THE UNIVERSITY OF TEXAS AT AUSTIN
Department of Statistics and Data Sciences
College of Natural Sciences

Advanced Predictive Models for Complex Data

Lecture 5: Clustering

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Clustering

- Given n data points, we want to divide them into K groups such that
  - datapoints in a group are very similar to each other
  - datapoints in two different groups are less similar

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- But how to define similarity?
- Let us start with something very simple. We will use the Euclidean distance as dis-similarity) between two points.

k-means clustering

- The k-means loss is given by:

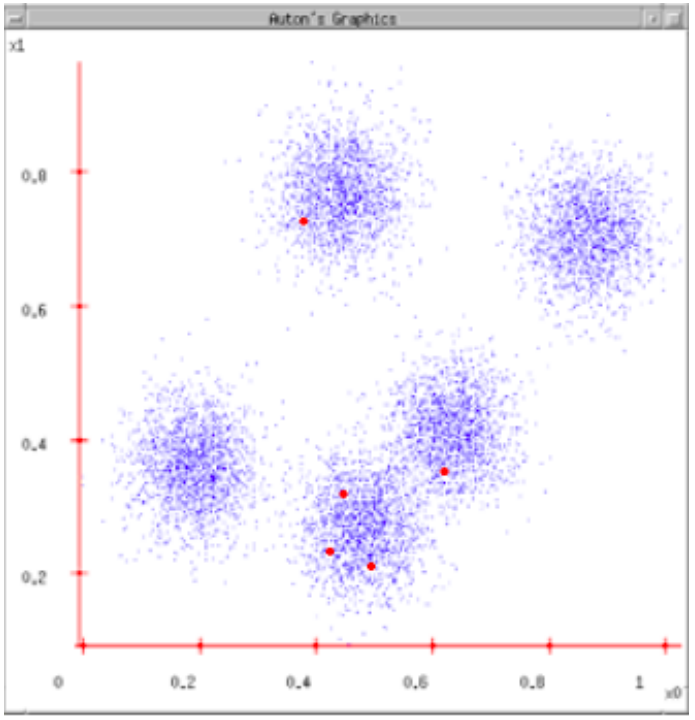
$$\sum_{k} \sum_{i \in C_k} \| x_i - \mu_k \|^2$$

The k^{th} cluster

k^{th} cluster center

The algorithm

- Initialization: randomly guess k cluster center.



Courtesy: Andrew W. Moore's k-means slides at CMU

The algorithm

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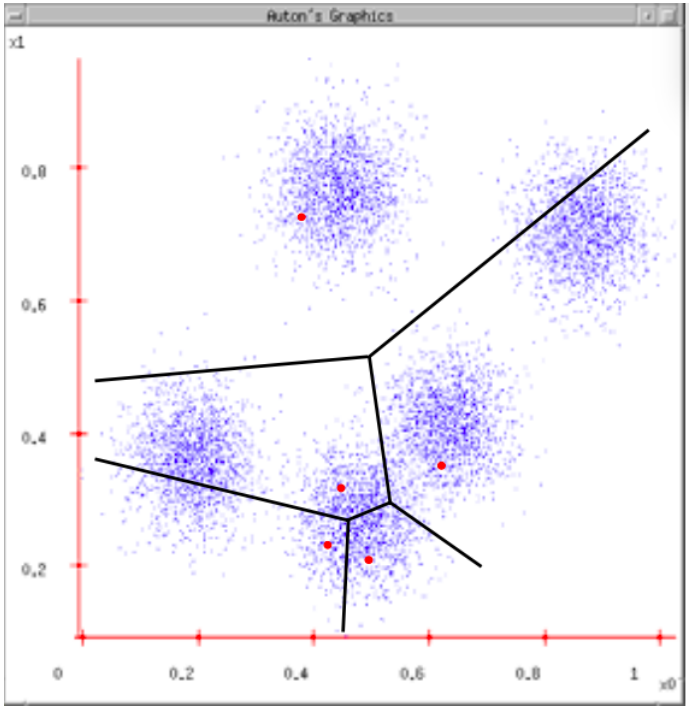
- In each iteration, each point finds out which cluster it is closest to.



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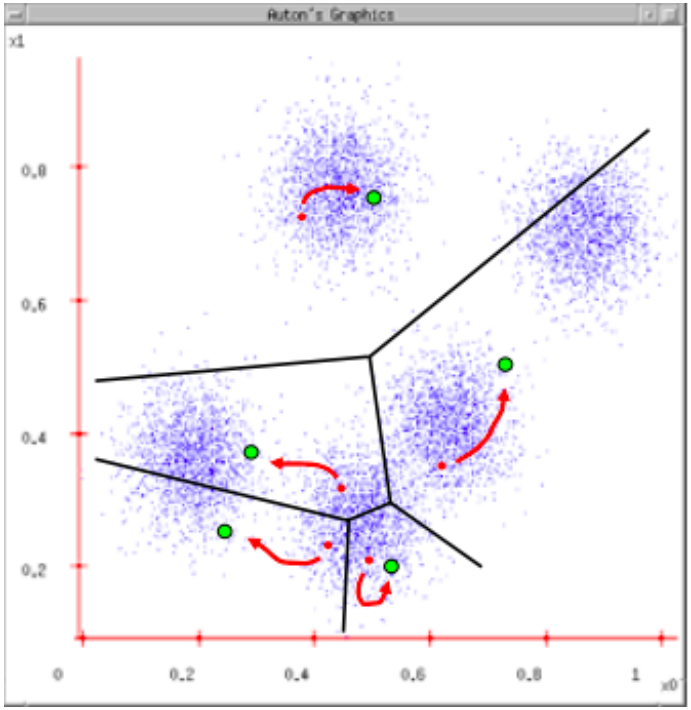

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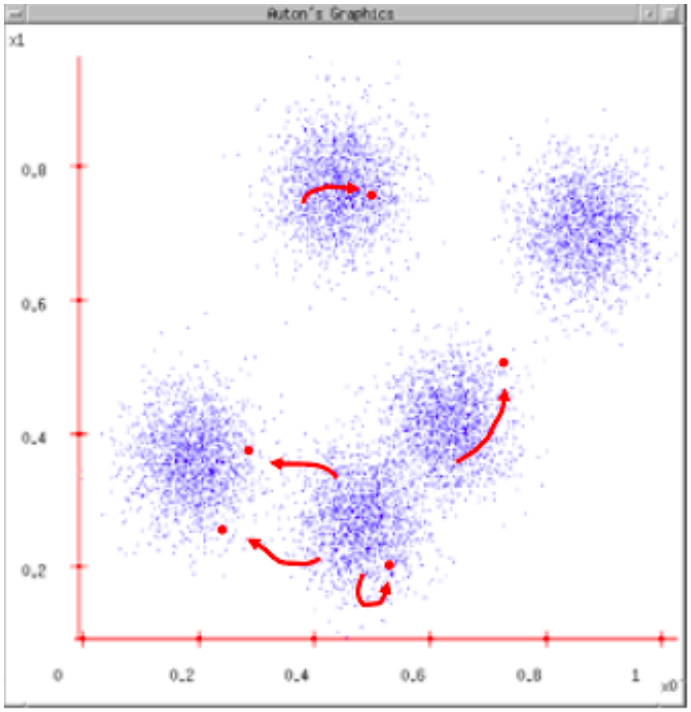
The algorithm

- Initialization: randomly guess k cluster center.
- In each iteration, each point finds out which cluster it is closest to.
- Each cluster computes the centroid of points belonging to it
- Make those the new centroids and continue.



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A video

https://miro.medium.com/max/335/1*JUm9BrH21dEiGpHg76AImw.gif

Courtest: Sunny K. Tuladhar

So all is well?

- The k-means algorithm will converge to a local optima, not necessarily a global one.
- A bad initialization may lead to a poor local optima.

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Figure 1: Courtesy: https://www.geeksforgeeks.org/ml-k-means-algorithm/

What if I give you funny looking clusters

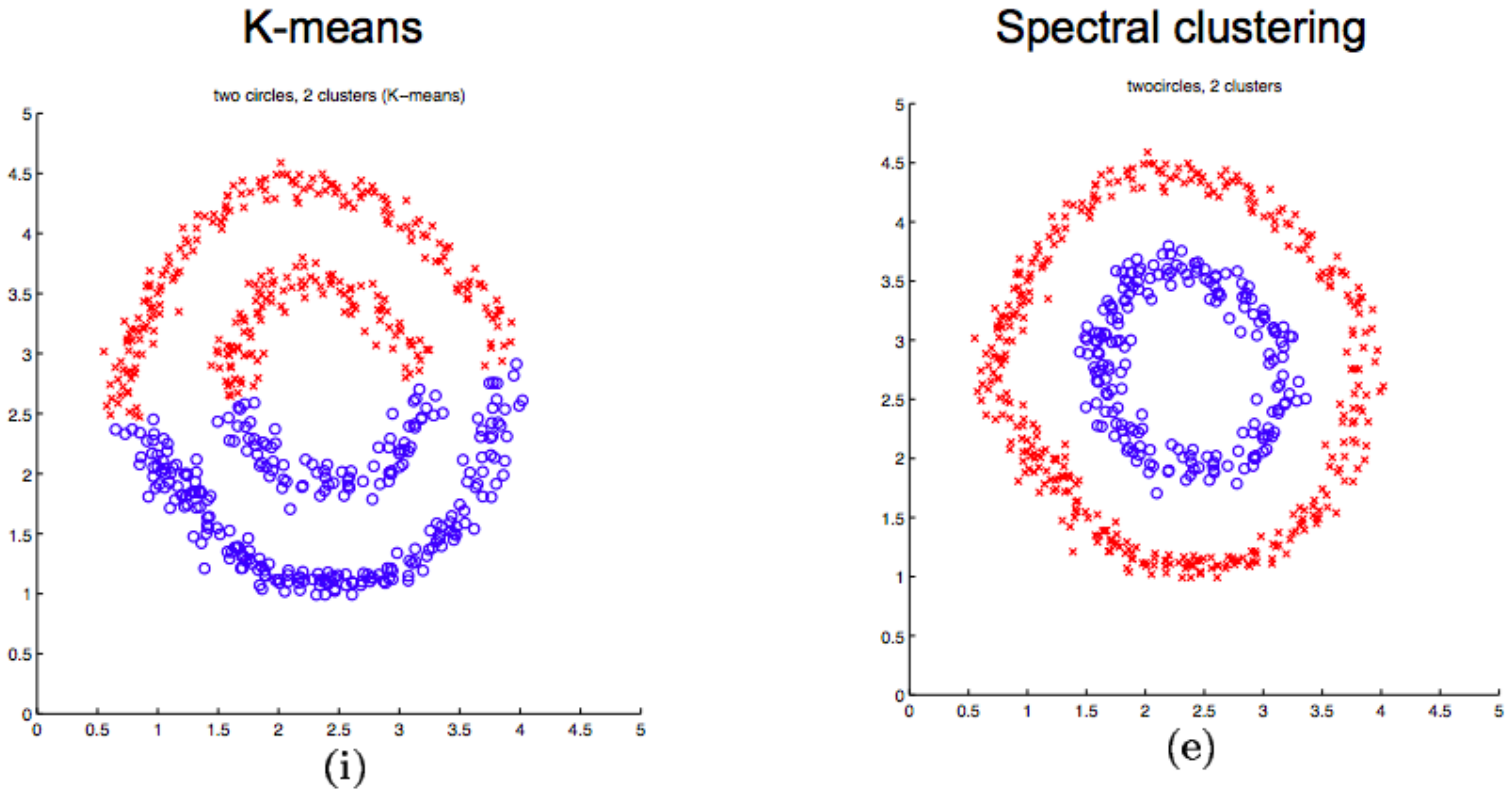


Figure 2: Shi and Malik '00; Ng, Jordan, and Weiss NIPS '01]

Spectral Clustering

The graph partitioning view

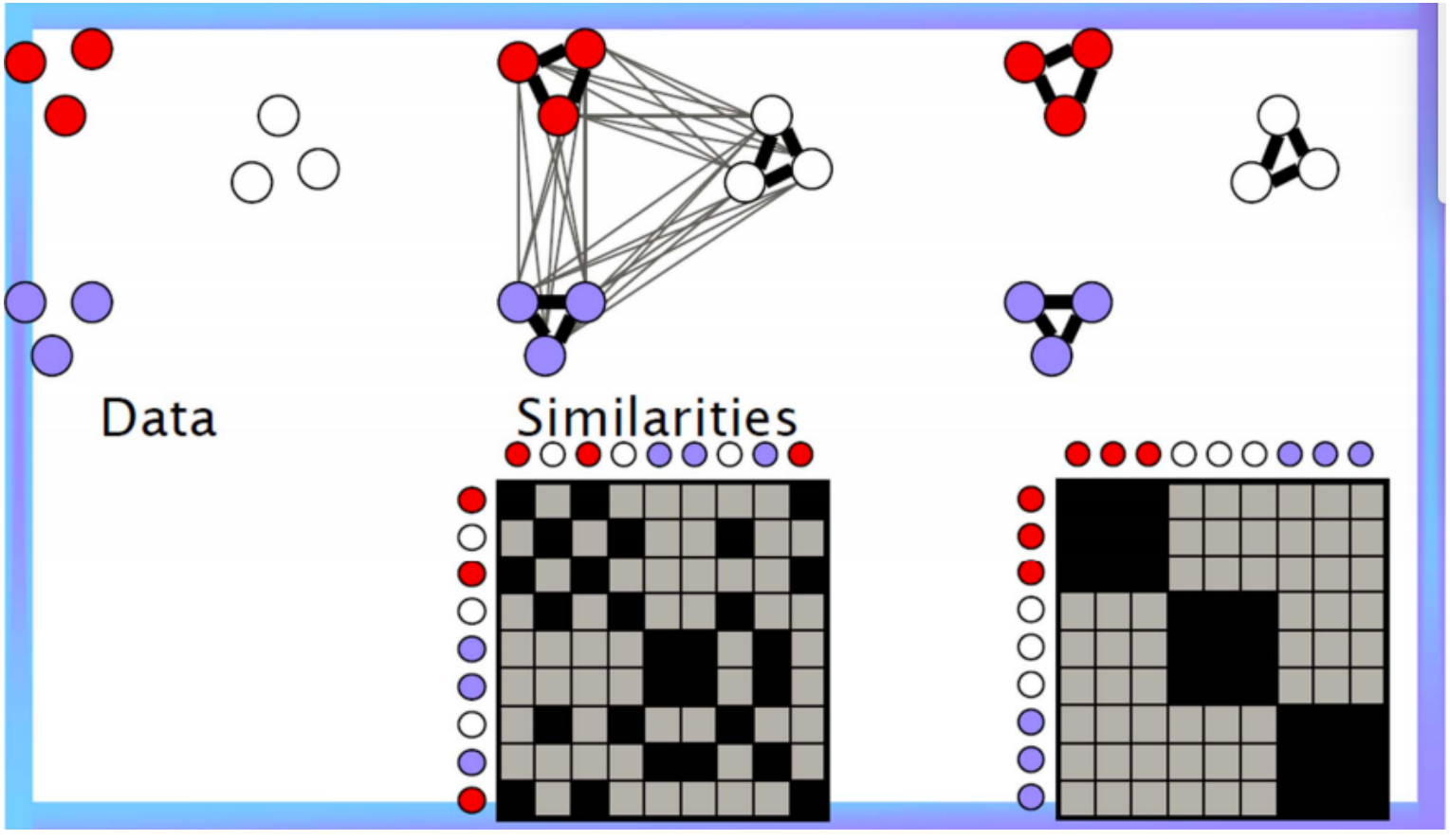


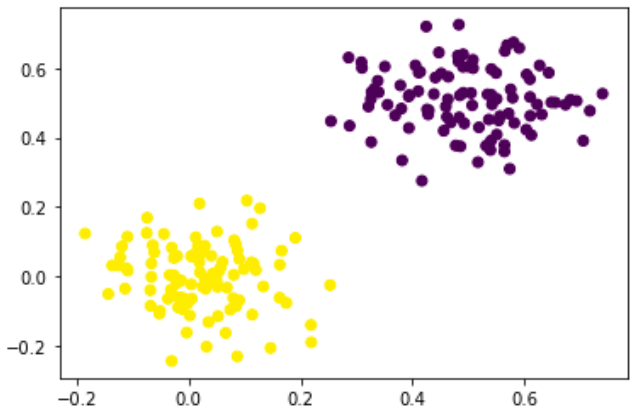
Figure 3: David Sontag's class notes

The Spectral Clustering algorithm in Ng, Jordan and Weiss

- Given dataset $x_1, \ldots x_n$ first form the affinity or similarity matrix $A \in \mathbb{R}^{n \times n}$ such that $A_{ij} = \exp(-\|x_i - x_j\|^2 / 2\sigma^2)$, and set the diagonal to zero.
- Let D be a diagonal matrix whose $D_{ii} = \sum_j A_{ij}$. Construct $L = D^{-1/2} A D^{-1/2}$
- Find the top K eigenvectors of L $v_1, \ldots v_K$ and build the matrix Y with these along the columns.
- Normalize the rows of Y to have length 1.
- Treating rows of Y as data points in K dimensions, run k-means with K clusters.

Try it out

- There are K Gaussians
- For each datapoint, you first decide which Gaussian it comes from by drawing from a multinomial with parameters $(\pi_1, \ldots, \pi_K)$
- If datapoint i comes from center i, then generate it from $N(\mu_i, \Sigma_i)$
- Goal: Given the data, figure out which gaussians/clusters/component it came from, and their parameters.



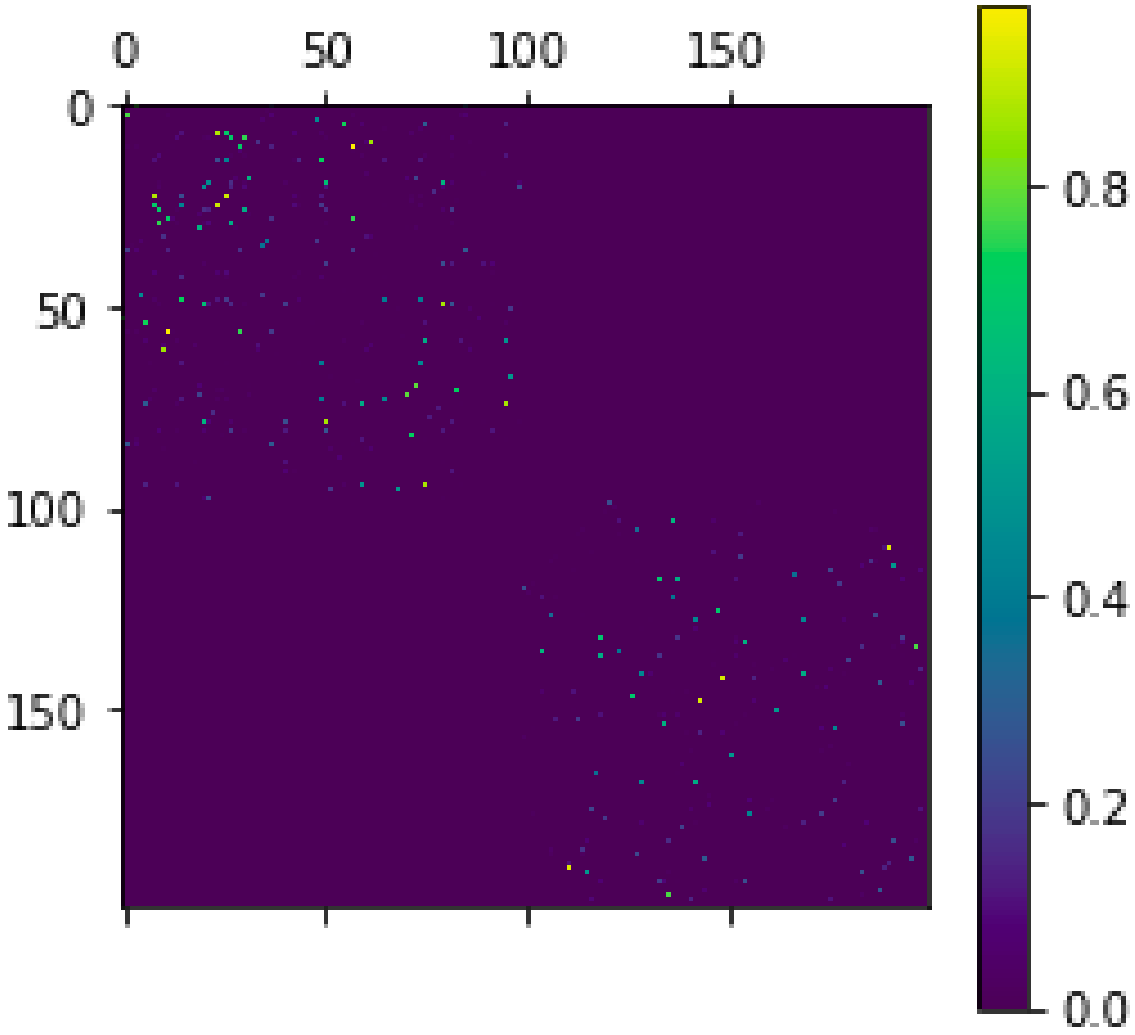
- $K = 2$
- $\pi = (.5, .5)$
- Spherical Gaussians

Try it out

```
: from scipy.spatial.distance import pdist, squareform
from sklearn import metrics
D=metrics.pairwise_distances(X,X)
s=.01
K=np.exp(-D**2/(2*s**2))
K=K-np.diag(np.diag(K))
D1=np.diag(sum(K,axis=0)**(-.5))
K1=D1.dot(K).dot(D1)
```

- Build the Kernel matrix and normalize it.

What does it look like with $s = .01$



- What do you see?

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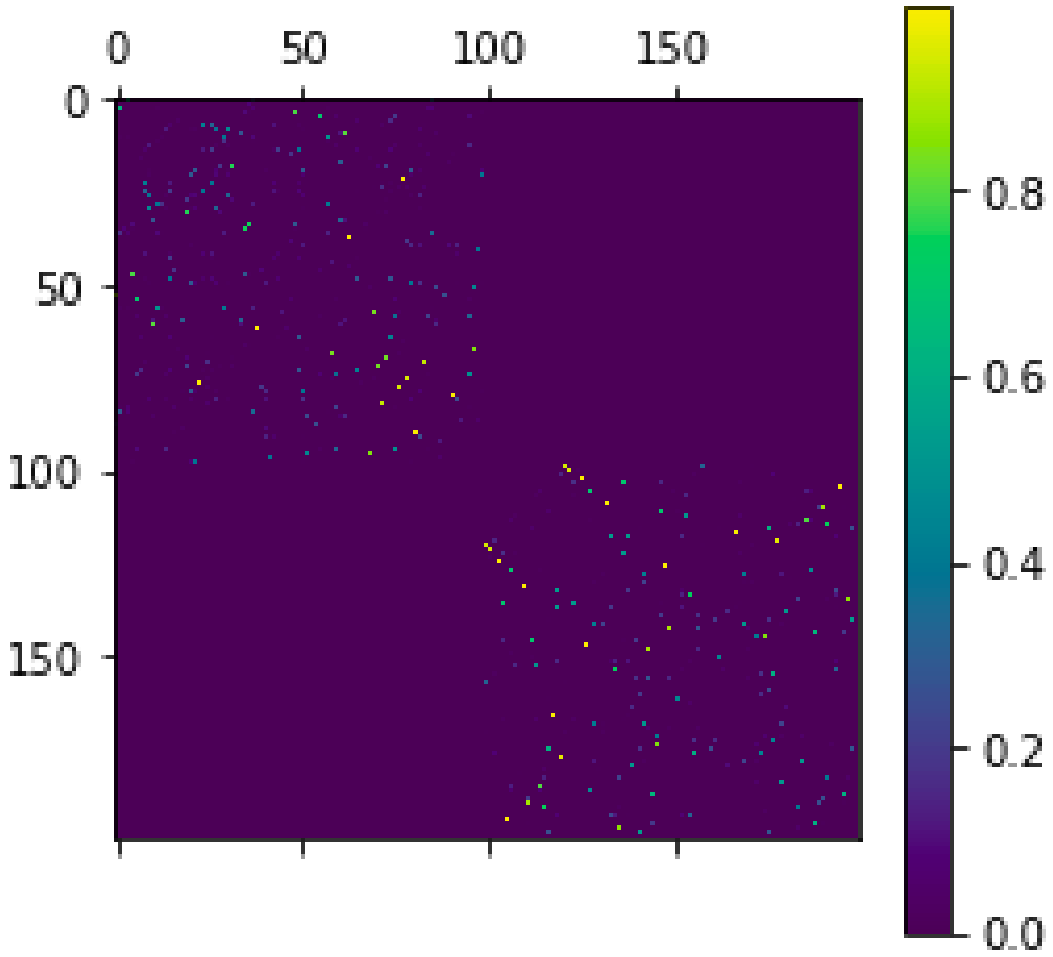
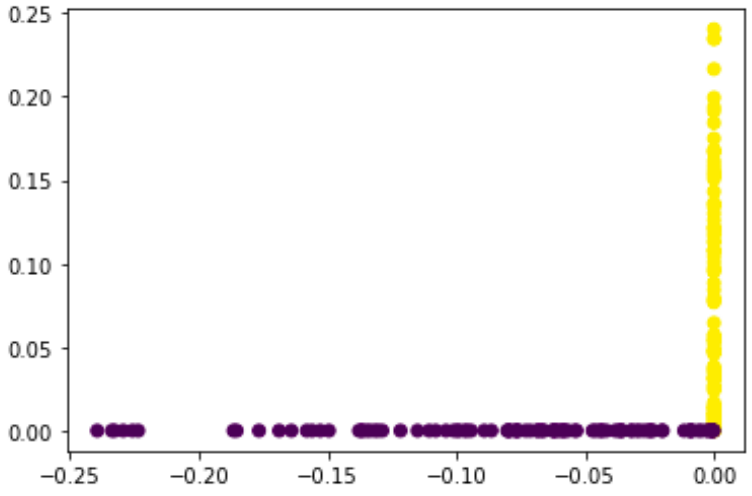


- What do you see?

Look at the eigenvectors

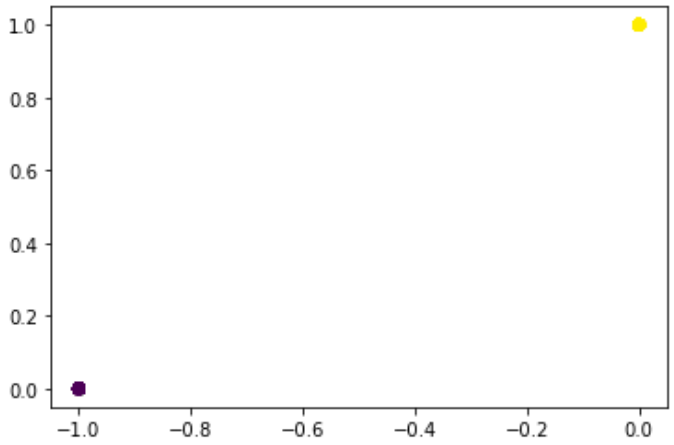


- This is the representation using the eigenvectors without normalization

Look at the eigenvectors-post normalization

```
plt.scatter(ul[:,0], ul[:,1],c=y)
```

```
<matplotlib.collections.PathCollection at 0x18ab63bb0>
```



- This is the representation using the eigenvectors with normalization
- Perfect accuracy

Wait, how do I measure accuracy or error

- Say you are given y_1 and y_2, two cluster assignments.
- You could do $\sum_i 1(y_1(i) \neq y_2(i))$
- Can you think for two minutes what is wrong with this?

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- You could do $\sum_i 1(y_1(i) \neq y_2(i))$
- Can you think for two minutes what is wrong with this?
- Well, clusterings are not identifiable up-to permutation.
- So the correct thing to do will be

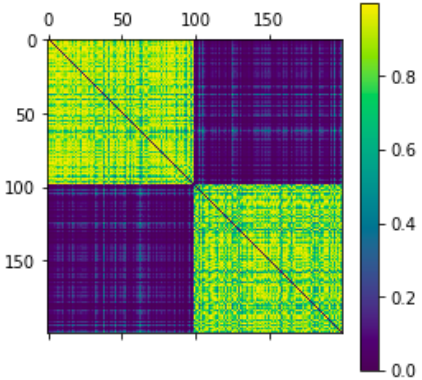
$$\min_{\pi \in \Pi_K} 1(\pi(y_1(i)) \neq y_2(i))$$

- Really costly when K is large, since we need to evaluate $K!$ permutations.
- You can use the Hungarian algorithm for mapping labels.

What does it look like with larger $s = 0.3$

```
In [336]: plt.matshow(K)
          plt.colorbar()

Out[336]: <matplotlib.colorbar.Colorbar at 0x190b6aac0>
```

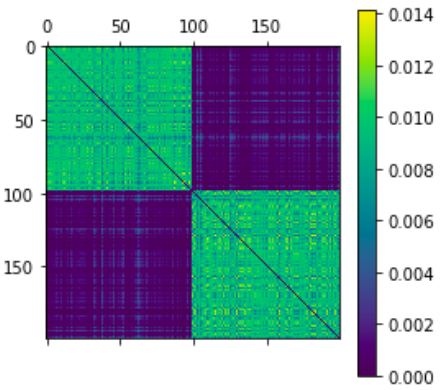


- What do you see?

What does it look like

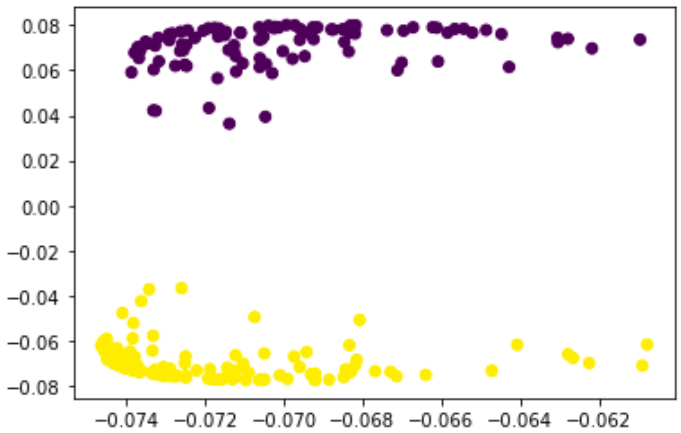
```
In [338]: plt.matshow(K1)
          plt.colorbar()

Out[338]: <matplotlib.colorbar.Colorbar at 0x190d40550>
```



- What do you see?

Look at the eigenvectors



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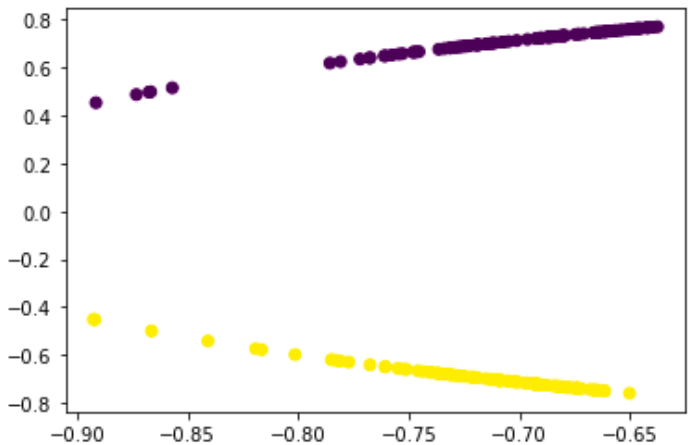
Look at the eigenvectors-post normalization

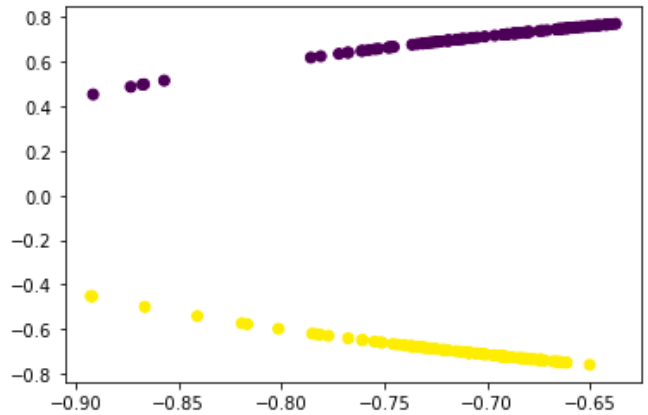


- This is the representation using the eigenvectors with normalization

Do k-means

```
kmeans = cluster.KMeans(2).fit(u1)
plt.scatter(u1[:,0], u1[:,1],c=kmeans.labels_)
```

```
<matplotlib.collections.PathCollection at 0x19134f640>
```



- This is the result labeled with k-means with 2 clusters
- Perfect accuracy, so pretty robust with selection of s

A tiny bit of theoretical insight

$$\hat{A} = \begin{bmatrix} A^{(11)} & 0 & 0 \\ 0 & A^{(22)} & 0 \\ 0 & 0 & A^{(33)} \end{bmatrix}; \quad \hat{L} = \begin{bmatrix} \hat{L}^{(11)} & 0 & 0 \\ 0 & \hat{L}^{(22)} & 0 \\ 0 & 0 & \hat{L}^{(33)} \end{bmatrix}$$

Figure 4: From Ng, Jordan, and Weiss 2001

- Consider an idealized setting, where there are no connections between the three clusters, and all elements of diagonal blocks are nonzero.
- Here after you normalize, for each of the smaller blocks there is exactly one eigenvalue 1, and all eigenvalues are strictly smaller.
- Call this $\hat{x}_1^{(i)}$

A tiny bit of theoretical insight

$$\hat{X} = \begin{bmatrix} x_1^{(1)} & \vec{0} & \vec{0} \\ \vec{0} & x_1^{(2)} & \vec{0} \\ \vec{0} & \vec{0} & x_1^{(3)} \end{bmatrix} \in \mathbb{R}^{n \times 3}.$$

Figure 5: From Ng, Jordan, and Weiss 2001

- Here padding the eigenvectors with zeros and then stacking them gives us eigenvectors of the bigger matrix.
- We need to be a bit careful, because all these eigenvalues are 1, so any 3 orthogonal vectors spanning this same subspace as the columns of the above will be eigenvectors too.

A tiny bit of theoretical insight

$$\begin{bmatrix} \vec{1} & \vec{0} & \vec{0} \\ \vec{0} & \vec{1} & \vec{0} \\ \vec{0} & \vec{0} & \vec{1} \end{bmatrix} R$$

Figure 6: From Ng, Jordan, and Weiss 2001

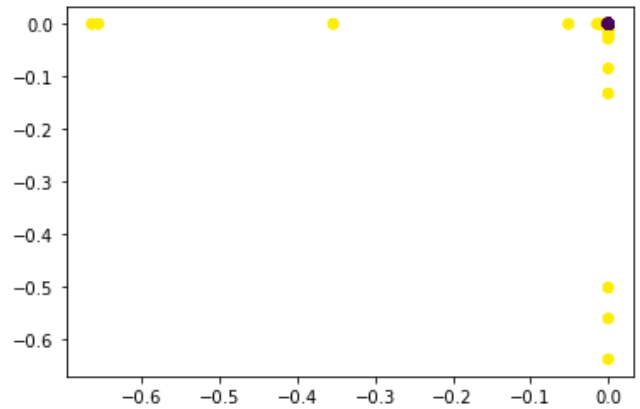
- R is a 3×3 orthogonal matrix, $R^T R = RR^T = I$
- When you normalize, all the points in cluster i get mapped to the i^{th} row of the orthogonal matrix R
- Typically, there will be some noise in the diagonal elements, and hence, *suitable conditions* we will have "tight" clusters around k well-separated points on the surface of the k sphere.

Why do the first normalization

```
u,s,vt=svd(K)
```

```
plt.scatter(u[:,0], u[:,1],c=y)
```

```
<matplotlib.collections.PathCollection at 0x18f055fd0>
```



- The very large entries in K take over and the top eigenvectors do not have any information about the cluster structure.