
```

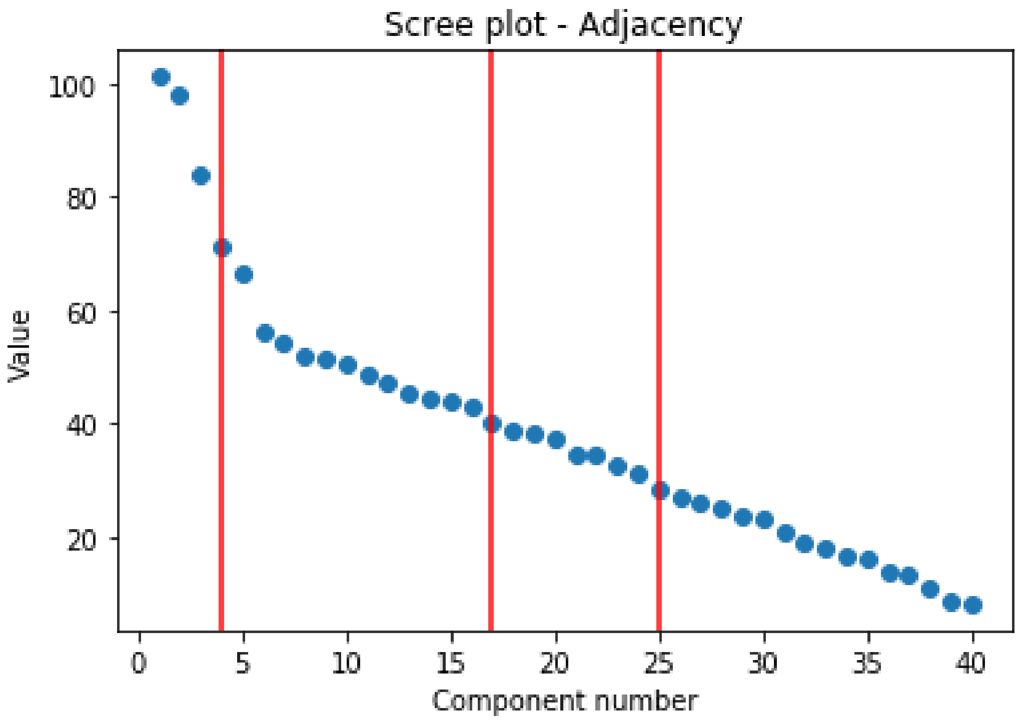
Out[67]: <matplotlib.text.Text at 0x26d7bca7ba8>




```
In [68]: # Dimension selection - Adjacency

fig, ax = plt.subplots(1, 1, figsize = (6, 4))

hp = jhu_primitives.dimselect.dimselect.Hyperparams # dimselect hyperparameters are:
                                                    # 'n_elbows': the number of elbow

hp = hp({'n_elbows': 3})

dimselector = jhu_primitives.DimensionSelection(hyperparams = hp)
d_hat = dimselector.produce(inputs = U**1/2).value # First three elbows for Laplacian

ax.scatter(arange(1,len(U) + 1), U**(1/2))
for elbow in d_hat:
```

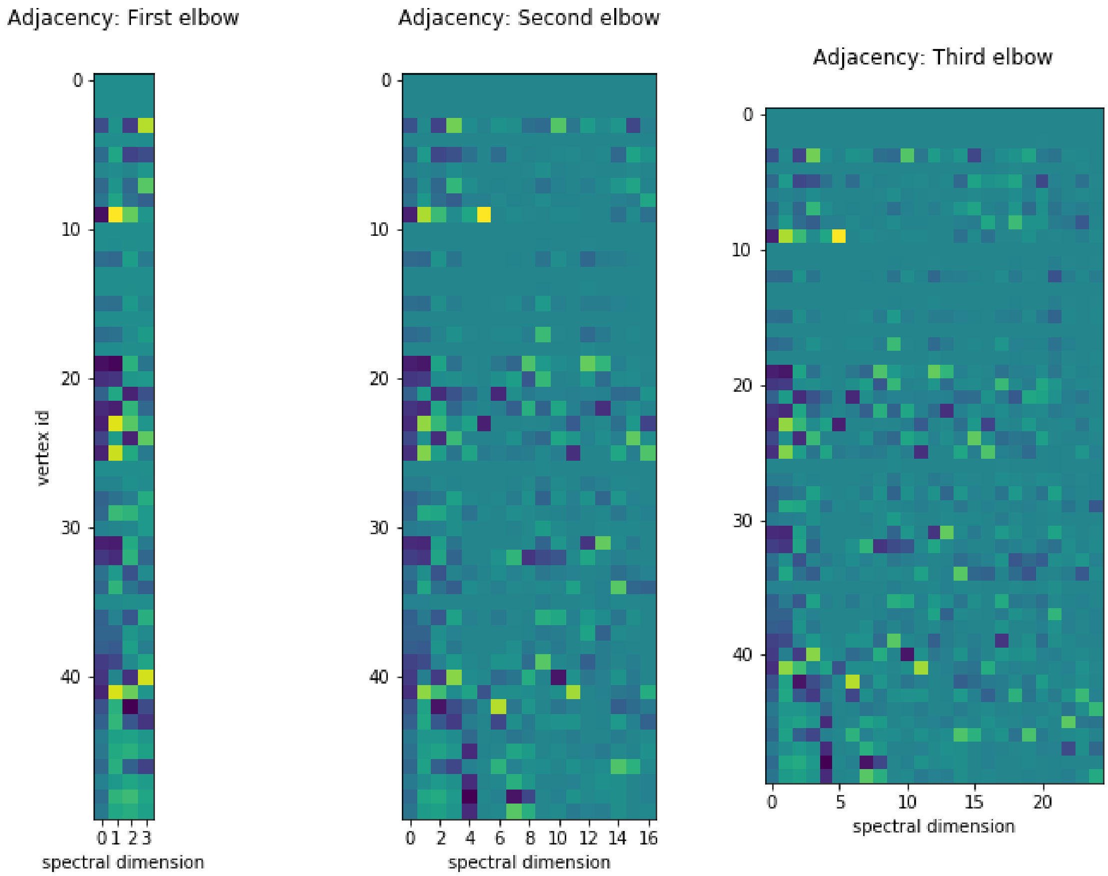
```
    ax.axvline(elbow, c = 'r')
ax.set_xlabel('Component number')
ax.set_ylabel('Value')
ax.set_title('Scree plot - Adjacency')
```

Out[68]: <matplotlib.text.Text at 0x26d7bf05128>



In [69]:
```
# ASE - first elbow

fig, (ax1, ax2, ax3) = subplots(1, 3, figsize = (12, 8))
ax1.matshow(V[:,:d_hat[0]])
ax1.set_xlabel('spectral dimension')
ax1.set_ylabel('vertex id')
ax1.set_title('Adjacency: First elbow')
plt.colorbar
ax1.xaxis.tick_bottom()

# ASE - second elbow

ax2.matshow(V[:,:d_hat[1]])
ax2.set_xlabel('spectral dimension')
#ax2.set_ylabel('vertex id')
ax2.set_title('Adjacency: Second elbow')
plt.colorbar
```

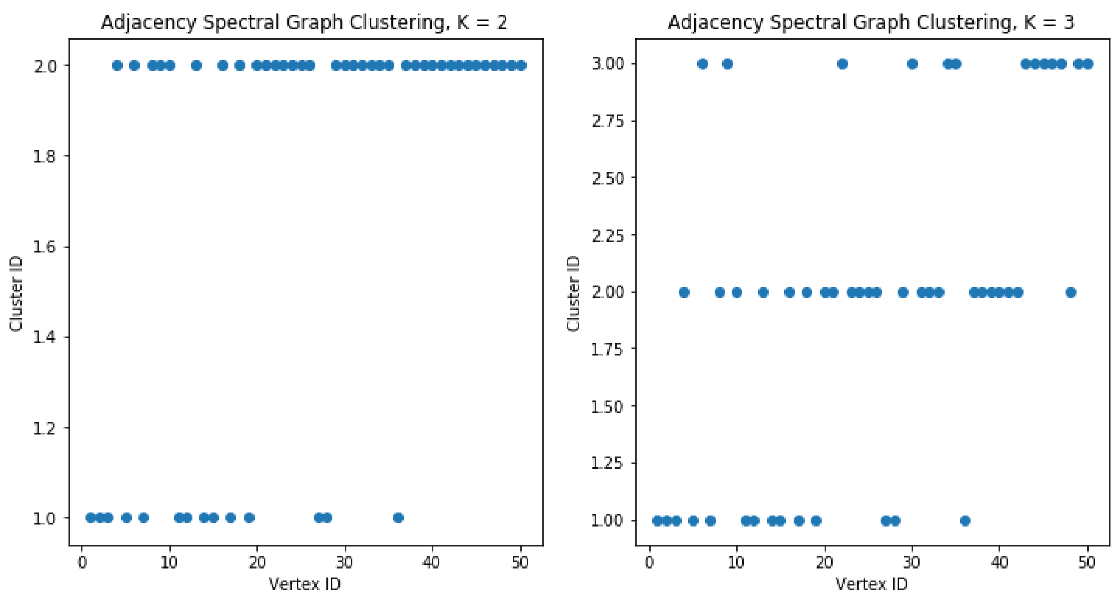
```
    ax2.xaxis.tick_bottom()

    # ASE - third elbow

    ax3.matshow(V[:,:d_hat[2]])
    ax3.set_xlabel('spectral dimension')
    #ax3.set_ylabel('vertex id')
    ax3.set_title('Adjacency: Third elbow')
    plt.colorbar
    ax3.xaxis.tick_bottom()
```

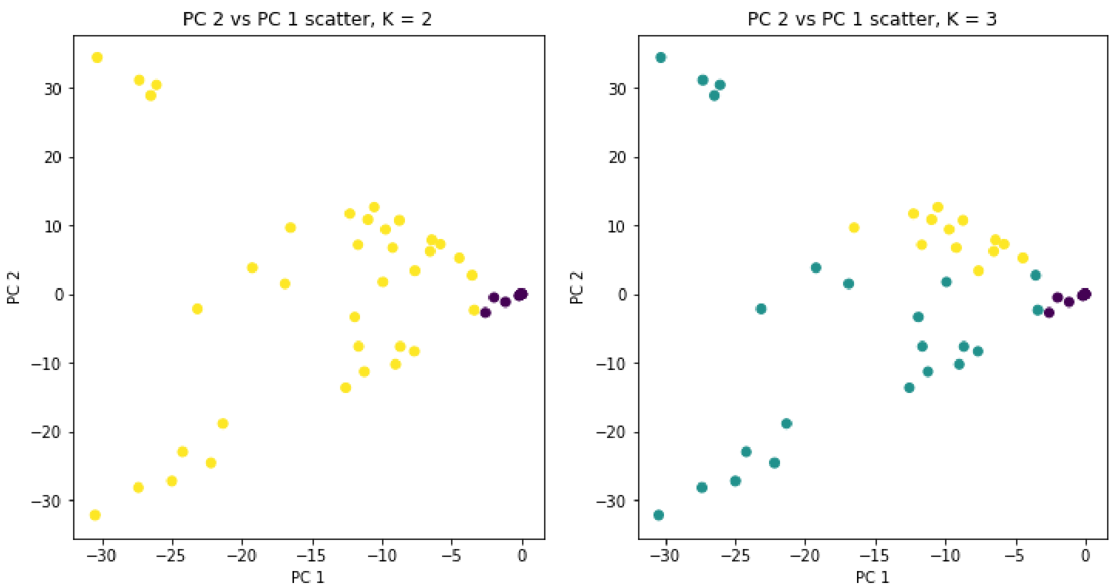



```
In [70]: # GaussianClustering - ASE - First Elbow

         hp = jhu_primitives.gclust.gclust.Hyperparams({'max_clusters': 2}) # gclust hyperpara
                                                                              # 'max_clusters' =
         gc = jhu_primitives.GaussianClustering(hyperparams = hp)
         ASEclustering_k2 = gc.produce(inputs = V[:,:int(d_hat[0])]).value

         hp = jhu_primitives.gclust.gclust.Hyperparams({'max_clusters': 3})
         gc = jhu_primitives.GaussianClustering(hyperparams = hp)
```

```
ASEclustering_k3 = gc.produce(inputs = V[:,:int(d_hat[0])]).value

fig, (ax1, ax2) = subplots(1, 2, figsize = (12, 6))
ax1.scatter(arange(1, len(ASEclustering_k2) + 1), ASEclustering_k2)
ax1.set_ylabel('Cluster ID')
ax1.set_xlabel('Vertex ID')
ax1.set_title('Adjacency Spectral Graph Clustering, K = 2')

ax2.scatter(arange(1, len(ASEclustering_k3) + 1), ASEclustering_k3)
ax2.set_ylabel('Cluster ID')
ax2.set_xlabel('Vertex ID')
ax2.set_title('Adjacency Spectral Graph Clustering, K = 3')

fig, (ax1, ax2) = plt.subplots(1, 2, figsize = (12, 6))
ax1.scatter(V[:,0], V[:, 1], c = ASEclustering_k2)
ax1.set_xlabel('PC 1')
ax1.set_ylabel('PC 2')
ax1.set_title('PC 2 vs PC 1 scatter, K = 2')

ax2.scatter(V[:,0], V[:, 1], c = ASEclustering_k3)
ax2.set_xlabel('PC 1')
ax2.set_ylabel('PC 2')
ax2.set_title('PC 2 vs PC 1 scatter, K = 3')
```

```
Out[70]: <matplotlib.text.Text at 0x26d7b991550>
```

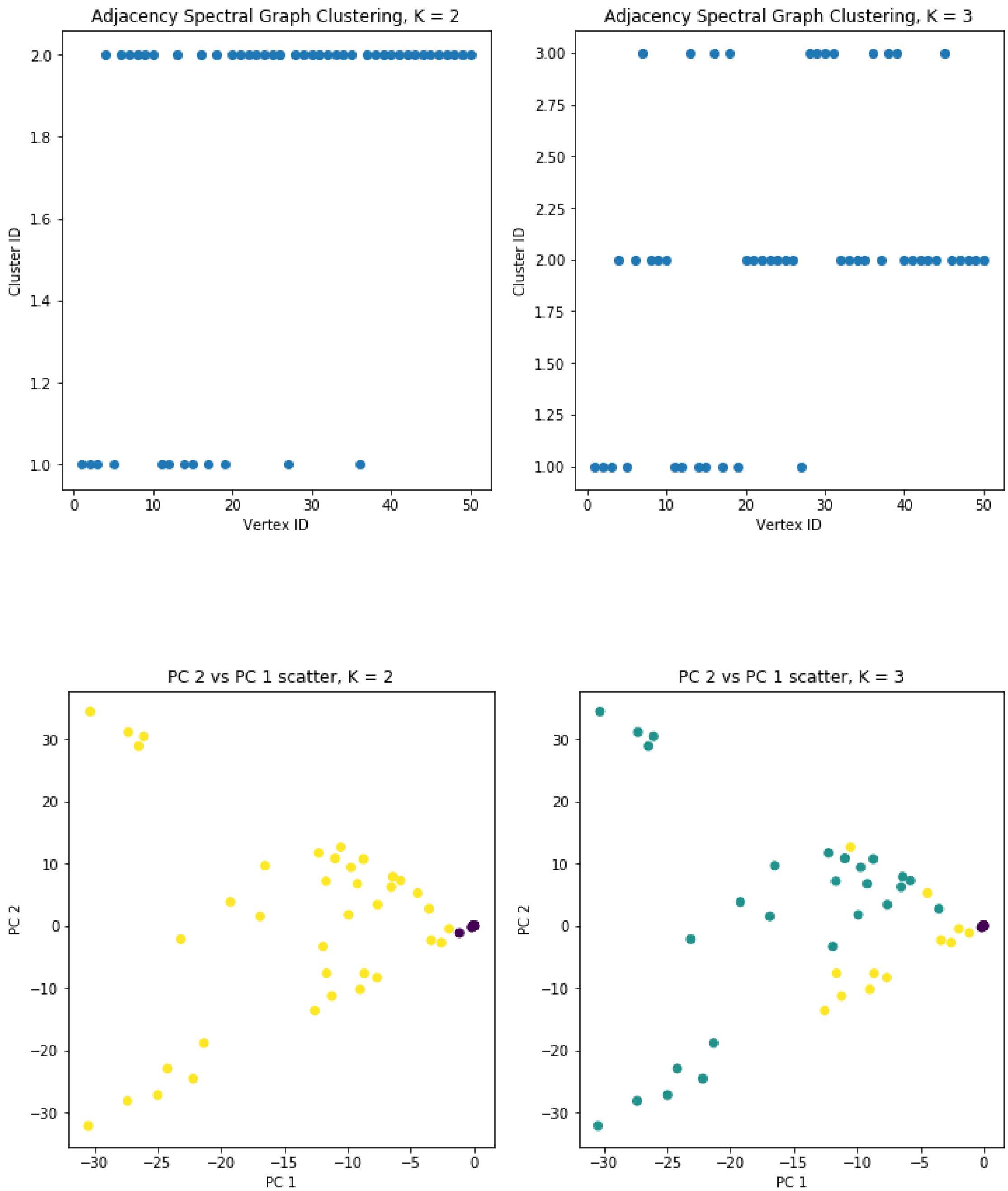




In [71]:
```
# GaussianClustering - ASE - Second Elbow

hp = jhu_primitives.gclust.gclust.Hyperparams({'max_clusters': 2}) # gclust hyperpara
                                                                    # 'max_clusters' =
gc = jhu_primitives.GaussianClustering(hyperparams = hp)
ASEclustering_k2 = gc.produce(inputs = V[:,:int(d_hat[1])]).value

hp = jhu_primitives.gclust.gclust.Hyperparams({'max_clusters': 3})
gc = jhu_primitives.GaussianClustering(hyperparams = hp)
ASEclustering_k3 = gc.produce(inputs = V[:,:int(d_hat[1])]).value

fig, (ax1, ax2) = subplots(1, 2, figsize = (12, 6))
ax1.scatter(arange(1, len(ASEclustering_k2) + 1), ASEclustering_k2)
ax1.set_ylabel('Cluster ID')
ax1.set_xlabel('Vertex ID')
ax1.set_title('Adjacency Spectral Graph Clustering, K = 2')

ax2.scatter(arange(1, len(ASEclustering_k3) + 1), ASEclustering_k3)
ax2.set_ylabel('Cluster ID')
ax2.set_xlabel('Vertex ID')
ax2.set_title('Adjacency Spectral Graph Clustering, K = 3')

fig, (ax1, ax2) = plt.subplots(1, 2, figsize = (12, 6))
ax1.scatter(V[:,0], V[:, 1], c = ASEclustering_k2)
ax1.set_xlabel('PC 1')
ax1.set_ylabel('PC 2')
ax1.set_title('PC 2 vs PC 1 scatter, K = 2')
```

```
ax2.scatter(V[:,0], V[:, 1], c = ASEclustering_k3)
ax2.set_xlabel('PC 1')
ax2.set_ylabel('PC 2')
ax2.set_title('PC 2 vs PC 1 scatter, K = 3')
```

Out[71]: <matplotlib.text.Text at 0x26d7b88e198>



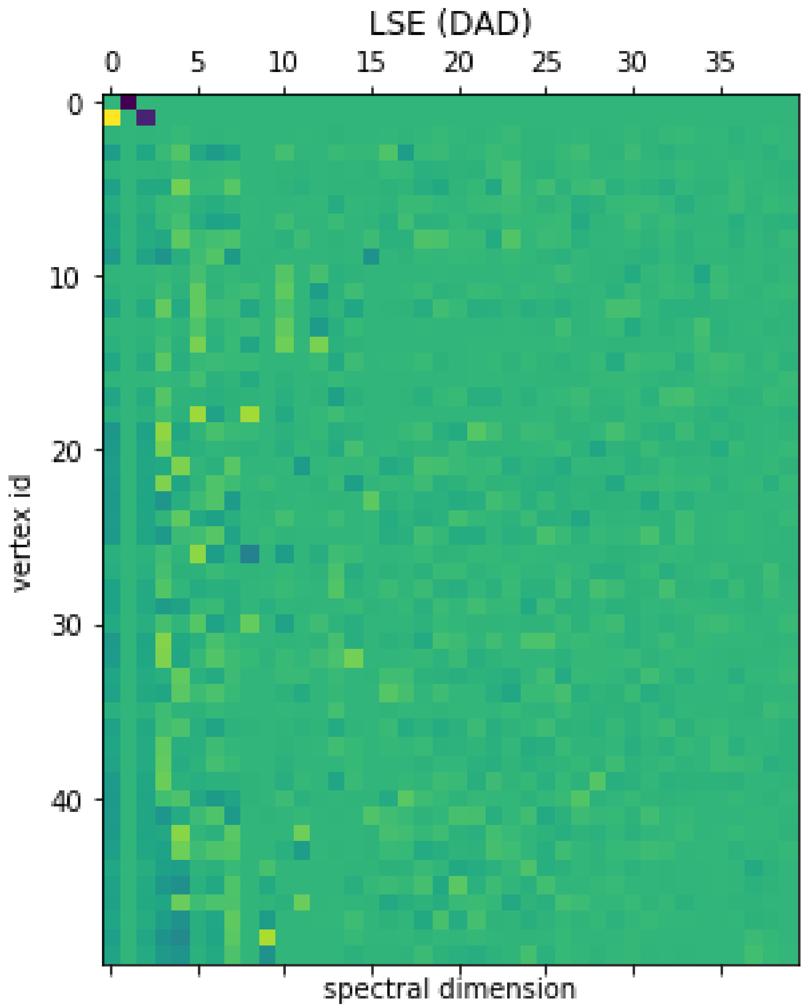

```
In [72]: gclustering == gclustering2 # including more/less dimensions can yield different clus
```

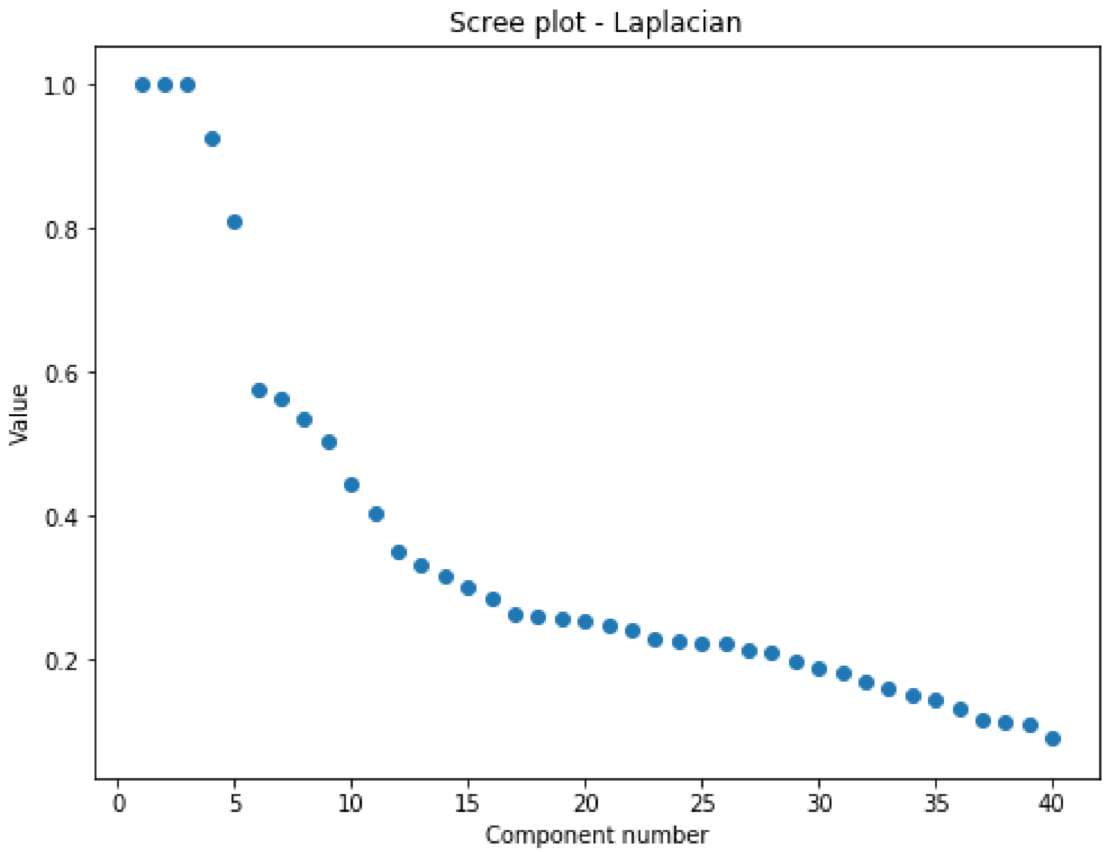
Out[72]: ndarray([True, True, True, True, True, True, False, True, True,
           True, True, True, True, True, True, True, True, True,
           True, True, True, True, True, True, True, True, True,
          False, True, True, True, True, True, True, True, True,
           True, True, True, True, True, True, True, True, True,
           True, True, True, True, True])

In [73]:
```
#LSE

d_max = 40

hp = jhu_primitives.lse.lse.Hyperparams
hp = hp({'max_dimension' : d_max})  # LSE hyperparameter(s) are:
                                    # 'max_dimension' = maximum embedding dimension (

LSE = jhu_primitives.LaplacianSpectralEmbedding(hyperparams = hp)
SVD = LSE.produce(inputs=A) # Uses the 'DAD' Laplacian
V_L = SVD.value[0]
U_L = SVD.value[1]
```

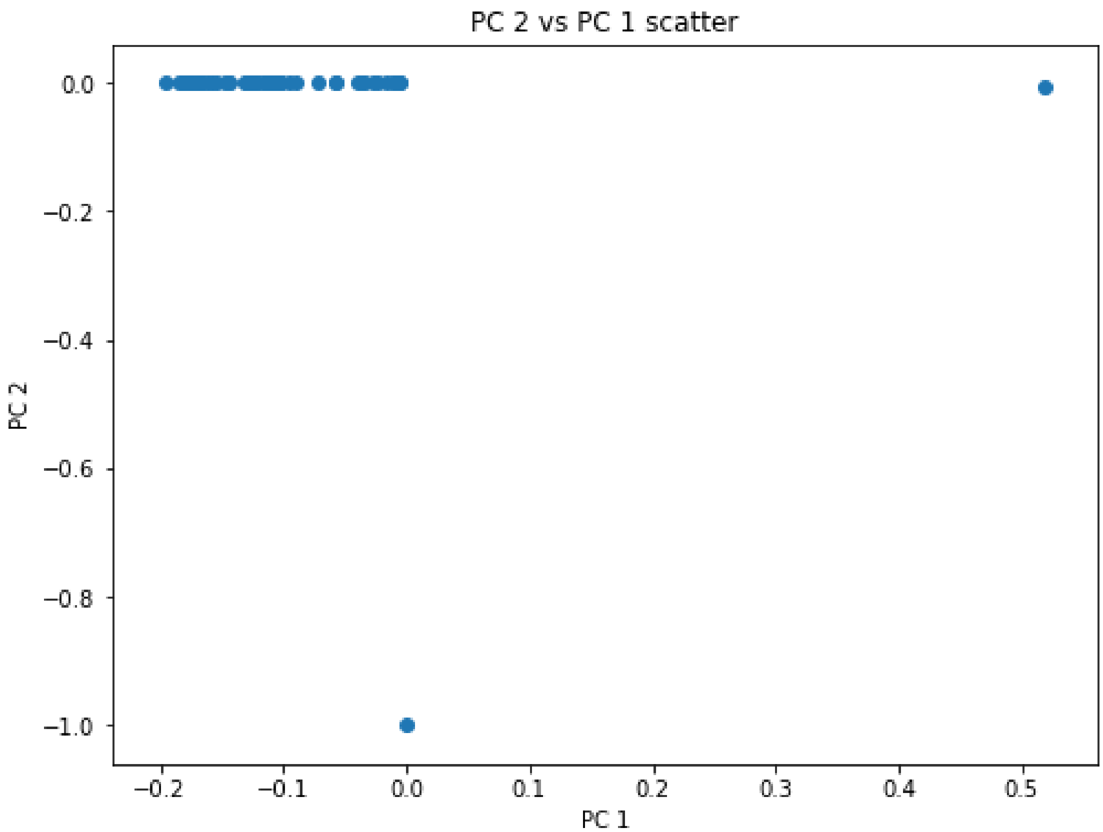
In [74]:
```
fig, ax1 = plt.subplots(1, 1, figsize = (8, 6))
ax1.matshow(V_L)
ax1.set_xlabel('spectral dimension')
ax1.set_ylabel('vertex id')
ax1.set_title('LSE (DAD)')

fig, ax2 = plt.subplots(1, 1, figsize = (8, 6))
ax2.scatter(arange(1,len(U_L) + 1), U_L**(1/2))
ax2.set_xlabel('Component number')
ax2.set_ylabel('Value')
ax2.set_title('Scree plot - Laplacian')

fig, ax3 = plt.subplots(1, 1, figsize = (8, 6))
ax3.scatter(V_L[:,0], V_L[:, 1])
ax3.set_xlabel('PC 1')
ax3.set_ylabel('PC 2')
ax3.set_title('PC 2 vs PC 1 scatter')
```

Out[74]: <matplotlib.text.Text at 0x26d160277f0>


LSE (DAD)
0
5
10
15
20
25
30
35
0
10
20
30
40
vertex id
spectral dimension

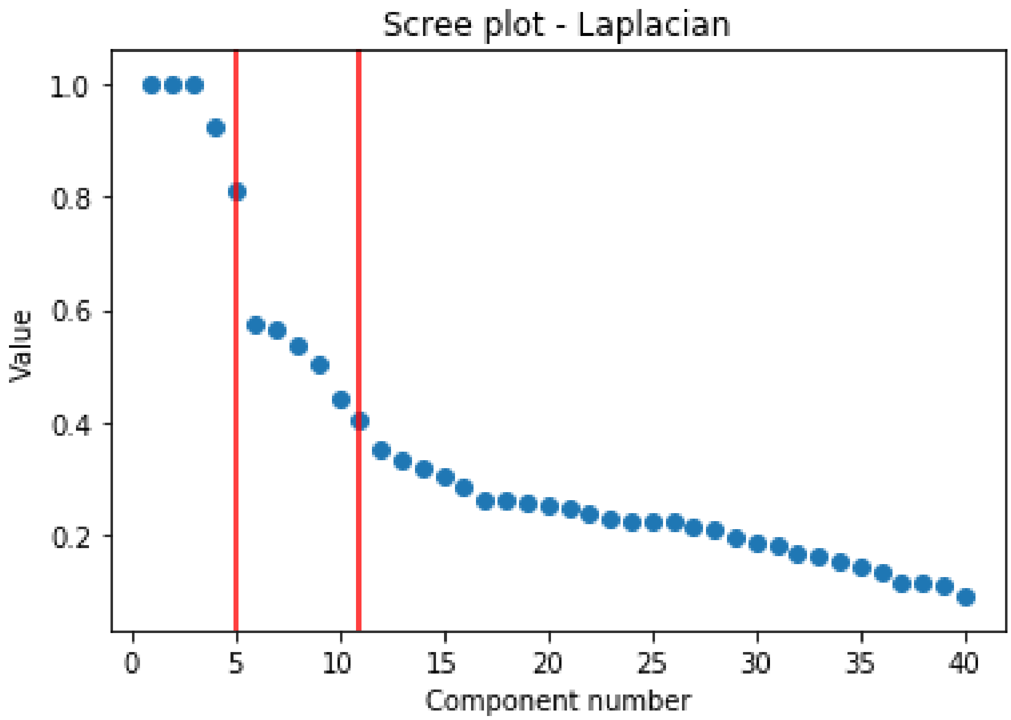


Scree plot - Laplacian
Value
Component number
1.0
0.8
0.6
0.4
0.2
0
5
10
15
20
25
30
35
40

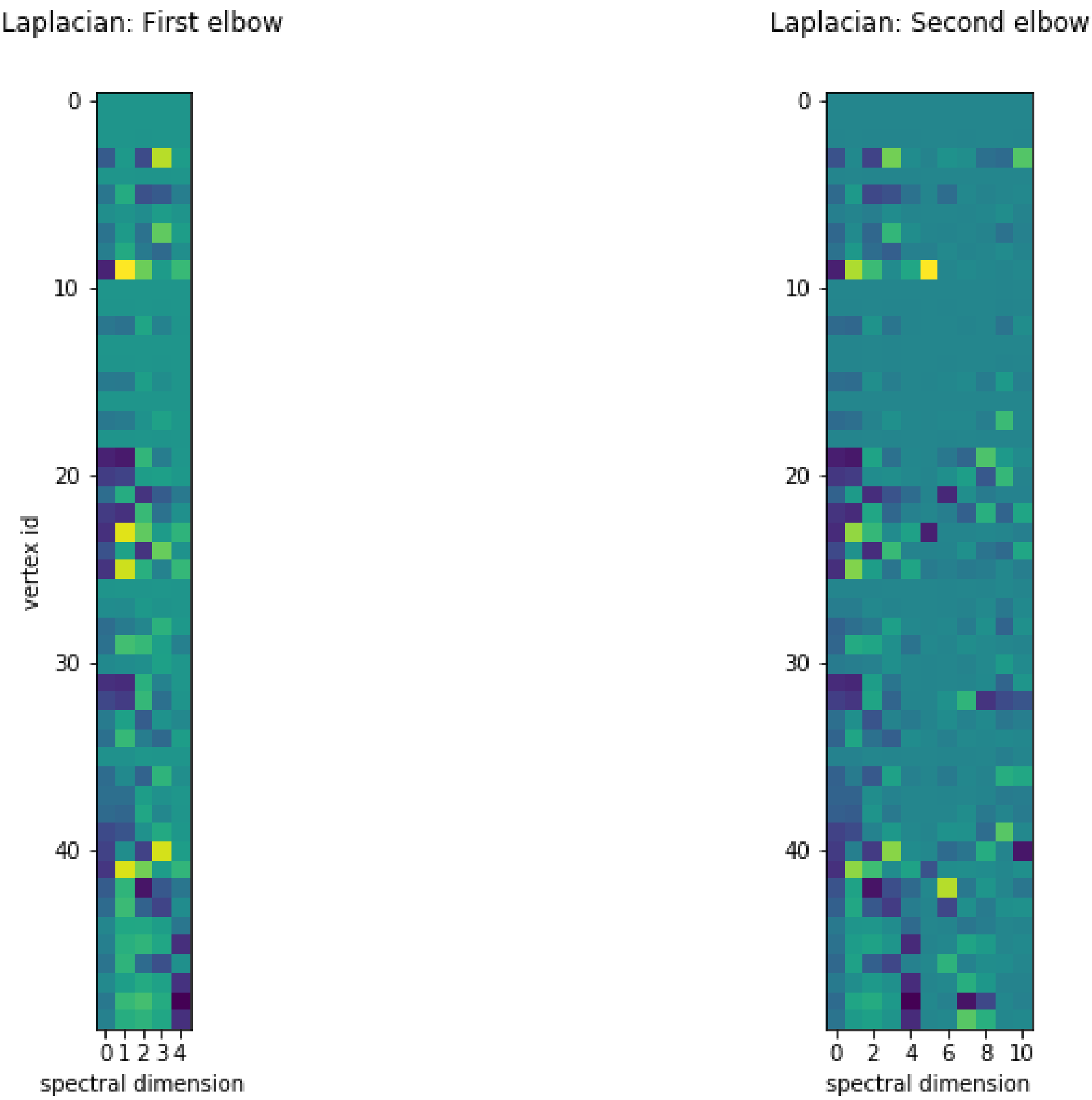


In [75]:
```
# DimensionSelection - Laplacian

fig, ax = plt.subplots(1, 1, figsize = (6, 4))
#V, U, _ = np.linalg.svd(A2)

hp = jhu_primitives.dimselect.dimselect.Hyperparams # dimselect hyperparameters are:
                                                    # 'n_elbows': the number of elbow
hp = hp({'n_elbows': 2})

dimselector = jhu_primitives.DimensionSelection(hyperparams = hp)
d_hat_L = dimselector.produce(inputs = U_L).value

ax.scatter(arange(1,len(U_L) + 1), U_L**(1/2))
for elbow in d_hat_L:
    ax.axvline(elbow, c = 'r')
ax.set_xlabel('Component number')
ax.set_ylabel('Value')
ax.set_title('Scree plot - Laplacian')
```

Out[75]:
```
<matplotlib.text.Text at 0x26d15f9af28>
```



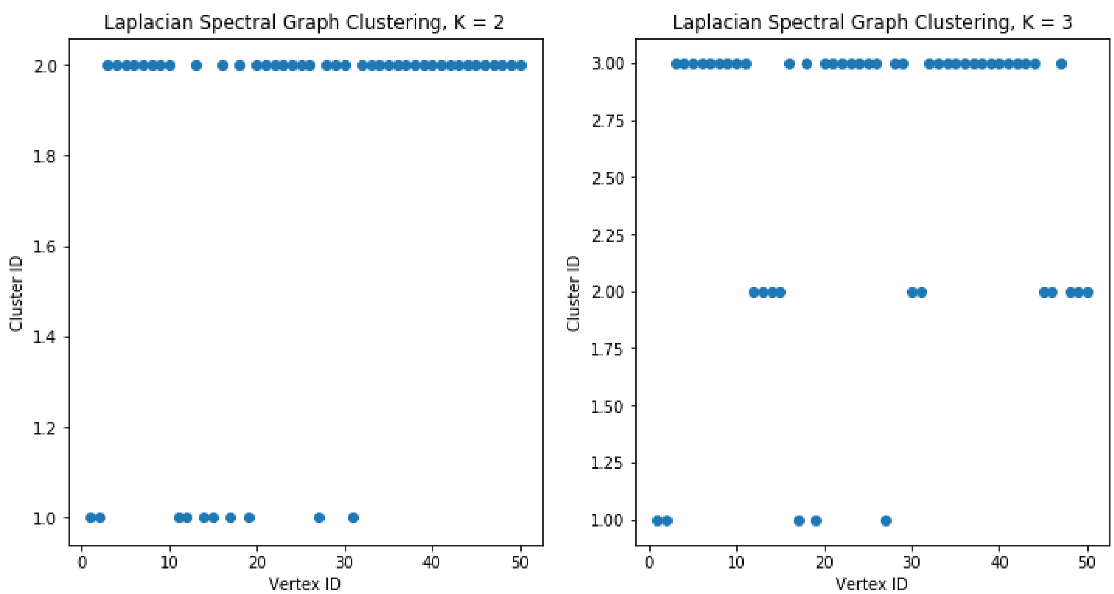

```
In [76]: # LSE - first elbow

         fig, (ax1, ax2) = subplots(1, 2, figsize = (12, 8))
         ax1.matshow(V[:,:d_hat_L[0]])
         ax1.set_xlabel('spectral dimension')
         ax1.set_ylabel('vertex id')
         ax1.set_title('Laplacian: First elbow')
         plt.colorbar
         ax1.xaxis.tick_bottom()

         # LSE - second elbow

         ax2.matshow(V[:,:d_hat_L[1]])
         ax2.set_xlabel('spectral dimension')
         ax2.set_title('Laplacian: Second elbow')
         plt.colorbar
         ax2.xaxis.tick_bottom()
```

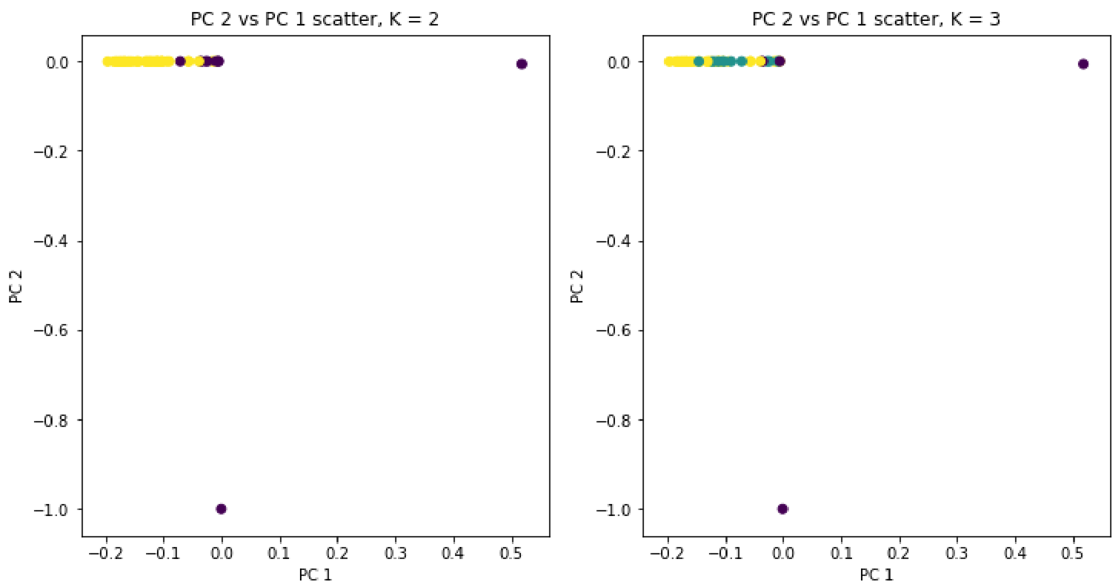



```
In [77]: # GaussianClustering - LSE - Second Elbow

         hp = jhu_primitives.gclust.gclust.Hyperparams({'max_clusters': 2}) # gclust hyperparam
         gc = jhu_primitives.GaussianClustering(hyperparams = hp)
         LSEclustering_k2 = gc.produce(inputs = V_L[:,:int(d_hat_L[1])]).value

         hp = jhu_primitives.gclust.gclust.Hyperparams({'max_clusters': 3})
         gc = jhu_primitives.GaussianClustering(hyperparams = hp)
         LSEclustering_k3 = gc.produce(inputs = V_L[:,:int(d_hat_L[1])]).value

         fig, (ax1, ax2) = subplots(1, 2, figsize = (12, 6))
         ax1.scatter(arange(1, len(LSEclustering_k2) + 1), LSEclustering_k2)
         ax1.set_ylabel('Cluster ID')
```

```python
ax1.set_xlabel('Vertex ID')
ax1.set_title('Laplacian Spectral Graph Clustering, K = 2')

ax2.scatter(arange(1, len(LSEclustering_k3) + 1), LSEclustering_k3)
ax2.set_ylabel('Cluster ID')
ax2.set_xlabel('Vertex ID')
ax2.set_title('Laplacian Spectral Graph Clustering, K = 3')

fig, (ax1, ax2) = plt.subplots(1, 2, figsize = (12, 6))
ax1.scatter(V_L[:,0], V_L[:, 1], c = LSEclustering_k2)
ax1.set_xlabel('PC 1')
ax1.set_ylabel('PC 2')
ax1.set_title('PC 2 vs PC 1 scatter, K = 2')

ax2.scatter(V_L[:,0], V_L[:, 1], c = LSEclustering_k3)
ax2.set_xlabel('PC 1')
ax2.set_ylabel('PC 2')
ax2.set_title('PC 2 vs PC 1 scatter, K = 3')
```

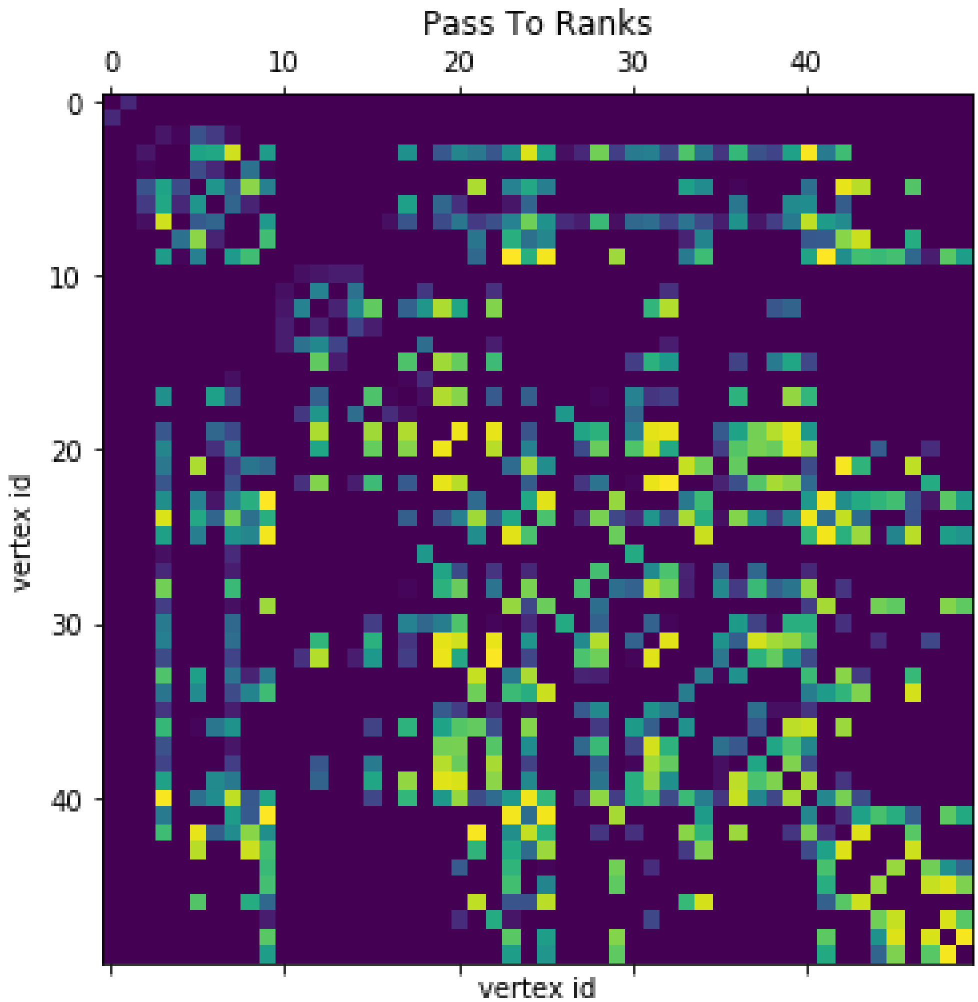
```
Out[77]: <matplotlib.text.Text at 0x26d7ba8a128>
```





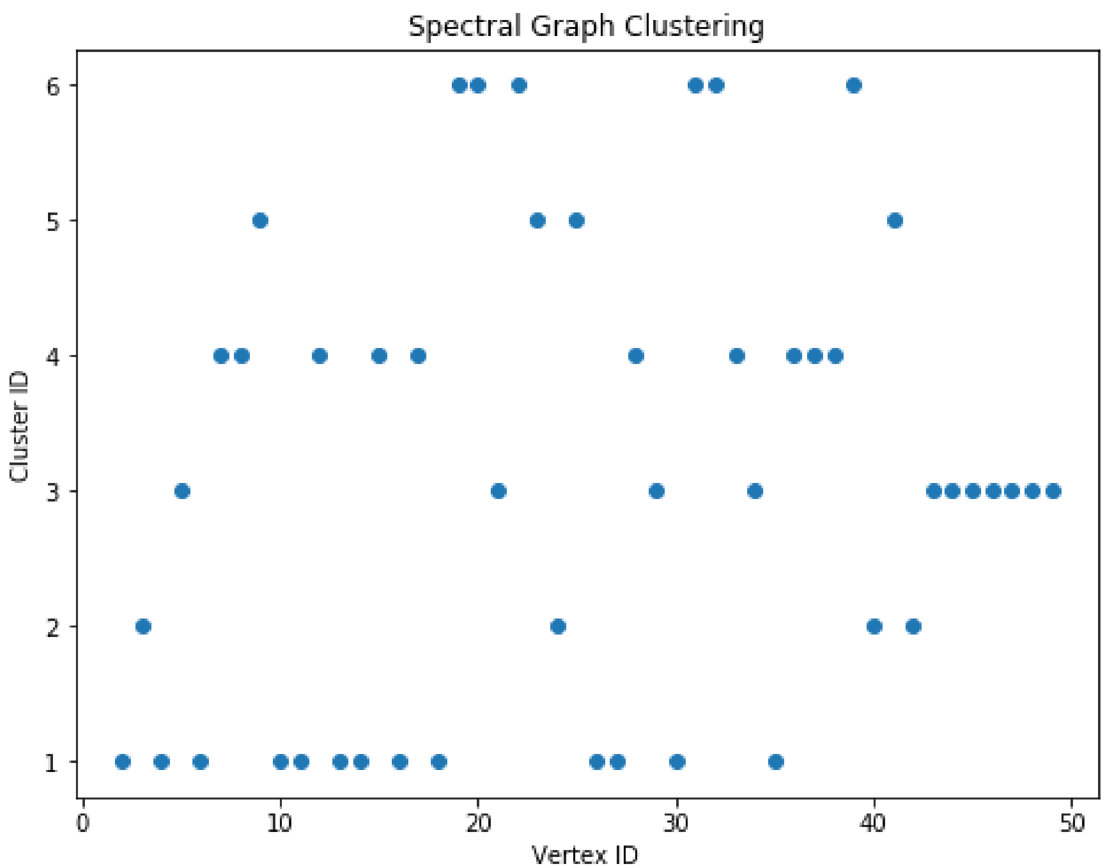
In [78]:
```python
# PassToRanks - For weighted graphs

hp = jhu_primitives.ptr.ptr.Hyperparams # PTR hyperparameters are:
                                         # None
hp = hp.defaults
ptr = jhu_primitives.PassToRanks(hyperparams = hp)
passtoranks = ptr.produce(inputs = A).value

fig, ax = subplots(1, 1, figsize=(8, 6))
ax.matshow(passtoranks)
ax.set_xlabel('vertex id')
ax.set_ylabel('vertex id')
ax.set_title('Pass To Ranks')
plt.colorbar
```

Out[78]: <function matplotlib.pyplot.colorbar>



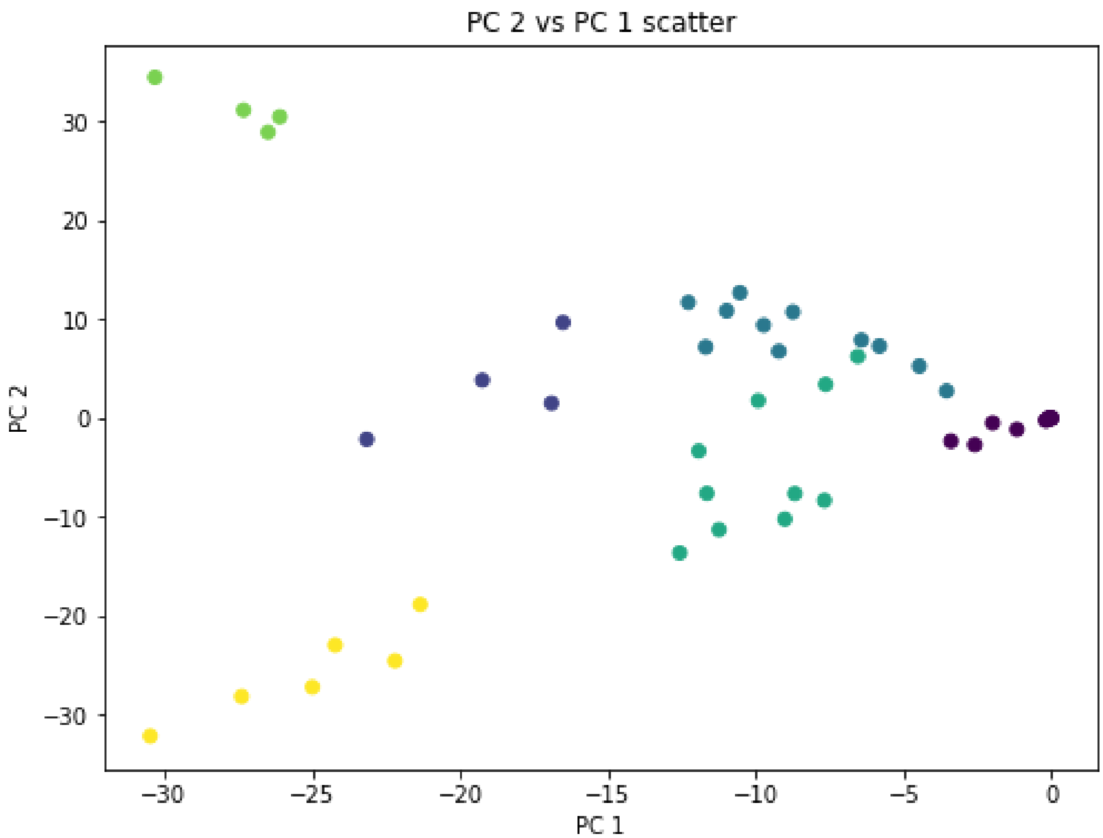

```
In [79]: # Spectral Graph Clustering - 'Super' primitive

         hp = jhu_primitives.sgc.sgc.Hyperparams # sgc hyperparameters are:
                                                 # None
         hp = hp.defaults()
         sgc = jhu_primitives.SpectralGraphClustering(hyperparams = hp)
         clusters = sgc.produce(inputs = A).value

         fig = plt.figure()
         ax = fig.add_subplot(111)
         ax.scatter(arange(2, 50), clusters)
         ax.set_ylabel('Cluster ID')
         ax.set_xlabel('Vertex ID')
         ax.set_title('Spectral Graph Clustering')
         fig.set_size_inches(8, 6)
         plt.show()
```

```python
print(len(clusters))

fig, ax3 = plt.subplots(1, 1, figsize = (8, 6))
ax3.scatter(V[2:, 0], V[2:, 1], c = clusters)
ax3.set_xlabel('PC 1')
ax3.set_ylabel('PC 2')
ax3.set_title('PC 2 vs PC 1 scatter')
```



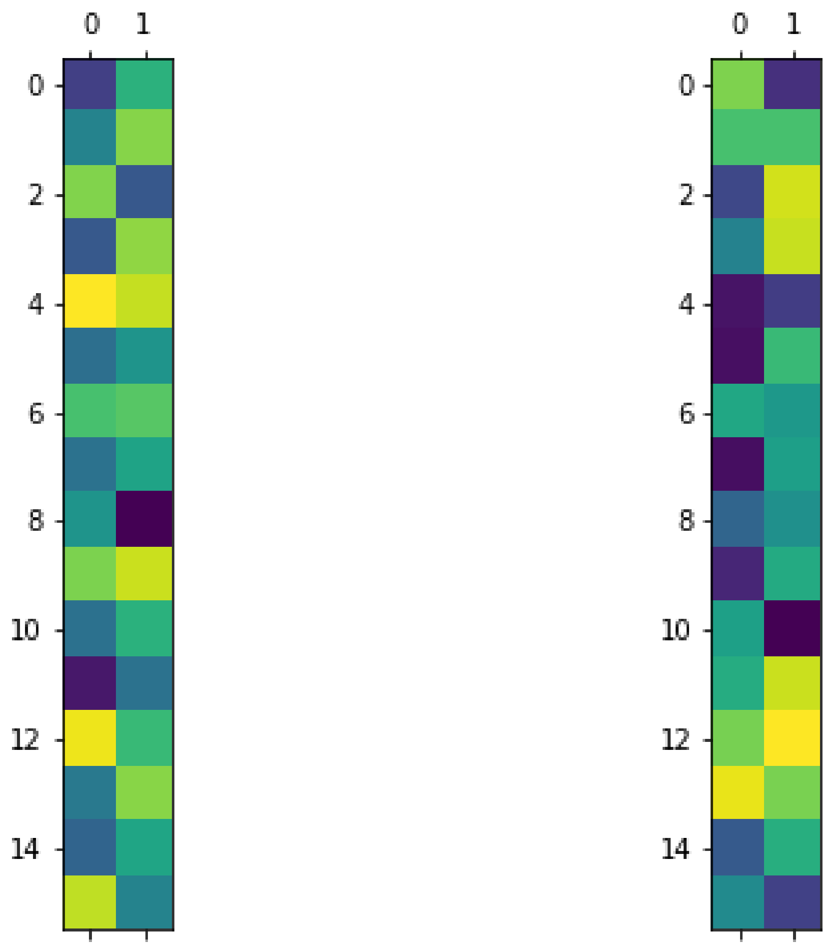
48

Out[79]: <matplotlib.text.Text at 0x26d15f2ca20>



In [80]:
```
# NonParametricCLustering

hp = jhu_primitives.nonpar.nonpar.Hyperparams  # NPC hyperparameter(s) are:
                                              # 'sigma' = scale of Gaussian (default
npc = jhu_primitives.NonParametricClustering(hyperparams = hp.defaults())

np.random.seed(1234)
xhat1 = np.random.random((16, 2))
xhat2 = np.random.random((16, 2))

fig, (ax1, ax2) = subplots(1,2, figsize = (8,6))
ax1.matshow(xhat1)
ax2.matshow(xhat2)

inputs = [xhat1, xhat2]

npc_clustering = npc.produce(inputs = inputs).value
npc_clustering
```

Out[80]:
```
ndarray([-1.01812157])
```




```
In [2]: graph1 = "C://Users/joshu/Documents/Research/d3m_summer/DS01876/DS01876_dataset/graphs/
        graph2 = "C://Users/joshu/Documents/Research/d3m_summer/DS01876/DS01876_dataset/graphs/
        g1 = nx.read_edgelist(graph1,nodetype=int, data=(('weight',float),))
        g2 = nx.read_edgelist(graph2,nodetype=int, data=(('weight',float),))
        g1 = g1.subgraph(np.arange(50)).copy()
        g2 = g2.subgraph(np.arange(50)).copy()
        g1 = nx.to_numpy_array(g1)
        nr,nc = g1.shape
        g1 = ro.r.matrix(g1, nrow=nr, ncol=nc)
        ro.r.assign("g1", g1)
        g2 = nx.to_numpy_array(g2)
        nr,nc = g2.shape
        g2 = ro.r.matrix(g2, nrow=nr, ncol=nc)
        ro.r.assign("g2", g2)
        data = np.array([g1,g2])
        hp = jhu_primitives.sgm.sgm.Hyperparams
        SGM = jhu_primitives.SeededGraphMatching(hyperparams=hp.defaults())
```

```
sgm_result = SGM.produce(inputs=data) #returns a permutation matrix
sgm_result.value
```

Out[2]:

```
ndarray([[1., 0., 0., ..., 0., 0., 0.],
         [0., 0., 0., ..., 0., 0., 0.],
         [0., 0., 0., ..., 0., 0., 0.],
         ...,
         [0., 0., 0., ..., 0., 0., 0.],
         [0., 0., 0., ..., 0., 0., 0.],
         [0., 0., 0., ..., 0., 0., 0.]])
```

In [13]:

```
# VNSGM -- in progress
#hp = jhu_primitives.vnsgm.vnsgm.Hyperparams
#VNSGM = jhu_primitives.VertexNominationSeededGraphMatching(hyperparams=hp.defaults()
#seeds = np.matrix([[2],[ 3]])
#nr,nc = seeds.shape
#seeds = ro.r.matrix(seeds,nrow=nr,ncol=nc)
#ro.r.assign("seeds",seeds)
#data = np.array([g1,g2,[1],seeds]) #1 is the vertex of interest, no seeds

#VNSGM_result = VNSGM.produce(inputs = data)
# TODO
```