# hw5

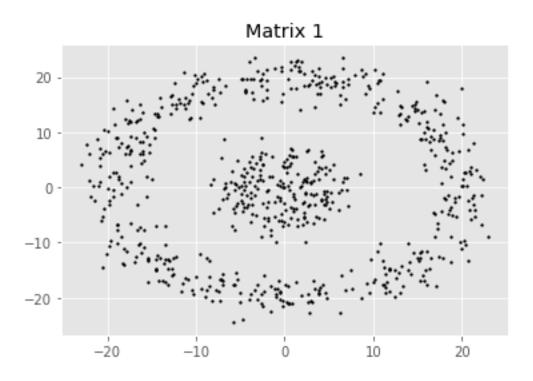
May 10, 2018

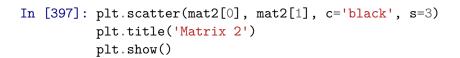
```
In [393]: import scipy.io
    import matplotlib.pyplot as plt
    import numpy as np
    import math
    import scipy

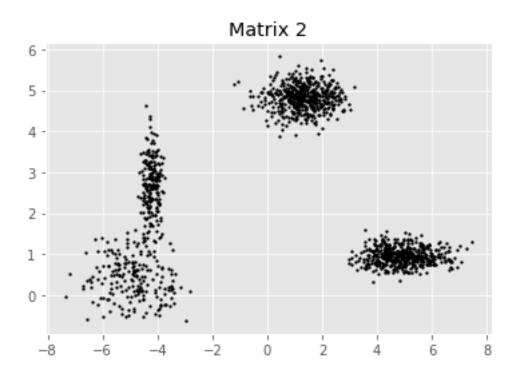
    %matplotlib inline
    plt.style.use('ggplot')
    np.random.seed(1)
```

### 1 Datasets

We have two datasets, mat1 and mat2, both consisting of 2 dimensional samples (700, 1400 respectively). We plot these on an 2D plot to examine our data before clustering.







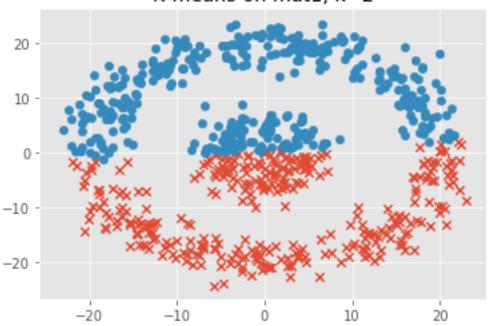
## 2 Problem 1, K-Means Clustering

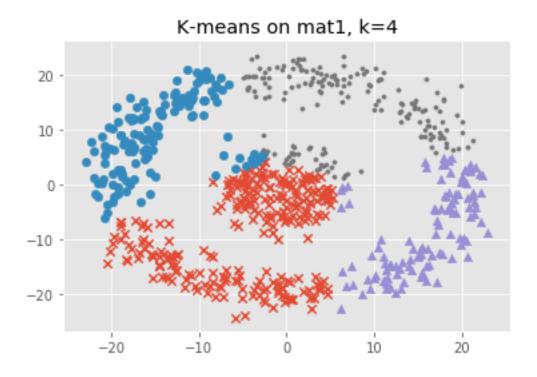
We now try out K-means. K-means can only separate clusters by linear boundaries, so we expect mat1 to be unseparable by KMeans.

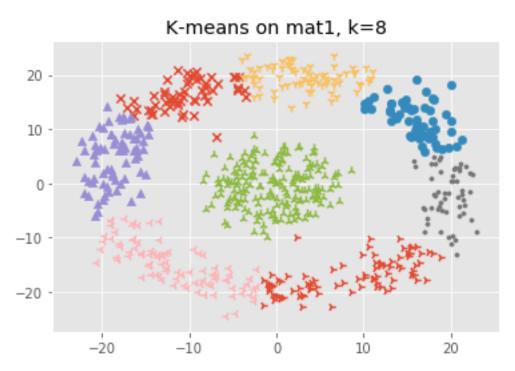
```
In [398]: def dist(a, b, ax=1):
              """ Euclidean distance """
              return np.linalg.norm(a-b, axis=ax)
In [399]: import copy
          def kmeans(X, k):
              C_x = np.random.uniform(0, np.max(X[0]), size=k)
              C_y = np.random.uniform(0, np.max(X[1]), size=k)
              C = np.array(list(zip(C_x, C_y)), dtype=np.float32)
              C_old = np.zeros(C.shape)
              clusters = np.zeros(X.shape[1])
              error = dist(C, C_old, None)
              flag = True
              while error != 0:
                  for i in range(X.shape[1]):
                      distances = dist((X[0][i], X[1][i]), C)
                      if numpy.isnan(distances).any() and flag:
                          flag = False
                          print(distances)
                          print("Coords: ")
                          print(X[0][i], X[1][i])
                          print("C: ")
                          print(C)
                      cluster = np.argmin(distances)
                      clusters[i] = cluster
                  C_old = copy.deepcopy(C)
                  for i in range(k):
                      points = np.array([(X[0][j], X[1][j]) for j in range(X.shape[1]) if clus
                      if len(points) == 0:
                          C[i] = 0
                      else:
                          C[i] = np.mean(points, axis=0)
                  error = dist(C, C_old, None)
```

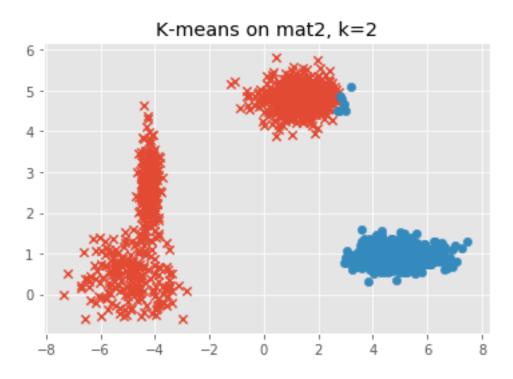
return clusters

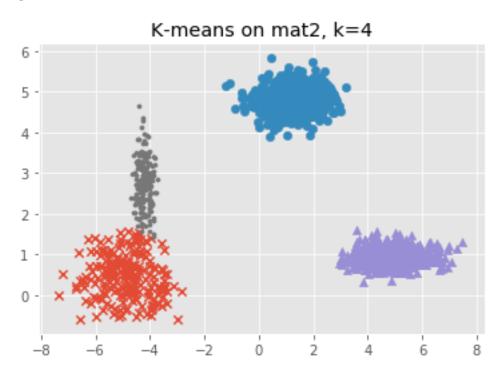
## K-means on mat1, k=2



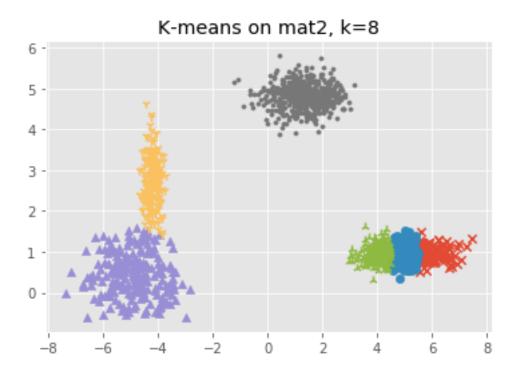








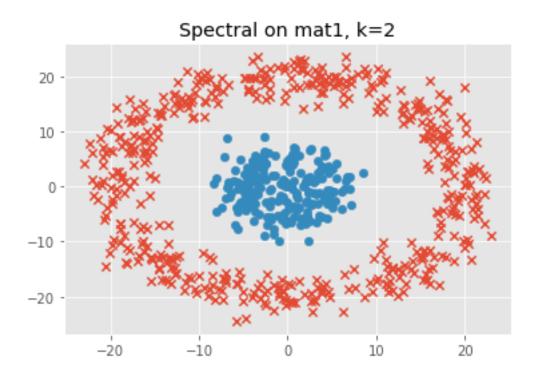
By inspection, we see that K-means clustering with 4 clusters successfully separates our mat2 data.



## 3 Problem 2, Spectral Clustering

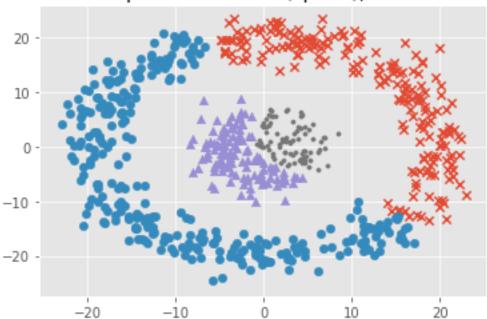
Spectral clustering, or affinity-based clustering, can handle non linearly separable classes, so it may work on mat1.

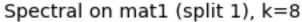
```
X = eigvec.real
              rows_norm = np.linalg.norm(X, axis=1, ord=2)
              labels = kmeans((X.T / rows_norm), k)
              return labels
In [1133]: def compute_affinity(X):
               def squared_exponential(x, y, sig=0.8, sig2=1):
                   """ Models smooth functions
                   Function from previous spectral clustering project from tut """
                   norm = numpy.linalg.norm(x - y)
                   dist = norm * norm
                   return numpy.exp(- dist / (2 * sig * sig2))
               N = X.shape[0]
               res = np.zeros((N, N))
               sig = []
               for i in range(N):
                   dists = []
                   for j in range(N):
                       dists.append(np.linalg.norm(X[i] - X[j]))
                   dists.sort()
                   sig.append(np.mean(dists[:5]))
               for i in range(N):
                   for j in range(N):
                       res[i][j] = squared_exponential(X[i], X[j], sig[i], sig[j])
               return res
In [555]: affinity1 = compute_affinity(mat1.T)
In [556]: affinity1
Out[556]: array([[1.00000000e+000, 9.07373112e-068, 2.13806994e-067, ...,
                  3.75536786e-156, 6.45797708e-058, 3.80635345e-104],
                 [9.07373112e-068, 1.00000000e+000, 1.28165649e-010, ...,
                  7.78220139e-177, 5.78066276e-003, 1.68477241e-160],
                 [2.13806994e-067, 1.28165649e-010, 1.00000000e+000, ...,
                  5.33745514e-118, 5.21226973e-015, 3.01382806e-099],
                 [3.75536786e-156, 7.78220139e-177, 5.33745514e-118, ...,
                  1.00000000e+000, 4.24887021e-210, 3.97603155e-019],
                 [6.45797708e-058, 5.78066276e-003, 5.21226973e-015, ...,
                  4.24887021e-210, 1.00000000e+000, 1.23857683e-179],
                 [3.80635345e-104, 1.68477241e-160, 3.01382806e-099, ...,
                  3.97603155e-019, 1.23857683e-179, 1.00000000e+000]])
In [697]: k1 = spectral_clustering(affinity1, 2)
          plot_clusters(mat1, k1, 2, "Spectral on mat1, k=2")
```

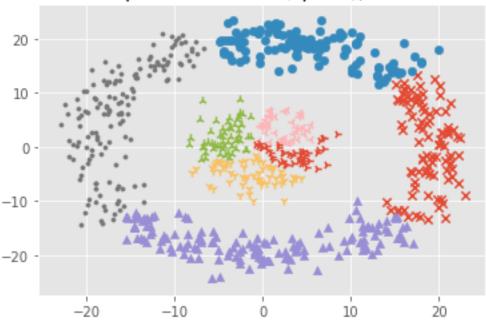


By inspection, we see that spectral clustering with 2 clusters successfully separates our mat1 data

# Spectral on mat1 (split 1), k=4







#### **Spectral Wrapper Functions**

```
In [592]: def spectral(M):
              affinity = compute_affinity(M.T)
              return spectral_clustering(affinity, 2), M
          def spectral4(M):
              Y, X = spectral(M)
              s1, s2 = M.T[[True if y==1 else False for y in Y]], X.T[[True if y==0 else False]]
              affinity1_1 = compute_affinity(s1)
              affinity1_2 = compute_affinity(s2)
              s1_labels = spectral_clustering(affinity1_1, 2)
              s2_labels = spectral_clustering(affinity1_2, 2)
              k2_labels = np.append(s1_labels, s2_labels+2)
              k2 = np.concatenate((s1, s2))
              return Y, X, k2_labels, k2
          def spectral8(M):
              Y1, X1, Y, X = \text{spectral4}(M)
              s3, s4, s5, s6 = X[[True if y==0 else False for y in Y]], X[[True if y==1 else False for y in Y]]
              affinity1_3 = compute_affinity(s3)
              affinity1_4 = compute_affinity(s4)
              affinity1_5 = compute_affinity(s5)
```

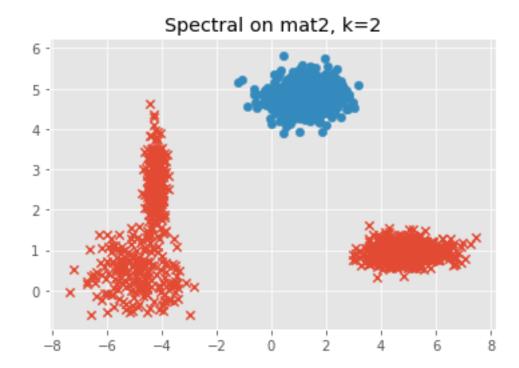
affinity1\_6 = compute\_affinity(s6)

```
s3_labels = spectral_clustering(affinity1_3, 2)
s4_labels = spectral_clustering(affinity1_4, 2)
s5_labels = spectral_clustering(affinity1_5, 2)
s6_labels = spectral_clustering(affinity1_6, 2)

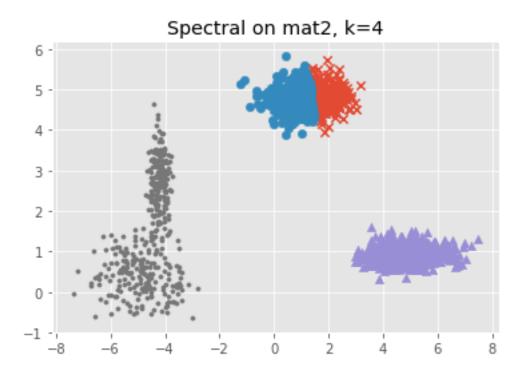
k8_labels = np.concatenate((s3_labels, s4_labels+2, s5_labels+4, s6_labels+6))
k8 = np.concatenate((s3, s4, s5, s6))
return Y1, X1, Y, X, k8_labels, k8
```

In [593]: Y1, X1, Y4, X4, Y8, X8 = spectral8(mat2)

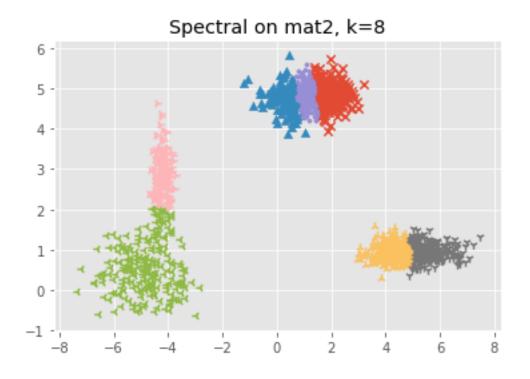
In [595]: plot\_clusters(X1, Y1, 2, "Spectral on mat2, k=2")



In [598]: plot\_clusters(X4.T, Y4, 4, "Spectral on mat2, k=4")



In [600]: plot\_clusters(X8.T, Y8, 8, "Spectral on mat2, k=8")



## 4 Problem 3: Comparison with Cost Functions

```
In [677]: def sum_squared_error(classes):
              Je = 0
              for cl in classes:
                  mean = np.mean(cl, axis=0)
                  for x in cl:
                      Je += np.inner(x-mean, x-mean)
              return Je
In [724]: def determinant(classes):
              S_W = 0
              for cl in classes:
                  mean = np.mean(cl, axis=0)
                  Si = 0
                  for i in range(np.array(cl).shape[0]):
                      S_i += np.outer(cl[:][i]-mean, cl[:][i]-mean)
                  S_W += S_i
              return np.linalg.det(S_W)
In [751]: import itertools as it
          def min_variance(classes):
              Je = 0
              for cl in classes:
                  si = np.sum([np.inner(x-y,x-y) for x,y in it.combinations(cl, 2)])
                  Je += si/np.array(cl).shape[0]
              return Je
In [737]: def transform(X, Y, n):
              arr = [[] for i in range(n)]
              for i in range(len(Y)):
                  arr[int(Y[i])].append(X[i])
              return arr
/usr/local/lib/python3.6/site-packages/numpy/core/fromnumeric.py:2957: RuntimeWarning: Mean of
  out=out, **kwargs)
/usr/local/lib/python3.6/site-packages/numpy/core/_methods.py:80: RuntimeWarning: invalid value
  ret = ret.dtype.type(ret / rcount)
In [744]: M2C2KMeans = transform(mat2.T, kmeans(mat2, k=2), 2)
          M2C4KMeans = transform(mat2.T, kmeans(mat2, k=4), 4)
          M2C8KMeans = transform(mat2.T, kmeans(mat2, k=8), 8)
          M2C2Spectral = transform(X1.T, Y1, 2)
          M2C4Spectral = transform(X4, Y4, 4)
          M2C8Spectral = transform(X8, Y8, 8)
          M1C2KMeans = transform(mat1.T, kmeans(mat1, k=2), 2)
```

```
M1C4KMeans = transform(mat1.T, kmeans(mat1, k=4), 4)
          M1C8KMeans = transform(mat1.T, kmeans(mat1, k=8), 8)
          M1C2Spectral = transform(mat1.T, k1, 2)
          M1C4Spectral = transform(k2, k2_labels, 4)
          M1C8Spectral = transform(k8, k8_labels, 8)
In [743]: e1 = sum_squared_error(M2C2KMeans)
          e2 = sum_squared_error(M2C4KMeans)
          e3 = sum_squared_error(M2C8KMeans)
          e4 = sum_squared_error(M2C2Spectral)
          e5 = sum_squared_error(M2C4Spectral)
          e6 = sum_squared_error(M2C8Spectral)
          e7 = sum_squared_error(M1C2KMeans)
          e8 = sum_squared_error(M1C4KMeans)
          e9 = sum_squared_error(M1C8KMeans)
          e10 = sum_squared_error(M1C2Spectral)
          e11 = sum_squared_error(M1C4Spectral)
          e12 = sum_squared_error(M1C8Spectral)
/usr/local/lib/python3.6/site-packages/numpy/core/fromnumeric.py:2957: RuntimeWarning: Mean of
  out=out, **kwargs)
/usr/local/lib/python3.6/site-packages/numpy/core/_methods.py:80: RuntimeWarning: invalid value
 ret = ret.dtype.type(ret / rcount)
4.0.1 Sum Squared Error
In [738]: print("Sum Squared Error, Dataset 2")
          print("C=2 | KMeans: " + str(e1) + " Spectral: " + str(e4))
          print("C=4 | KMeans: " + str(e2) + " Spectral: " + str(e5))
          print("C=8 | KMeans: " + str(e3) + " Spectral: " + str(e6))
Sum Squared Error, Dataset 2
C=2 | KMeans: 11523.462641572416 Spectral: 12980.544476534591
C=4 | KMeans: 1308.589852762342 Spectral: 1367.4907262152626
C=8 | KMeans: 1249.690428419723 Spectral: 556.4301312921771
In [739]: print("Sum Squared Error, Dataset 1")
          print("C=2 | KMeans: " + str(e7) + " Spectral: " + str(e10))
          print("C=4 | KMeans: " + str(e8) + " Spectral: " + str(e11))
          print("C=8 | KMeans: " + str(e9) + " Spectral: " + str(e12))
Sum Squared Error, Dataset 1
C=2 | KMeans: 131904.90415142267 Spectral: 207710.95870316675
C=4 | KMeans: 67243.97450008814 Spectral: 129584.95960087515
C=8 | KMeans: 20491.671457244076 Spectral: 44623.695784612944
```

**Discussion** These results do not compare well with the visual observations given by the above clustering algorithms. When we increase the number of clusters, the numerical error obviously decreases. However, we see that dataset 1 (mat1) obviously has only 2 classes, so k=2 is the best (and is visually so, with the spectral clustering), but the numerical error decreases as we increase k. For dataset 2 which is linearly separable, KMeans and Spectral almost perform the same. This is not the case for dataset 1, where with K=2 Spectral successfully separates the clusters but KMeans does not. And yet, Spectral's sum squared error is 207710 > KMean's SSE of 139335.

#### 4.0.2 Determinant

```
In [745]: e1 = determinant(M2C2KMeans)
          e2 = determinant(M2C4KMeans)
          e3 = determinant(M2C8KMeans)
          e4 = determinant(M2C2Spectral)
          e5 = determinant(M2C4Spectral)
          e6 = determinant(M2C8Spectral)
          e7 = determinant(M1C2KMeans)
          e8 = determinant(M1C4KMeans)
          e9 = determinant(M1C8KMeans)
          e10 = determinant(M1C2Spectral)
          e11 = determinant(M1C4Spectral)
          e12 = determinant(M1C8Spectral)
/usr/local/lib/python3.6/site-packages/numpy/core/fromnumeric.py:2957: RuntimeWarning: Mean of
  out=out, **kwargs)
/usr/local/lib/python3.6/site-packages/numpy/core/_methods.py:80: RuntimeWarning: invalid value
 ret = ret.dtype.type(ret / rcount)
In [746]: print("Determinant, Dataset 2")
          print("C=2 | KMeans: " + str(e1) + " Spectral: " + str(e4))
          print("C=4 | KMeans: " + str(e2) + " Spectral: " + str(e5))
          print("C=8 | KMeans: " + str(e3) + " Spectral: " + str(e6))
Determinant, Dataset 2
C=2 | KMeans: 8107128.413448382 Spectral: 26358947.80734672
C=4 | KMeans: 145456.4670150636 Spectral: 446531.7034244581
C=8 | KMeans: 84989.73206552764 Spectral: 72199.32401656003
In [747]: print("Determinant, Dataset 1")
          print("C=2 | KMeans: " + str(e7) + " Spectral: " + str(e10))
          print("C=4 | KMeans: " + str(e8) + " Spectral: " + str(e11))
          print("C=8 | KMeans: " + str(e9) + " Spectral: " + str(e12))
Determinant, Dataset 1
C=2 | KMeans: 3285283551.736198 Spectral: 10751492347.651451
C=4 | KMeans: 975897318.337423 Spectral: 2557848611.074802
C=8 | KMeans: 120141496.7612552 Spectral: 494209586.2569458
```

#### 4.0.3 Min Variance

```
In [753]: e1 = min_variance(M2C2KMeans)
          e2 = min_variance(M2C4KMeans)
          e3 = min_variance(M2C8KMeans)
          e4 = min_variance(M2C2Spectral)
          e5 = min_variance(M2C4Spectral)
          e6 = min_variance(M2C8Spectral)
          e7 = min_variance(M1C2KMeans)
          e8 = min_variance(M1C4KMeans)
          e9 = min_variance(M1C8KMeans)
          e10 = min_variance(M1C2Spectral)
          e11 = min_variance(M1C4Spectral)
          e12 = min_variance(M1C8Spectral)
/usr/local/lib/python3.6/site-packages/ipykernel_launcher.py:7: RuntimeWarning: invalid value
  import sys
In [756]: print("Min Variance, Dataset 2")
          print("C=2 | KMeans: " + str(e1) + " Spectral: " + str(e4))
          print("C=4 | KMeans: " + str(e2) + " Spectral: " + str(e5))
          print("C=8 | KMeans: " + str(e3) + " Spectral: " + str(e6))
Min Variance, Dataset 2
C=2 | KMeans: 11523.46264157244 Spectral: 12980.544476534602
C=4 | KMeans: 955.5036139177143 Spectral: 1367.4907262152633
C=8 | KMeans: 637.8077128578185 Spectral: nan
In [757]: print("Min Variance, Dataset 1")
          print("C=2 | KMeans: " + str(e7) + " Spectral: " + str(e10))
          print("C=4 | KMeans: " + str(e8) + " Spectral: " + str(e11))
          print("C=8 | KMeans: " + str(e9) + " Spectral: " + str(e12))
Min Variance, Dataset 1
C=2 | KMeans: 131839.5046818803 Spectral: 207710.95870316686
C=4 | KMeans: 63969.713173109674 Spectral: 129584.9596008751
C=8 | KMeans: 22066.58996087212 Spectral: 44623.69578461293
```

**Discussion** We also note that Min Variance and Sum Squared Error are equivalent in this case.

## 5 Problem 4: Expectation Maximization

We use expectation maximization with gaussian assumption (gaussian mixture model) to find parameters (means, covariances, and priors) for the gaussian PDF. Once we converge (or in this case, run for 100 iterations), we use the last cluster result as our clustering.

This should be the slower of the three algorithms on this dataset without algorithmic optimization.

In [761]: mat2.shape

```
Out[761]: (2, 1400)
In [781]: for i in range(2,9):
              # find priors, means, and covariances
              print(i)
2
3
4
5
6
7
8
In [1081]: from scipy.stats import multivariate_normal
           def prob(val, mean, cov, prior):
               p = prior
               for i in range(len(val)):
                   try:
                       p *= multivariate_normal.pdf(val[i], mean[i], cov[i][i])
                   except IndexError:
                       p *= 1.0
               return p
5.0.1 Part A: Expectation Maximization
In [1094]: C_results = dict()
           for C in [2,4,8]:
               # initial parameters
               means = np.array([np.random.uniform(-5,5,2) for i in range(C)])
               covs = np.array([np.eye(2) for i in range(C)])
               priors = np.array([1.0/c] * C)
               clusters = []
               for i in range(10):
                   # evaluate most likely clusters for every point, given current parameters
                   clusters[:] = []
                   for i in range(mat2.shape[1]):
                       point = mat2[0][i], mat2[1][i]
                       cluster = np.argmax([prob(point, means[cl], covs[cl], priors[cl]) for cl
```

clusters.append(cluster)

```
# reestimate parameters given current clusters
assignments = np.array([np.concatenate(np.argwhere(np.array(clusters)==i)) :
populations = np.array([len(i) for i in assignments])
ratios = populations / np.sum(populations)

means = np.array([np.mean(np.squeeze(np.dstack((mat2[0][assignments[i]], matcovs = np.array([np.cov(np.squeeze(np.dstack((mat2[0][assignments[i]], mat2priors = np.array(ratios)

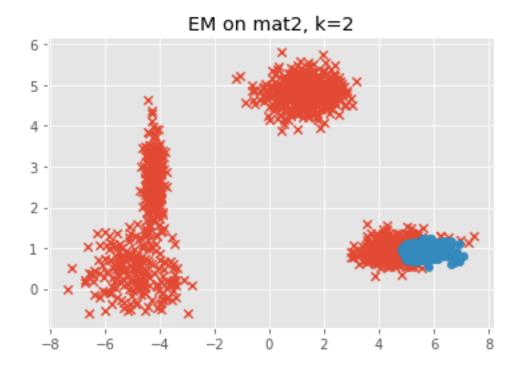
# get final clusters
for i in range(mat2.shape[1]):
    point = mat2[0][i], mat2[1][i]
    cluster = np.argmax([prob(point, means[cl], covs[cl], priors[cl]) for cl in clusters.append(cluster)

C_results[C] = clusters, means, covs, priors
```

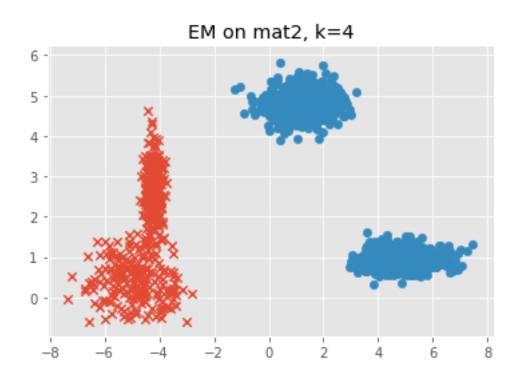
We use 10 iterations instead of 100 because of computer heating issues, and because of reasonable convergence with 10 iterations.

#### 5.0.2 Part B: Clustering

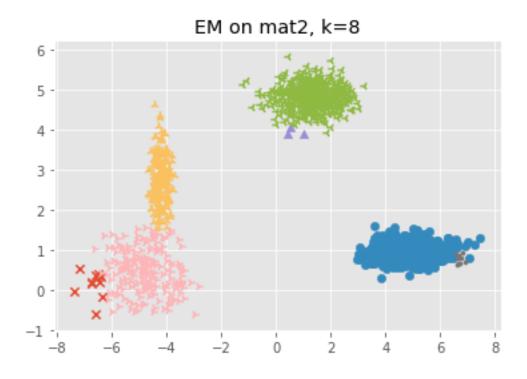
In [1095]: plot\_clusters(mat2, C\_results[2][0], 2, "EM on mat2, k=2")



```
In [1096]: plot_clusters(mat2, C_results[4][0], 4, "EM on mat2, k=4")
```



In [1097]: plot\_clusters(mat2, C\_results[8][0], 8, "EM on mat2, k=8")



#### 5.0.3 Comparison with Cost Functions

```
In [1116]: M2C2EM = transform(mat2.T, C_results[2][0][:1400], 2)
           M2C4EM = transform(mat2.T, C_results[4][0][:1400], 4)
          M2C8EM = transform(mat2.T, C_results[8][0][:1400], 8)
In [1130]: e1 = sum_squared_error(M2C2KMeans)
           e2 = sum_squared_error(M2C4KMeans)
           e3 = sum_squared_error(M2C8KMeans)
           e4 = sum_squared_error(M2C2Spectral)
           e5 = sum_squared_error(M2C4Spectral)
           e6 = sum_squared_error(M2C8Spectral)
           e7 = sum_squared_error(M2C2EM)
           e8 = sum_squared_error(M2C4EM)
           e9 = sum_squared_error(M2C8EM)
/usr/local/lib/python3.6/site-packages/numpy/core/fromnumeric.py:2957: RuntimeWarning: Mean of
  out=out, **kwargs)
/usr/local/lib/python3.6/site-packages/numpy/core/_methods.py:80: RuntimeWarning: invalid value
 ret = ret.dtype.type(ret / rcount)
In [1118]: print("Sum Squared Error, Dataset 2")
           print("C=2 | KMeans: " + str(e1) + " Spectral: " + str(e4) + " EM: " + str(e7))
           print("C=4 | KMeans: " + str(e2) + " Spectral: " + str(e5) + " EM: " + str(e8))
           print("C=8 | KMeans: " + str(e3) + " Spectral: " + str(e6) + " EM: " + str(e9))
Sum Squared Error, Dataset 2
C=2 | KMeans: 11523.462641572429 Spectral: 12980.544476534591 EM: 19650.16853656148
C=4 | KMeans: 955.5036139177154 Spectral: 1367.4907262152626 EM: 8523.805188355976
C=8 | KMeans: 637.8077128578192 Spectral: 556.4301312921771 EM: 877.5695135612715
In [1126]: e1 = min_variance(M2C2KMeans)
           e2 = min_variance(M2C4KMeans)
           e3 = min_variance(M2C8KMeans)
           e4 = min_variance(M2C2Spectral)
           e5 = min_variance(M2C4Spectral)
           e6 = min_variance(M2C8Spectral)
           e7 = min_variance(M2C2EM)
           e8 = min_variance(M2C4EM)
           e9 = min_variance(M2C8EM)
/usr/local/lib/python3.6/site-packages/ipykernel_launcher.py:7: RuntimeWarning: invalid value
  import sys
In [1131]: print("Min Variance, Dataset 2")
          print("C=2 | KMeans: " + str(e1) + " Spectral: " + str(e4) + " EM: " + str(e7))
           print("C=4 | KMeans: " + str(e2) + " Spectral: " + str(e5) + " EM: " + str(e8))
```

print("C=8 | KMeans: " + str(e3) + " Spectral: " + str(e6) + " EM: " + str(e9))

```
Min Variance, Dataset 2
C=2 | KMeans: 11523.462641572429 Spectral: 12980.544476534591 EM: 19650.16853656148
C=4 | KMeans: 955.5036139177154 Spectral: 1367.4907262152626 EM: 8523.805188355976
C=8 | KMeans: 637.8077128578192 Spectral: 556.4301312921771 EM: 877.5695135612715
In [1128]: e1 = determinant(M2C2KMeans)
           e2 = determinant(M2C4KMeans)
           e3 = determinant(M2C8KMeans)
           e4 = determinant(M2C2Spectral)
           e5 = determinant(M2C4Spectral)
           e6 = determinant(M2C8Spectral)
           e7 = determinant(M2C2EM)
           e8 = determinant(M2C4EM)
           e9 = determinant(M2C8EM)
/usr/local/lib/python3.6/site-packages/numpy/core/fromnumeric.py:2957: RuntimeWarning: Mean of
  out=out, **kwargs)
/usr/local/lib/python3.6/site-packages/numpy/core/_methods.py:80: RuntimeWarning: invalid value
  ret = ret.dtype.type(ret / rcount)
In [1129]: print("Min Variance, Dataset 2")
           print("C=2 | KMeans: " + str(e1) + " Spectral: " + str(e4) + " EM: " + str(e7))
           print("C=4 | KMeans: " + str(e2) + " Spectral: " + str(e5) + " EM: " + str(e8))
           print("C=8 | KMeans: " + str(e3) + " Spectral: " + str(e6) + " EM: " + str(e9))
Min Variance, Dataset 2
C=2 | KMeans: 8107128.413448382 Spectral: 26358947.80734672 EM: 64168696.66829248
C=4 | KMeans: 145456.4670150636 Spectral: 446531.7034244581 EM: 6951116.3744544815
C=8 | KMeans: 84989.73206552764 Spectral: 72199.32401656003 EM: 128323.23851540437
   Problem 5: HMMs
Transitions P(S1 \mid S1) = 0.8, P(S2 \mid S1) = 0.2, P(S1 \mid S2) = 0.2, P(S2 \mid S2) = 0.8
Emissions P(A \mid S1) = 0.4, P(C \mid S1) = 0.1, P(G \mid S1) = 0.4, P(T \mid S1) = 0.1
   P(A \mid S2) = 0.1, P(C \mid S2) = 0.4, P(G \mid S2) = 0.1, P(T \mid S2) = 0.4
Priors P(S1) = 0.5, P(S2) = 0.5
   Please see the P5.pdf
```