Problem 2: Spectral Clustering.

1. Compute the “Laplacian matrix”, L = D−A, where D is a diagonal matrix with Dii = $\sum$ j Aij for all i. Argue that this matrix is positive semidefinite

In [1]:
```
import numpy as np
import pandas as pd
from sklearn.cluster import KMeans
import matplotlib.pyplot as plt
```

In [2]:
```
def compute_laplacian(A):
    m, n = A.shape
    D = np.zeros((m, m))
    for i in range(m):
        D[i, i] = A[i].sum()
    return D - A
```

In [3]:
```
def compute_similarity_matrix(X, sigma):
    shape = X.shape
    if len(shape) == 2:
        m, n = shape
    else:
        m = shape[0]
    K = np.zeros((m, m))
    X_sq = -2 * np.dot(X, X.T)
    X_sq = X_sq.astype(np.float64)
    X_sq += (X ** 2).sum(axis=1).reshape(-1, 1)
    X_sq += (X ** 2).sum(axis=1)
    K = X_sq / (-2 * (sigma ** 2))
    np.exp(K, K)
    return K
```

2. Compute the eigenvectors of the Laplacian using eig() in MATLAB (numpy in Python).

3. Construct a matrix V ∈ R n×k whose columns are the eigenvectors that correspond to the k smallest eigenvalues of L.

4. Let y1, . . . , yn denote the rows of V . Use the kmeans() algorithm in MATLAB (scikit-learn in Python) to cluster the rows of V into clusters S1, . . . , Sk.

5. The final clusters C1, . . . , Ck should be given by assigning vertex i of the input set to cluster Cj if yi ∈ Sj .

In [4]:
```
def form_clusters(labels, X, K):
    clusters = {}
    for i in range(len(X)):
        clusters[labels[i]] = X[i]
    return clusters

def spectral_clustering(A, K=2):
    L  =  compute_laplacian(A)
    eigen_val, eigen_vectors = np.linalg.eigh(L)
    idx = eigen_val.argsort()[0:K]
    k_eigen_val = eigen_val[idx]
    V = eigen_vectors[:,idx]
    V = np.nan_to_num(V)
    spectral = KMeans(n_clusters=K).fit(V)
    labels = spectral.labels_
    clusters = form_clusters(labels, V, K)
    return clusters, labels
```

A Simple Comparison

1. Use the spectral clustering algorithm above to compute the clustering for the matrix of twodimensional points returned by the function circs() (attached to this problem set) above with k = 2 and different values of σ.

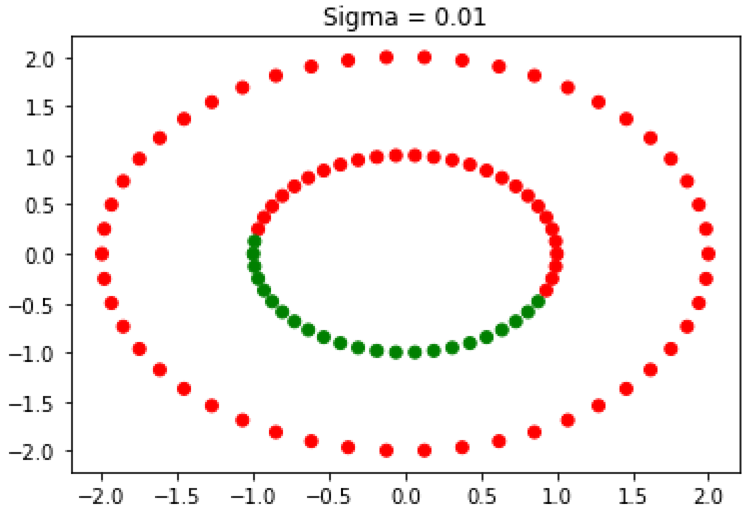
In [5]:
```
def circs():

    #X = zeros(2,100);
    #y = 0;
    #for i = 0:pi/25:2*pi
        #y = y + 1;
        #X(1, y) = cos(i);
        #X(2, y) = sin(i);
    #end
    #for i = 0:pi/25:2*pi
        #y = y + 1;
        #X(1, y) = 2*cos(i);
        #X(2, y) = 2*sin(i);
    #end


    X = np.zeros((2, 100))
    y = 0

    for i in np.arange(0, 2*np.pi, np.pi/25.0):
        X[0, y] = np.cos(i)
        X[1, y] = np.sin(i)
        y += 1

    for i in np.arange(0, 2*np.pi, np.pi/25.0):
        X[0, y] = 2*np.cos(i)
        X[1, y] = 2*np.sin(i)
        y += 1
    return X
```

In [6]:
```
X = circs().T
K = 2
```

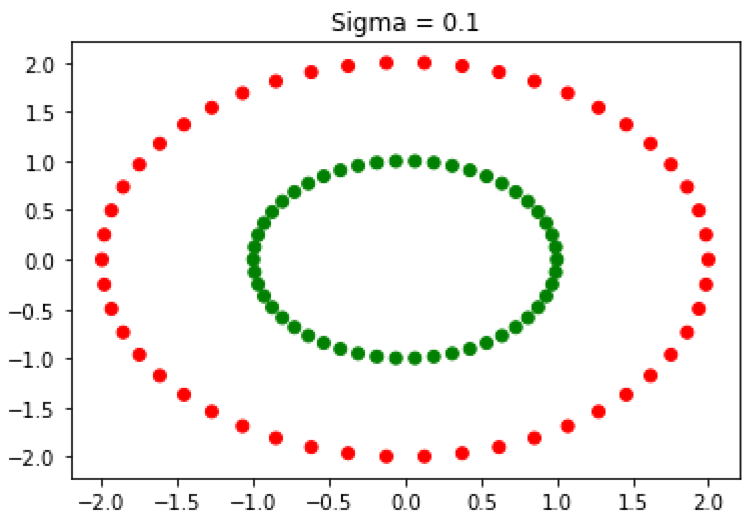
In [7]:
```
sigma_list = [0.01, 0.1, 1, 10, 100]
```

In [8]:
```
for sigma in sigma_list:
    A = compute_similarity_matrix(X, sigma)
    clusters, labels = spectral_clustering(A, K)
    label_colors = ['r' if l else 'g' for l in labels]
    plt.title(f'Sigma = {sigma}')
    plt.scatter(X[:, 0], X[:, 1], c=label_colors)
    plt.show()
```

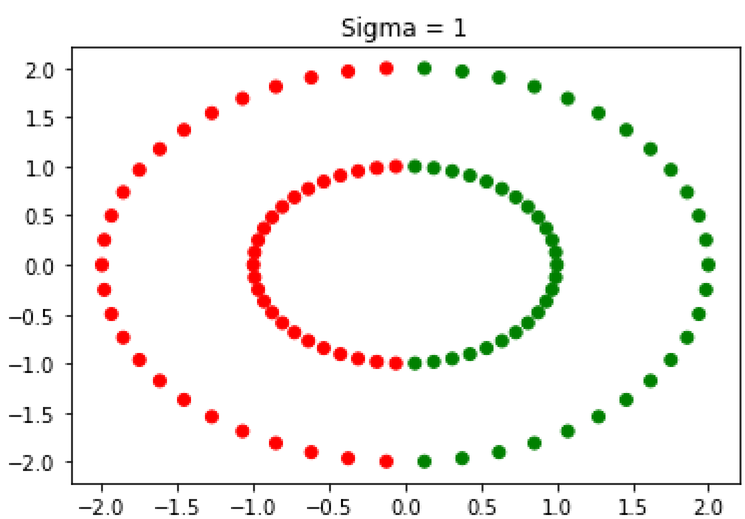
```
Laplacian Computed
Eigen values computed
```



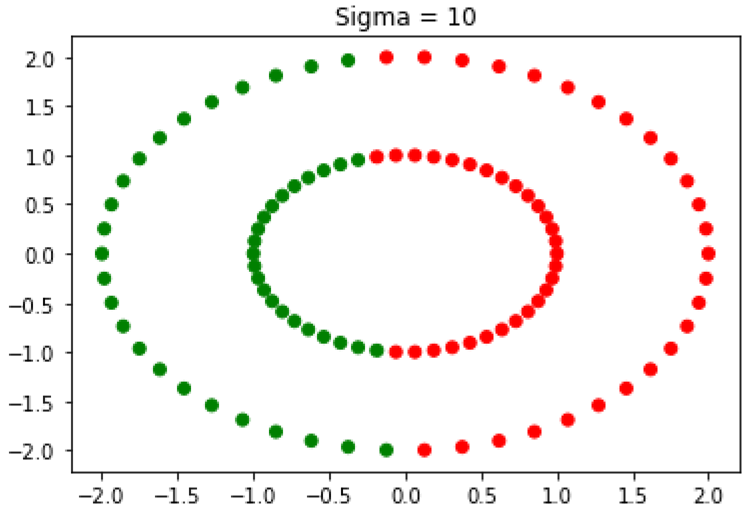

```
Laplacian Computed
Eigen values computed
```



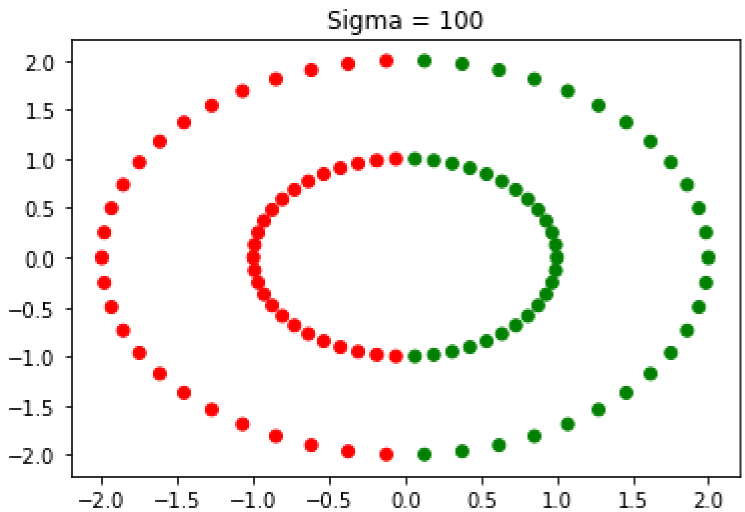

```
Laplacian Computed
Eigen values computed
```



```
Laplacian Computed
Eigen values computed
```

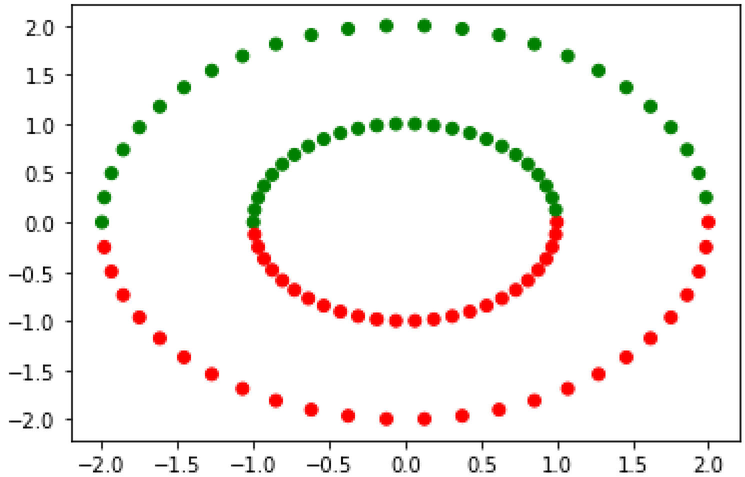



```
Laplacian Computed
Eigen values computed
```



Use the k-means algorithm in MATLAB/Python to compute an alternative clustering.

In [9]:
```
kmeans = KMeans(n_clusters=K).fit(X)
label_color = ['r' if l else 'g' for l in kmeans.labels_]
plt.scatter(X[:, 0], X[:, 1], c=label_color)
plt.show()
```



3. Find a choice of σ such that the spectral method outperforms k-means. How do you know that there is no k-means solution (i.e., a choice of centers and clusters) that performs this well? Include the output of your code in your submission

$\sigma = 0.1$ produces a good clustering compared to k-means

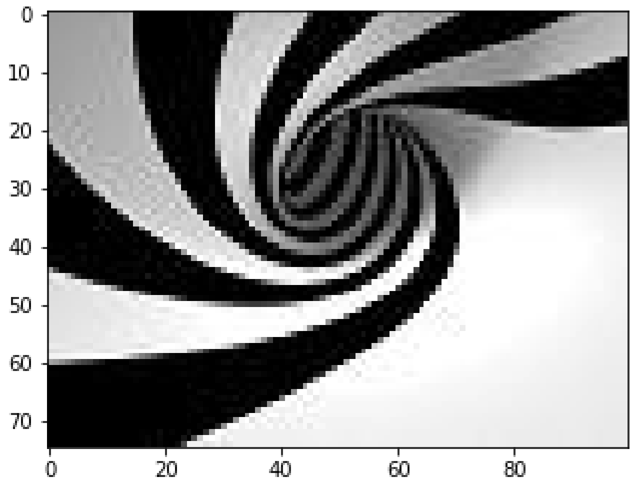
k-means is well suited for linearly separable data. This dataset with k = 2 is not linearly separable and k-means will perform poorly. However, spectral clustering is similar to applying feature map to data and then performing k-means clustering on higher dimensions where the data would be linearly separable.

Partitioning Images

1. We can use the same spectral technique to partition images. Here, we consider each pixel of a grayscale image as a single intensity and construct a similarity matrix for pairs of pixels just as before

2. Perform the same comparison of spectral clustering and k-means as before using the image bw.jpg that was attached as part of the homework. Again, set k = 2. You can use imread() to read an image from a file in MATLAB.

In [10]:
```
img = plt.imread('bw.jpg')
plt.imshow(img, cmap='gray')
h, w = img.shape
img = img.ravel()
img = img.reshape(-1,1)
```

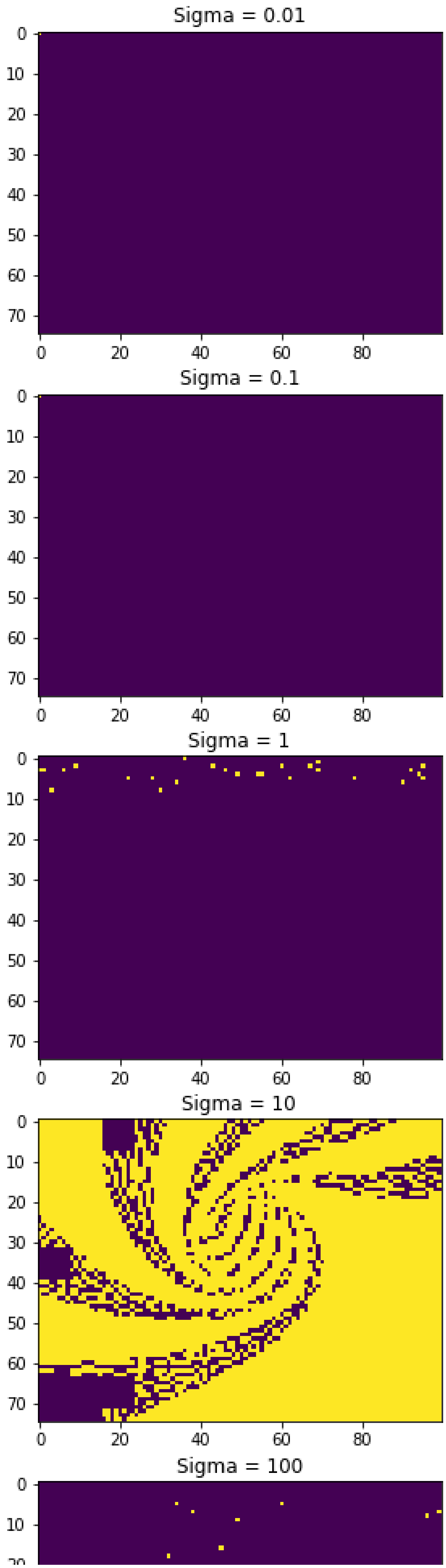


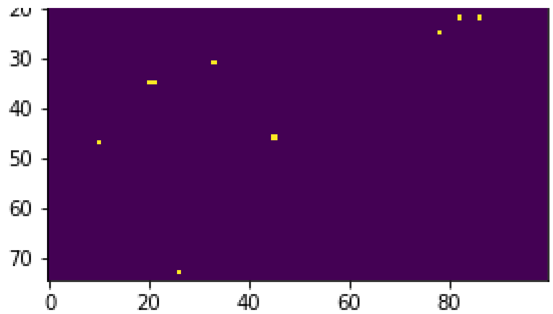
In [16]:
```
for sigma in sigma_list:
    print(f"computing for Sigma = {sigma}")
    A = compute_similarity_matrix(img, sigma)
    clusters, labels = spectral_clustering(A, K)
    image_labels = np.array(labels).astype(np.float)
    image_labels = np.reshape(image_labels, (h, w))
    plt.imsave(f'bw{sigma}.png',image_labels)
```

```
computing for Sigma = 0.01

/home/xnkr/ml/lib/python3.6/site-packages/ipykernel_launcher.py:13: RuntimeWa
rning: overflow encountered in exp
  del sys.path[0]

computing for Sigma = 0.1

/home/xnkr/ml/lib/python3.6/site-packages/ipykernel_launcher.py:13: RuntimeWa
rning: overflow encountered in exp
  del sys.path[0]

computing for Sigma = 1
computing for Sigma = 10
computing for Sigma = 100
```

In [41]:

```
fig,a =  plt.subplots(5,1,figsize=(20,20))
it = 0
for i in range(5):
    s = sigma_list[i]
    k = plt.imread(f'bw{s}.png')
    a[i].set_title(f'Sigma = {s}')
    a[i].imshow(k)
plt.show()
```


Sigma = 0.01
Sigma = 0.1
Sigma = 1
Sigma = 10
Sigma = 100



In [25]:
```
kmeans = KMeans(n_clusters=2).fit(img)
clusters_kmeans = form_clusters(kmeans.labels_, img, K)
image_labels = np.reshape(kmeans.labels_, (75, 100))
plt.imsave('bw-kmeans.jpg',image_labels)
plt.title('k-means')
plt.imshow(image_labels)
```

Out[25]: <matplotlib.image.AxesImage at 0x7fccae0d69b0>