

# Practice

- Fill in the missing plots:

$$\Sigma = \mathbf{X}^T \mathbf{J} \mathbf{J} \mathbf{X} = \mathbf{Z}^T \mathbf{J} \mathbf{J} \mathbf{Z}$$

$$\mathbf{V} \mathbf{S} \mathbf{V}^T = \text{eig}(\Sigma) \quad \mathbf{J} = \mathbf{I} - \mathbf{1} \mathbf{1}^T / n$$

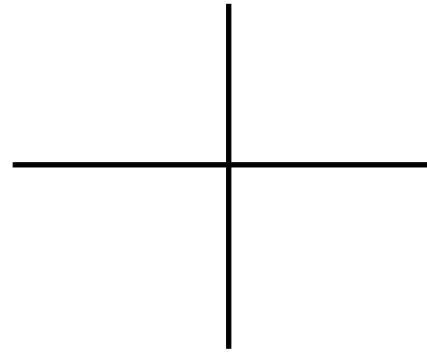
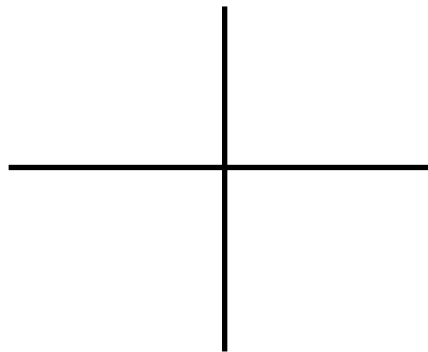
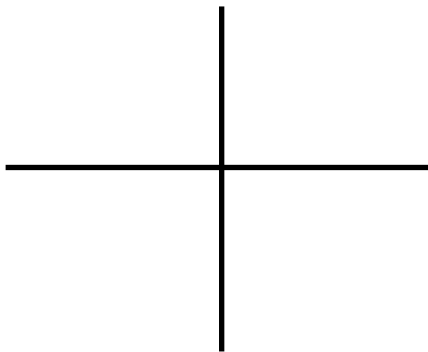
$$\mu_X = \mathbf{X}^T \mathbf{1} / n \quad \mu_Z = \mathbf{Z}^T \mathbf{1} / n$$

**X**

**Z**

$\mu_X - \mu_Z$

$\mathbf{V} \mathbf{S}^{-1/2} \mathbf{V}^T (\mu_X - \mu_Z)$





# Matrix Completion

Machine Learning – CSE546

Kevin Jamieson

University of Washington

November 15, 2016

# Singular Value Decomposition (SVD)

**Theorem (SVD):** Let  $\mathbf{A} \in \mathbb{R}^{m \times n}$  with rank  $r \leq \min\{m, n\}$ . Then  $\mathbf{A} = \mathbf{U}\mathbf{S}\mathbf{V}^T$  where  $\mathbf{S} \in \mathbb{R}^{r \times r}$  is diagonal with positive entries,  $\mathbf{U}^T\mathbf{U} = \mathbf{I}$ ,  $\mathbf{V}^T\mathbf{V} = \mathbf{I}$ .

$$\mathbf{U} = [u_1, \dots, u_r] \quad \mathbf{V} = [v_1, \dots, v_r]$$

$$\mathbf{A}^T \mathbf{A} v_i = \mathbf{S}_{i,i}^2 v_i$$

$$\mathbf{A} \mathbf{A}^T u_i = \mathbf{S}_{i,i}^2 u_i$$

$\mathbf{V}$  are the first  $r$  eigenvectors of  $\mathbf{A}^T \mathbf{A}$  with eigenvalues  $\text{diag}(\mathbf{S})$   
 $\mathbf{U}$  are the first  $r$  eigenvectors of  $\mathbf{A} \mathbf{A}^T$  with eigenvalues  $\text{diag}(\mathbf{S})$

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$$\mathbf{U} = [u_1, \dots, u_r] \quad \mathbf{V} = [v_1, \dots, v_r] \quad \mathbf{S} = \text{diag}(s_1, \dots, s_r)$$

$$\mathbf{A} = \sum_{k=1}^r u_k v_k^T s_k$$

$$s_1 \geq s_2 \geq \dots \geq s_r$$

Best rank-1 approximation  $\sigma > 0$  and unit vectors  $x \in \mathbb{R}^m$ ,  $y \in \mathbb{R}^n$  minimizes:  
 $\|\sigma xy^T - \mathbf{A}\|_F^2 =$

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Best rank-1 approximation  $\sigma > 0$  and unit vectors  $x \in \mathbb{R}^m$ ,  $y \in \mathbb{R}^n$  minimizes:

$$\begin{aligned} \|\sigma xy^T - \mathbf{A}\|_F^2 &= \sigma^2 + \text{Tr}(\mathbf{A}^T \mathbf{A}) - 2\sigma x^T \mathbf{A} y \\ &= \sigma^2 + \left( \sum_{k=1}^r s_k^2 \right) - 2\sigma \left( \sum_{k=1}^r x^T u_k v_k^T y s_k \right) \end{aligned}$$

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In general: 
$$\sum_{k=1}^p u_k v_k^T s_k = \arg \min_{\mathbf{Z}: \text{rank}(\mathbf{Z})=p} \|\mathbf{Z} - \mathbf{A}\|_F^2$$

# Matrix completion

Given historical data on how users rated movies in past:

17,700 movies, 480,189 users, 99,072,112 ratings



(Sparsity: 1.2%)

Predict how the same users will rate movies in the future (for \$1 million prize)

						...
Alice	1	?	?	4	?	
Bob	?	2	5	?	?	
Carol	?	?	4	5	?	
Dave	5	?	?	?	4	
⋮						

# Matrix completion

n movies, m users, |S| ratings

$$\arg \min_{U \in \mathbb{R}^{m \times d}, V \in \mathbb{R}^{n \times d}} \sum_{(i,j,s) \in \mathcal{S}} \|(UV^T)_{i,j} - s_{i,j}\|_2^2$$

How do we solve it? With full information?



# Matrix completion

n movies, m users, |S| ratings

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Practical techniques to solve:

- Alternating minimization (Fix U, minimize V. Then fix V and minimize U)
- Stochastic gradient descent on U, V
- Nuclear norm regularization (convex)



# Clustering

# K-means

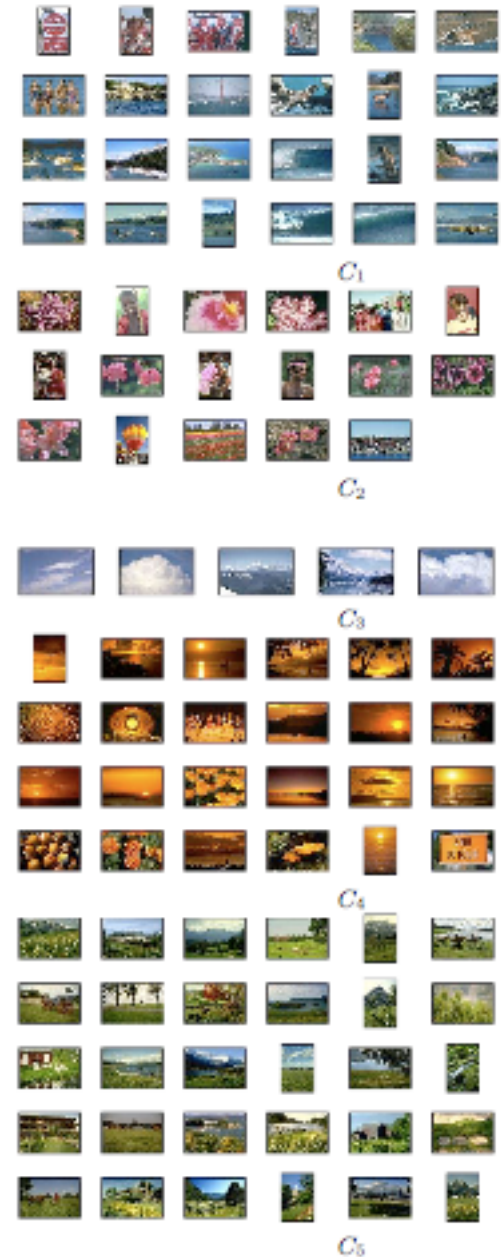
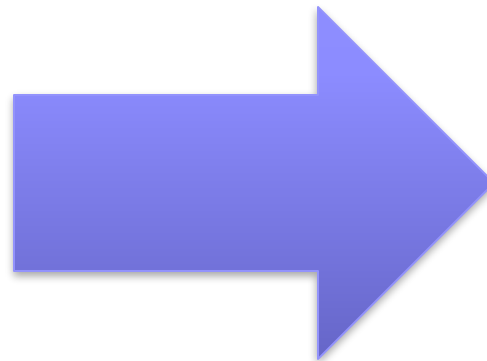
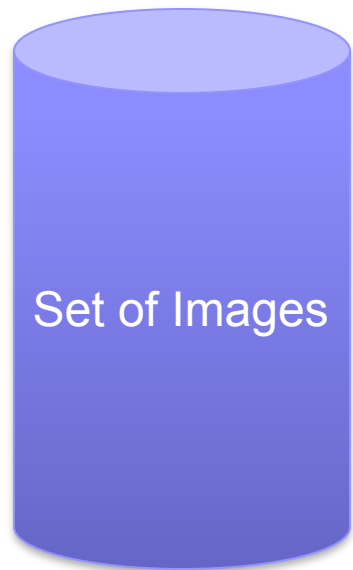
Machine Learning – CSE546

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# Clustering images



# Clustering web search results

The screenshot shows the Clusty search engine interface. At the top, there's a navigation bar with links for 'web', 'news', 'images', 'wikipedia', 'blogs', 'jobs', and 'more'. The search bar contains the word 'race'. Below the search bar, there are tabs for 'clusters', 'sources', and 'sites'. The 'clusters' tab is active, showing a list of clusters on the left and search results on the right. The 'Human' cluster is selected, containing 8 documents. The search results list 7 items, each with a title, a brief description, and a URL. The first result is 'Race (classification of human beings) - Wikipedia, the free ...', the second is 'Race - Wikipedia, the free encyclopedia', the third is 'Publications | Human Rights Watch', the fourth is 'Amazon.com: Race: The Reality Of Human Differences: Vincent Sarich ...', the fifth is 'AAPA Statement on Biological Aspects of Race', the sixth is 'race: Definition from Answers.com', and the seventh is 'Dopefish.com'.

web news images wikipedia blogs jobs more »

Clusty

race Search advanced preferences

clusters sources sites

All Results (238) remix

- Car (28)
  - Race cars (7)
  - Photos, Races Scheduled (5)
  - Game (4)
  - Track (3)
  - Nascar (2)
  - Equipment And Safety (2)
  - Other Topics (7)
- Photos (22)
- Game (14)
- Definition (13)
- Team (18)
- Human (8)**
  - Classification Of Human (2)
  - Statement, Evolved (2)
  - Other Topics (4)
- Weekend (8)
- Ethnicity And Race (7)
- Race for the Cure (8)
- Race Information (8)

more | all clusters

find in clusters: Find

Cluster Human contains 8 documents.

Search Results

- [Race \(classification of human beings\) - Wikipedia, the free ...](#)

The term **race** or racial group usually refers to the concept of dividing **humans** into populations or groups on the basis of various sets of characteristics. The most widely used **human** racial categories are based on visible traits (especially skin color, cranial or facial features and hair texture), and self-identification. Conceptions of **race**, as well as specific ways of grouping **races**, vary by culture and over time, and are often controversial for scientific as well as social and political reasons. History · Modern debates · Political and ...  
[en.wikipedia.org/wiki/Race\\_\(classification\\_of\\_human\\_beings\)](http://en.wikipedia.org/wiki/Race_(classification_of_human_beings)) - [cache] - Live, Ask
- [Race - Wikipedia, the free encyclopedia](#)

General. **Racing** competitions The **Race** (yachting **race**), or La course du millénaire, a no-rules round-the-world sailing event; **Race** (biology), classification of flora and fauna; **Race** (classification of **human** beings) **Race** and ethnicity in the United States Census, official definitions of "**race**" used by the US Census Bureau; **Race** and genetics, notion of racial classifications based on genetics. Historical definitions of **race**; **Race** (bearing), the inner and outer rings of a rolling-element bearing. **RACE** in molecular biology "Rapid ... General · Surnames · Television · Music · Literature · Video games  
[en.wikipedia.org/wiki/Race](http://en.wikipedia.org/wiki/Race) - [cache] - Live, Ask
- [Publications | Human Rights Watch](#)

The use of torture, unlawful rendition, secret prisons, unfair trials, ... Risks to Migrants, Refugees, and Asylum Seekers in Egypt and Israel ... In the run-up to the Beijing Olympics in August 2008, ...  
[www.hrw.org/background/usa/race](http://www.hrw.org/background/usa/race) - [cache] - Ask
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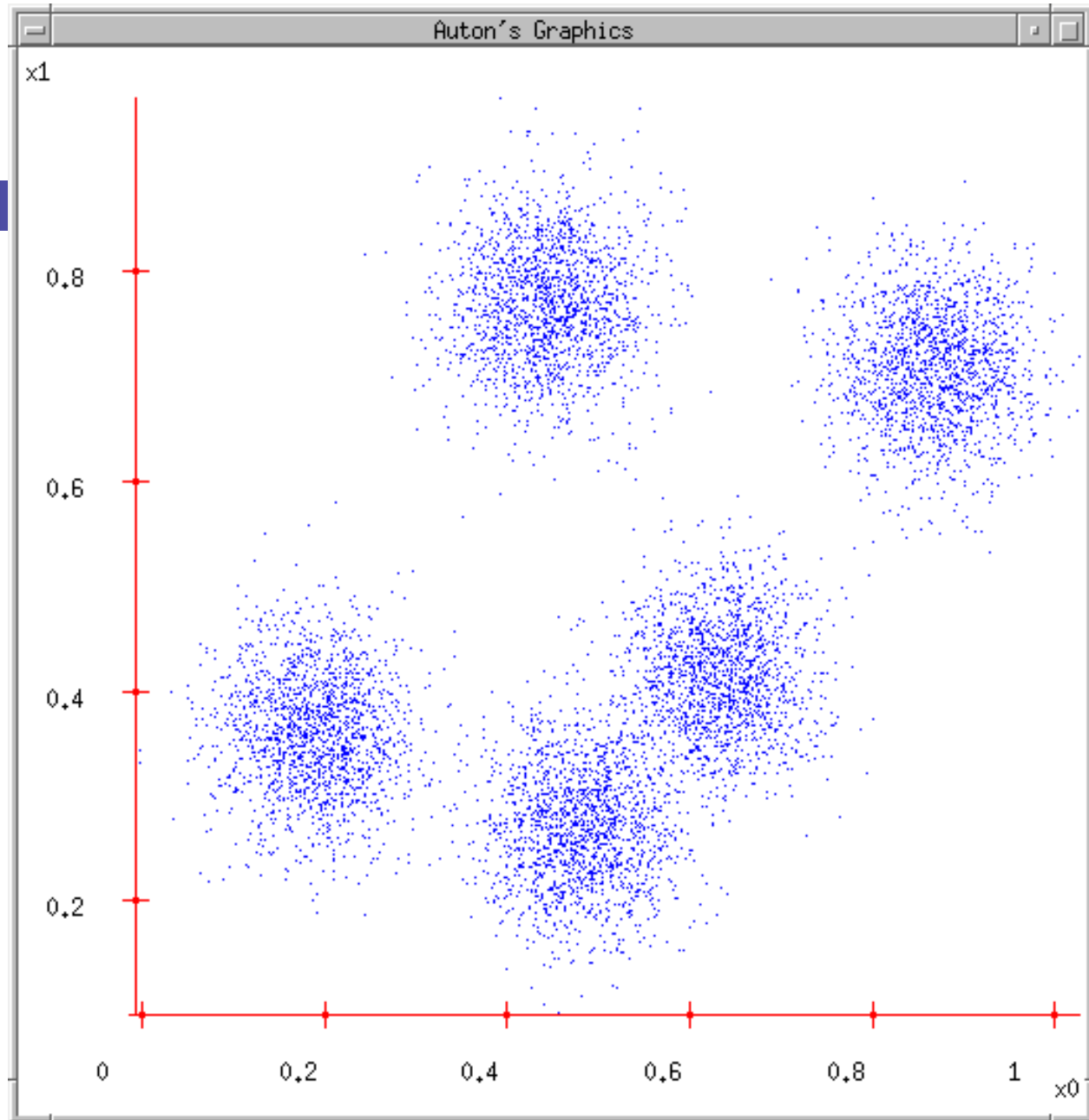
Amazon.com: **Race: The Reality Of Human Differences: Vincent Sarich, Frank Miele: Books ...** From Publishers Weekly Sarich, a Berkeley emeritus anthropologist, and Miele, an editor ...  
[www.amazon.com/Race-Reality-Differences-Vincent-Sarich/dp/0813340861](http://www.amazon.com/Race-Reality-Differences-Vincent-Sarich/dp/0813340861) - [cache] - Live
- [AAPA Statement on Biological Aspects of Race](#)

AAPA Statement on Biological Aspects of **Race** ... Published in the American Journal of Physical Anthropology, vol. 101, pp 569-570, 1996 ... PREAMBLE As scientists who study **human** evolution and variation, ...  
[www.physanth.org/positions/race.html](http://www.physanth.org/positions/race.html) - [cache] - Ask
- [race: Definition from Answers.com](#)

**race** n. A local geographic or global **human** population distinguished as a more or less distinct group by genetically transmitted physical  
[www.answers.com/topic/race-1](http://www.answers.com/topic/race-1) - [cache] - Live
- [Dopefish.com](#)

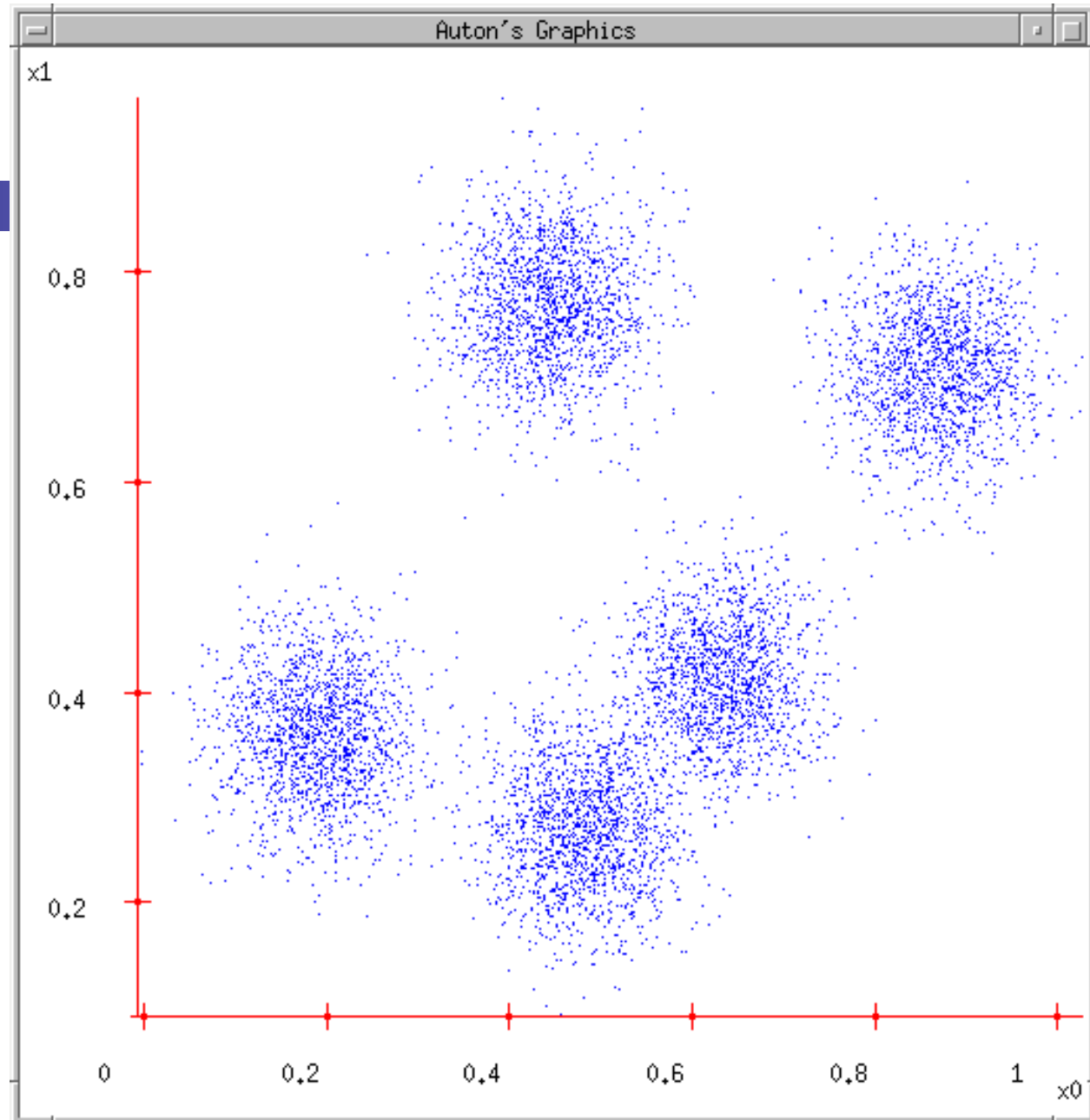
Site for newbies as well as experienced Dopefish followers, chronicling the birth of the Dopefish, its numerous appearances in several computer games, and its eventual take-over of the **human** **race**. Maintained by Mr. Dopefish himself, Joe Siegler of Apogee Software.  
[www.dopefish.com](http://www.dopefish.com) - [cache] - Open Directory

# Some Data



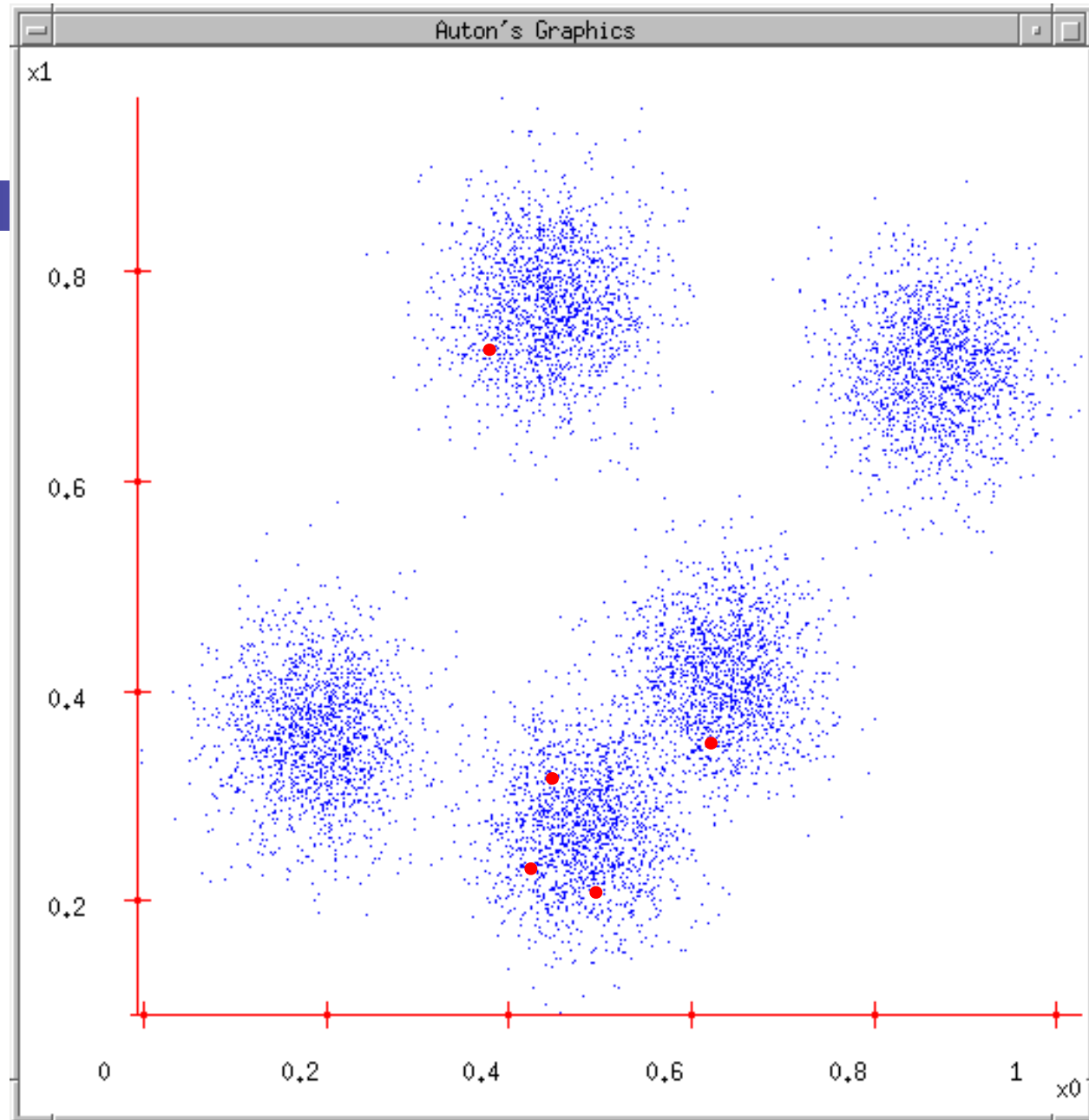
# K-means

1. Ask user how many clusters they'd like.  
(e.g.  $k=5$ )



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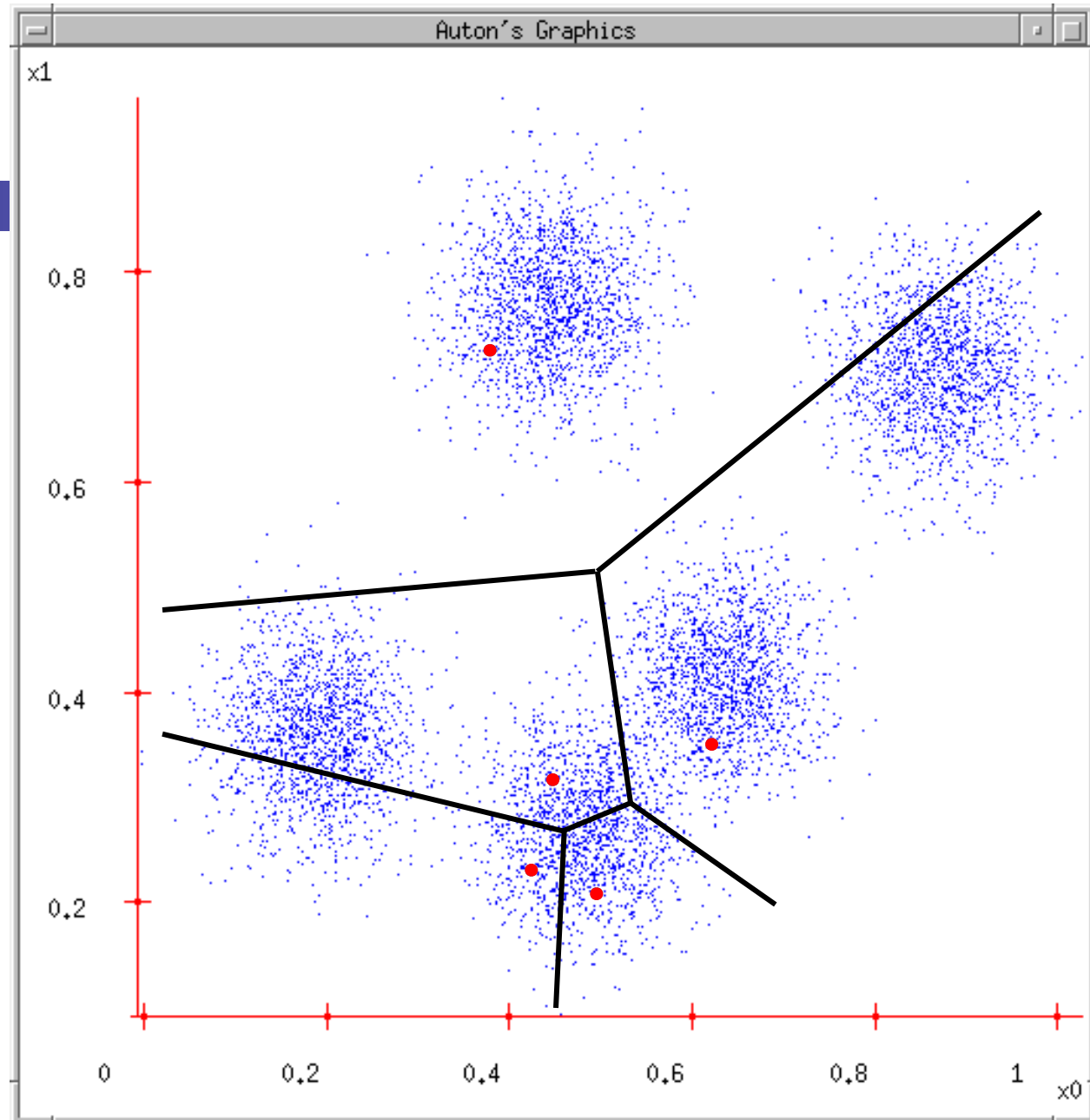
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2. Randomly guess  $k$  cluster Center locations





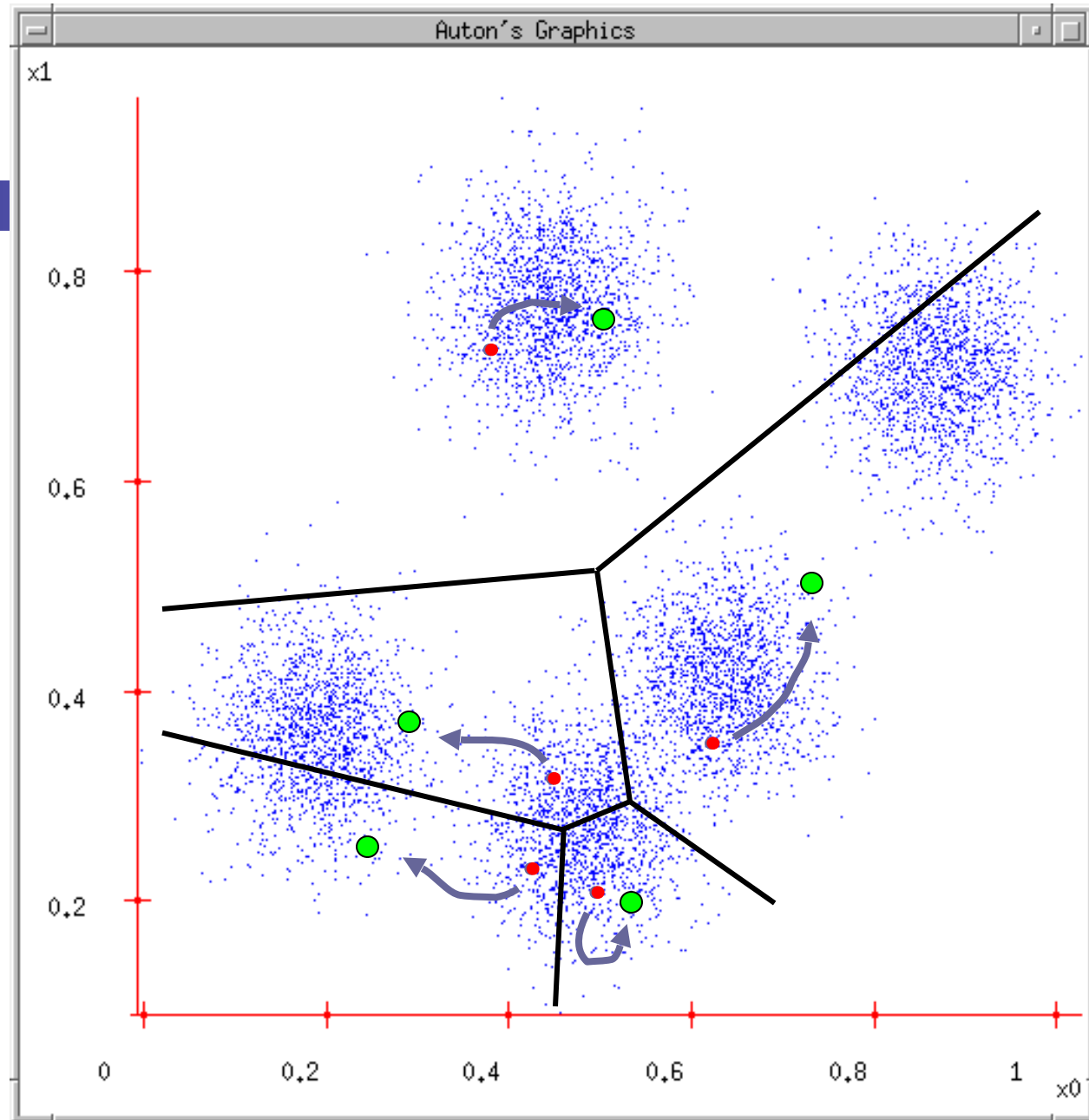
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2. Randomly guess  $k$  cluster Center locations
3. Each datapoint finds out which Center it's closest to. (Thus each Center "owns" a set of datapoints)



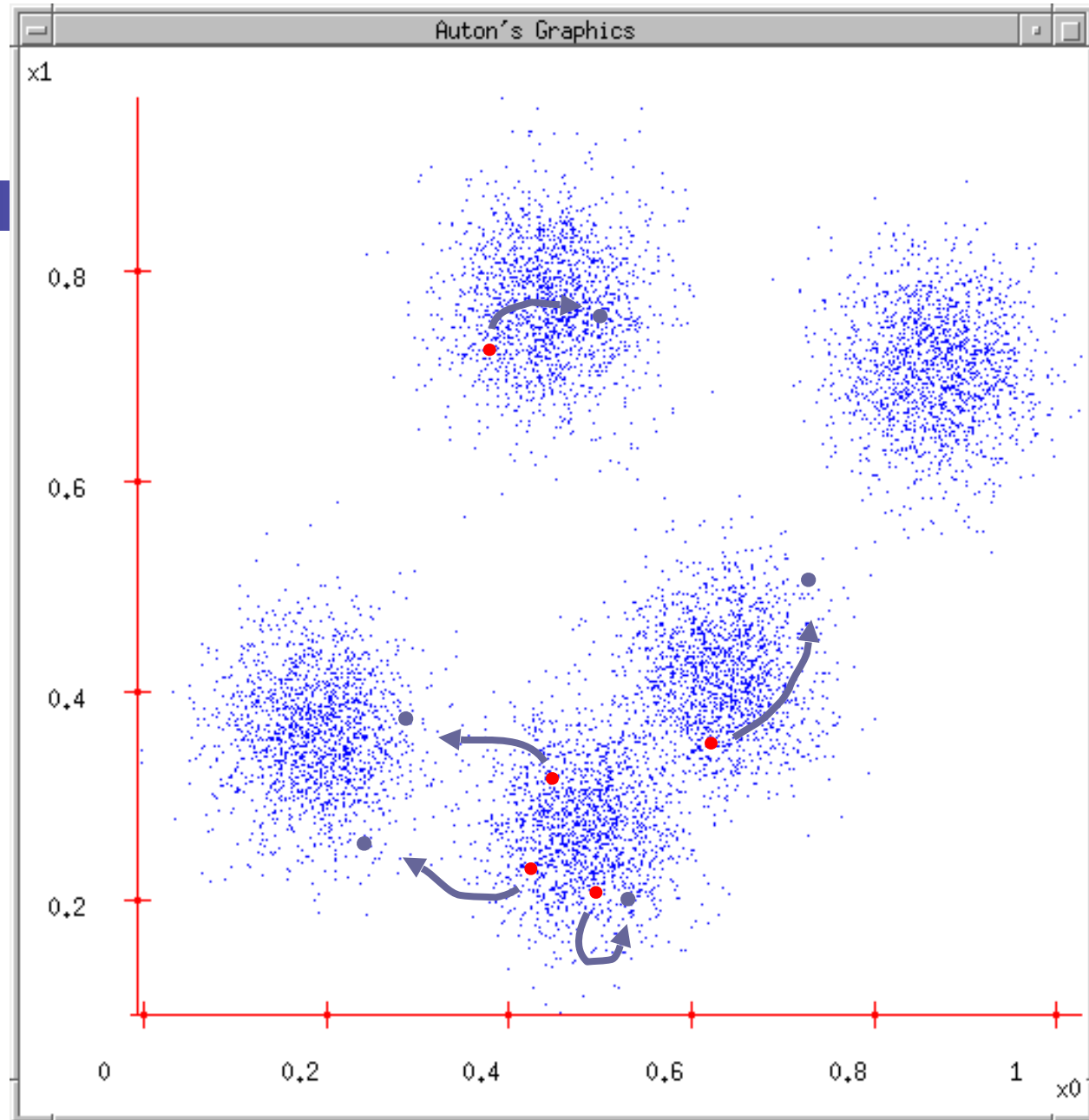
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3. Each datapoint finds out which Center it's closest to.
4. Each Center finds the centroid of the points it owns...
5. ...and jumps there
6. ...Repeat until terminated!



# K-means

- Randomly initialize  $k$  centers
  - $\mu^{(0)} = \mu_1^{(0)}, \dots, \mu_k^{(0)}$
- **Classify:** Assign each point  $j \in \{1, \dots, N\}$  to nearest center:
  - $C^{(t)}(j) \leftarrow \arg \min_i \|\mu_i - x_j\|^2$
- **Recenter:**  $\mu_i$  becomes centroid of its point:
  - $\mu_i^{(t+1)} \leftarrow \arg \min_{\mu} \sum_{j: C(j)=i} \|\mu - x_j\|^2$
  - Equivalent to  $\mu_i \leftarrow$  average of its points!

# Does K-means converge??? Part 1

- Optimize potential function:

$$\min_{\mu} \min_C F(\mu, C) = \min_{\mu} \min_C \sum_{i=1}^k \sum_{j:C(j)=i} \|\mu_i - x_j\|^2$$

- Fix  $\mu$ , optimize C

# Does K-means converge??? Part 2

- Optimize potential function:

$$\min_{\mu} \min_C F(\mu, C) = \min_{\mu} \min_C \sum_{i=1}^k \sum_{j:C(j)=i} \|\mu_i - x_j\|^2$$

- Fix C, optimize  $\mu$

# Vector Quantization, Fisher Vectors

## Vector Quantization (for compression)

1. Represent image as grid of patches
2. Run k-means on the patches to build code book
3. Represent each patch as a code word.



**FIGURE 14.9.** *Sir Ronald A. Fisher (1890 – 1962) was one of the founders of modern day statistics, to whom we owe maximum-likelihood, sufficiency, and many other fundamental concepts. The image on the left is a  $1024 \times 1024$  grayscale image at 8 bits per pixel. The center image is the result of  $2 \times 2$  block VQ, using 200 code vectors, with a compression rate of 1.9 bits/pixel. The right image uses only four code vectors, with a compression rate of 0.50 bits/pixel*

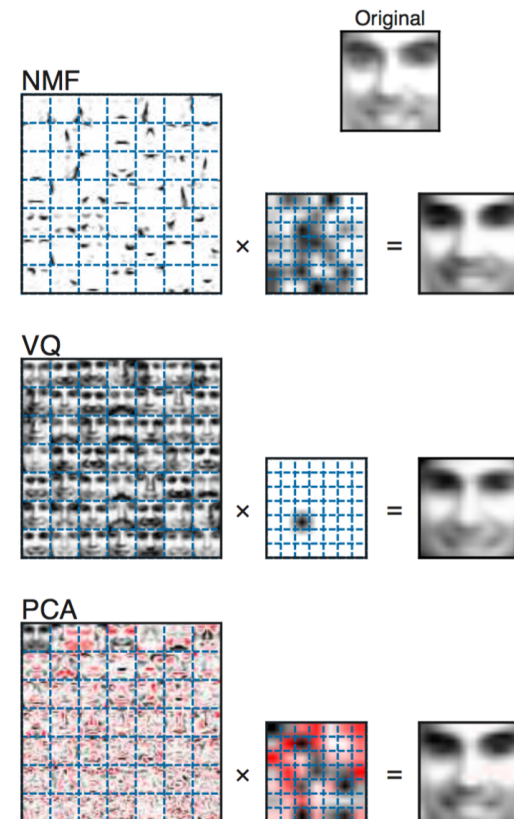
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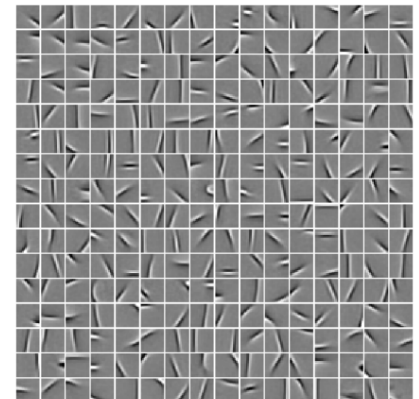
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Typical output of k-means  
on patches



Similar reduced representation can be used as a feature vector

Coates, Ng, *Learning Feature Representations with K-means*, 2012

# Spectral Clustering

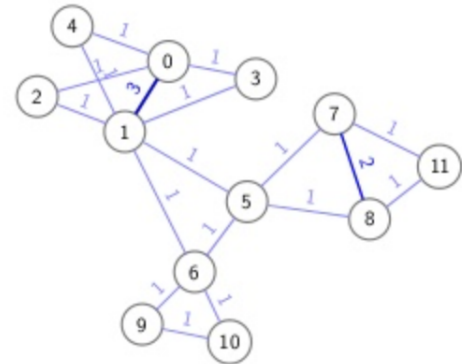
Adjacency matrix:  $\mathbf{W}$

$\mathbf{W}_{i,j}$  = weight of edge  $(i, j)$

$$\mathbf{D}_{i,i} = \sum_{j=1}^n \mathbf{W}_{i,j} \quad \mathbf{L} = \mathbf{D} - \mathbf{W}$$

Given feature vectors, could construct:

- k-nearest neighbor graph with weights in  $\{0,1\}$
- weighted graph with arbitrary *similarities*  $\mathbf{W}_{i,j} = e^{-\gamma\|x_i - x_j\|^2}$



Let  $f \in \mathbb{R}^n$  be a function over the nodes

$$\begin{aligned} \mathbf{f}^T \mathbf{L} \mathbf{f} &= \sum_{i=1}^N g_i f_i^2 - \sum_{i=1}^N \sum_{i'=1}^N f_i f_{i'} w_{ii'} \\ &= \frac{1}{2} \sum_{i=1}^N \sum_{i'=1}^N w_{ii'} (f_i - f_{i'})^2. \end{aligned}$$

# Spectral Clustering

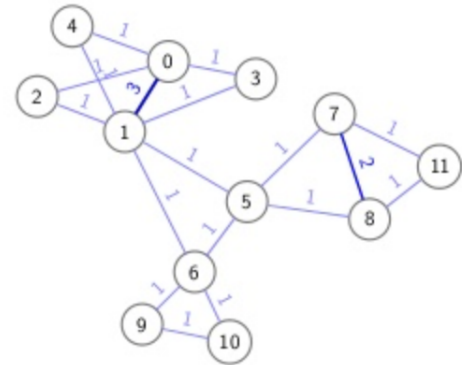
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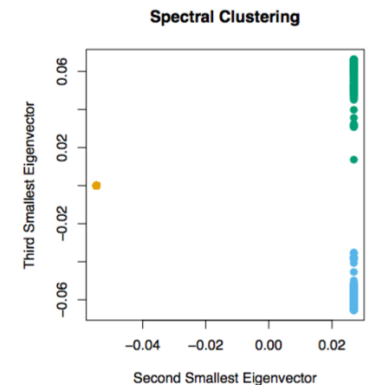
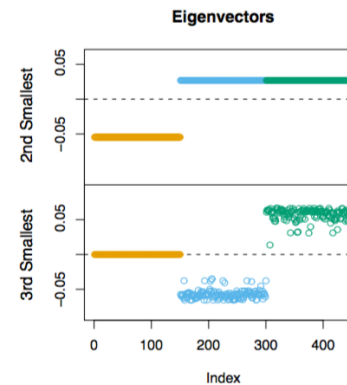
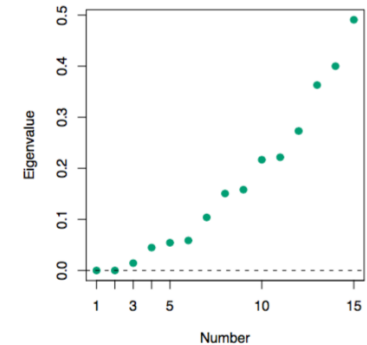
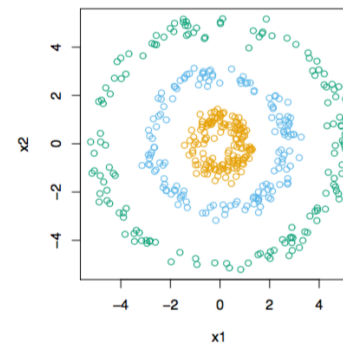
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Given feature vectors, could construct:

- (k=10)-nearest neighbor graph with weights in  $\{0,1\}$





# Mixtures of Gaussians

Machine Learning – CSE546

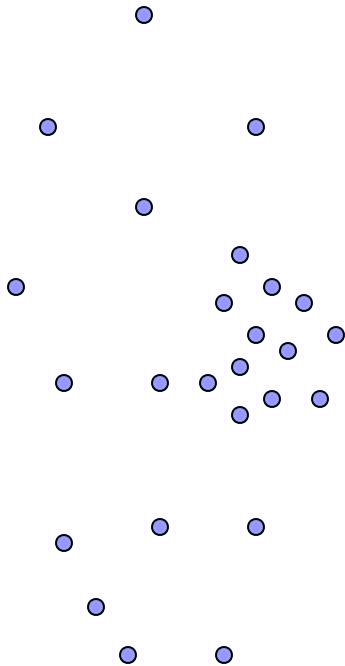
Kevin Jamieson

University of Washington

November 15, 2016

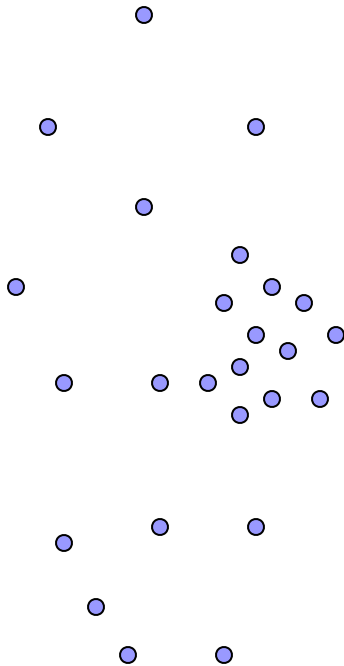
# (One) bad case for k-means

- Clusters may overlap
- Some clusters may be “wider” than others



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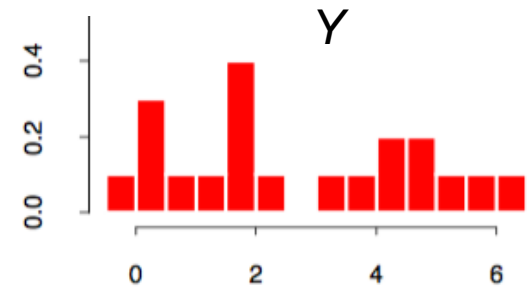
# Mixture models

$$Y_1 \sim N(\mu_1, \sigma_1^2),$$

$$Y_2 \sim N(\mu_2, \sigma_2^2),$$

$$Y = (1 - \Delta) \cdot Y_1 + \Delta \cdot Y_2,$$

$$\Delta \in \{0, 1\} \text{ with } \Pr(\Delta = 1) = \pi$$



$\mathbf{Z} = \{y_i\}_{i=1}^n$  is observed data

If  $\phi_\theta(x)$  is Gaussian density with parameters  $\theta = (\mu, \sigma^2)$  then

$$\ell(\theta; \mathbf{Z}) = \sum_{i=1}^n \log[(1 - \pi)\phi_{\theta_1}(y_i) + \pi\phi_{\theta_2}(y_i)]$$



# Mixture models

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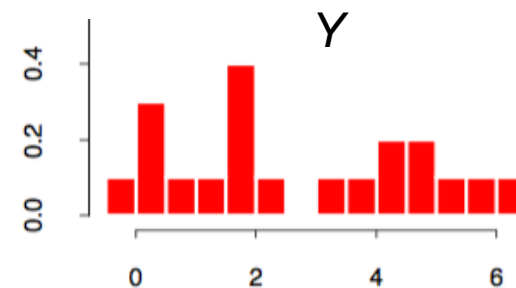
$$\Delta \in \{0, 1\} \text{ with } \Pr(\Delta = 1) = \pi$$

$$\theta = (\pi, \theta_1, \theta_2) = (\pi, \mu_1, \sigma_1^2, \mu_2, \sigma_2^2)$$

If  $\phi_\theta(x)$  is Gaussian density with parameters  $\theta = (\mu, \sigma^2)$  then

$$\ell(\theta; y_i, \Delta_i = 0) =$$

$$\ell(\theta; y_i, \Delta_i = 1) =$$



$\mathbf{Z} = \{y_i\}_{i=1}^n$  is observed data

$\mathbf{\Delta} = \{\Delta_i\}_{i=1}^n$  is unobserved data

# Mixture models

$$Y_1 \sim N(\mu_1, \sigma_1^2),$$

$$Y_2 \sim N(\mu_2, \sigma_2^2),$$

$$Y = (1 - \Delta) \cdot Y_1 + \Delta \cdot Y_2,$$

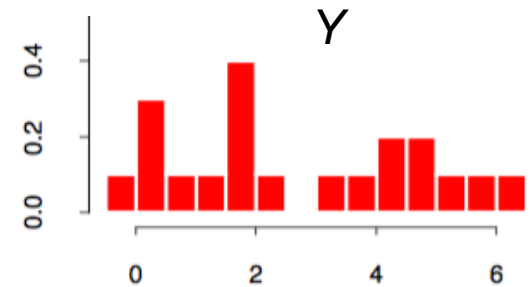
$$\Delta \in \{0, 1\} \text{ with } \Pr(\Delta = 1) = \pi$$

$$\theta = (\pi, \theta_1, \theta_2) = (\pi, \mu_1, \sigma_1^2, \mu_2, \sigma_2^2)$$

If  $\phi_\theta(x)$  is Gaussian density with parameters  $\theta = (\mu, \sigma^2)$  then

$$\ell(\theta; \mathbf{Z}, \mathbf{\Delta}) = \sum_{i=1}^n (1 - \Delta_i) \log[(1 - \pi)\phi_{\theta_1}(y_i)] + \Delta_i \log(\pi\phi_{\theta_2}(y_i))$$

If we knew  $\mathbf{\Delta}$ , how would we choose  $\theta$ ?



$\mathbf{Z} = \{y_i\}_{i=1}^n$  is observed data

$\mathbf{\Delta} = \{\Delta_i\}_{i=1}^n$  is unobserved data

# Mixture models

$$Y_1 \sim N(\mu_1, \sigma_1^2),$$

$$Y_2 \sim N(\mu_2, \sigma_2^2),$$

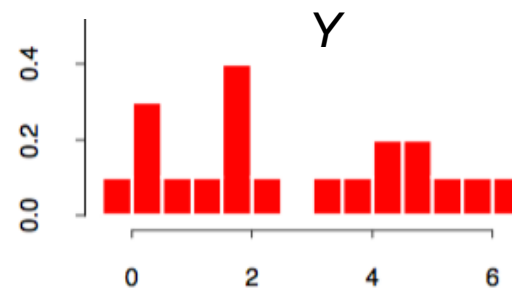
$$Y = (1 - \Delta) \cdot Y_1 + \Delta \cdot Y_2,$$

$$\Delta \in \{0, 1\} \text{ with } \Pr(\Delta = 1) = \pi$$

$$\theta = (\pi, \theta_1, \theta_2) = (\pi, \mu_1, \sigma_1^2, \mu_2, \sigma_2^2)$$

If  $\phi_\theta(x)$  is Gaussian density with parameters  $\theta = (\mu, \sigma^2)$  then

$$\ell(\theta; \mathbf{Z}, \mathbf{\Delta}) = \sum_{i=1}^n (1 - \Delta_i) \log[(1 - \pi)\phi_{\theta_1}(y_i)] + \Delta_i \log(\pi\phi_{\theta_2}(y_i))$$



$\mathbf{Z} = \{y_i\}_{i=1}^n$  is observed data

$\mathbf{\Delta} = \{\Delta_i\}_{i=1}^n$  is unobserved data

If we knew  $\theta$ , how would we choose  $\mathbf{\Delta}$ ?

# Mixture models

$$Y_1 \sim N(\mu_1, \sigma_1^2),$$

$$Y_2 \sim N(\mu_2, \sigma_2^2),$$

$$Y = (1 - \Delta) \cdot Y_1 + \Delta \cdot Y_2,$$

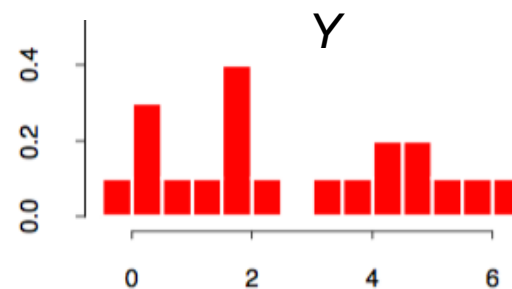
$$\Delta \in \{0, 1\} \text{ with } \Pr(\Delta = 1) = \pi$$

$$\theta = (\pi, \theta_1, \theta_2) = (\pi, \mu_1, \sigma_1^2, \mu_2, \sigma_2^2)$$

If  $\phi_\theta(x)$  is Gaussian density with parameters  $\theta = (\mu, \sigma^2)$  then

$$\ell(\theta; \mathbf{Z}, \mathbf{\Delta}) = \sum_{i=1}^n (1 - \Delta_i) \log[(1 - \pi)\phi_{\theta_1}(y_i)] + \Delta_i \log(\pi\phi_{\theta_2}(y_i))$$

$$\gamma_i(\theta) = \mathbb{E}[\Delta_i | \theta, \mathbf{Z}] =$$



$\mathbf{Z} = \{y_i\}_{i=1}^n$  is observed data

$\mathbf{\Delta} = \{\Delta_i\}_{i=1}^n$  is unobserved data

# Mixture models

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**Algorithm 8.1** *EM Algorithm for Two-component Gaussian Mixture.*

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1. Take initial guesses for the parameters  $\hat{\mu}_1, \hat{\sigma}_1^2, \hat{\mu}_2, \hat{\sigma}_2^2, \hat{\pi}$  (see text).
2. *Expectation Step*: compute the responsibilities

$$\hat{\gamma}_i = \frac{\hat{\pi} \phi_{\hat{\theta}_2}(y_i)}{(1 - \hat{\pi}) \phi_{\hat{\theta}_1}(y_i) + \hat{\pi} \phi_{\hat{\theta}_2}(y_i)}, \quad i = 1, 2, \dots, N. \quad (8.42)$$

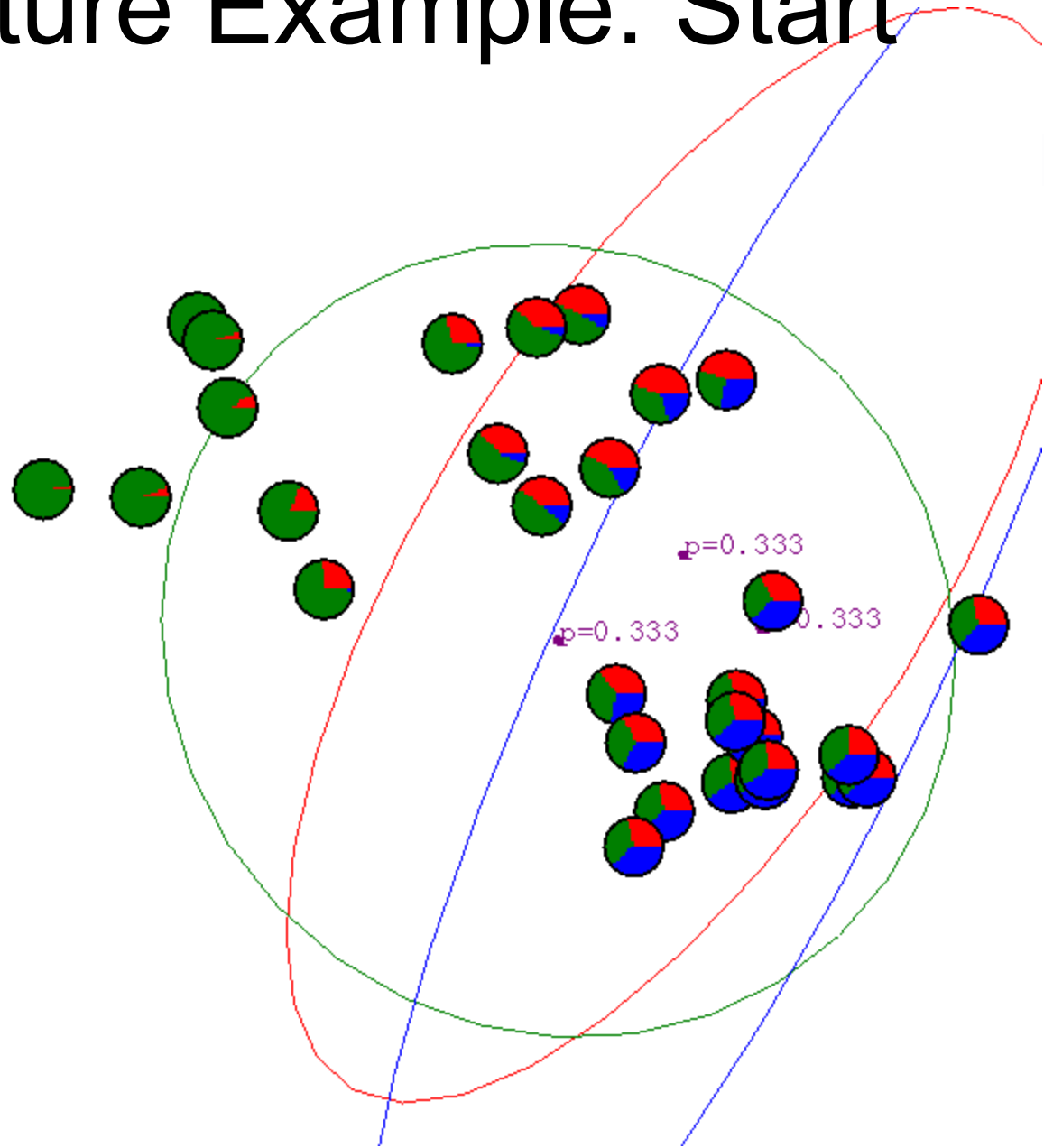
3. *Maximization Step*: compute the weighted means and variances:

$$\hat{\mu}_1 = \frac{\sum_{i=1}^N (1 - \hat{\gamma}_i) y_i}{\sum_{i=1}^N (1 - \hat{\gamma}_i)}, \quad \hat{\sigma}_1^2 = \frac{\sum_{i=1}^N (1 - \hat{\gamma}_i) (y_i - \hat{\mu}_1)^2}{\sum_{i=1}^N (1 - \hat{\gamma}_i)},$$
$$\hat{\mu}_2 = \frac{\sum_{i=1}^N \hat{\gamma}_i y_i}{\sum_{i=1}^N \hat{\gamma}_i}, \quad \hat{\sigma}_2^2 = \frac{\sum_{i=1}^N \hat{\gamma}_i (y_i - \hat{\mu}_2)^2}{\sum_{i=1}^N \hat{\gamma}_i},$$

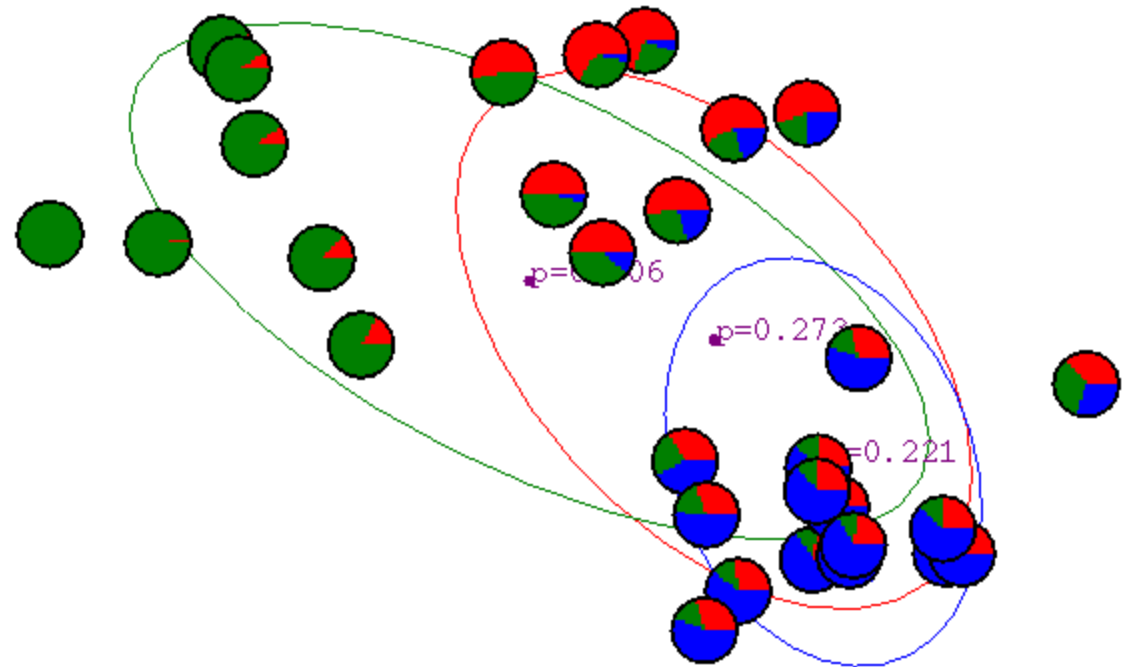
and the mixing probability  $\hat{\pi} = \sum_{i=1}^N \hat{\gamma}_i / N$ .

4. Iterate steps 2 and 3 until convergence.
-

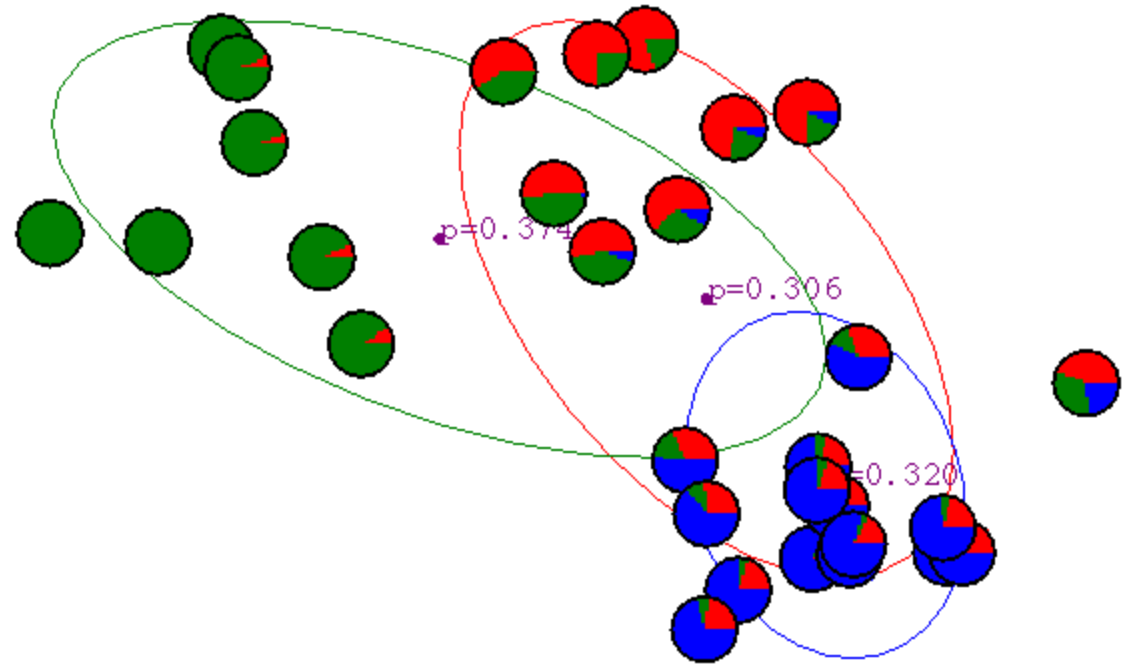
# Gaussian Mixture Example: Start



# After first iteration

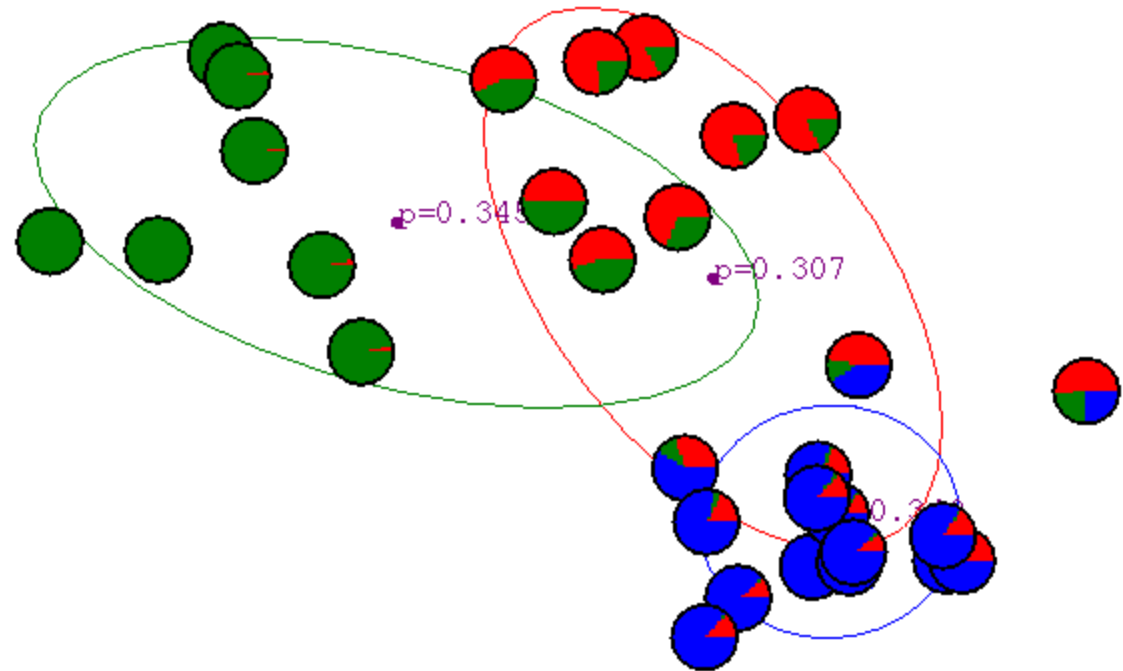


# After 2nd iteration

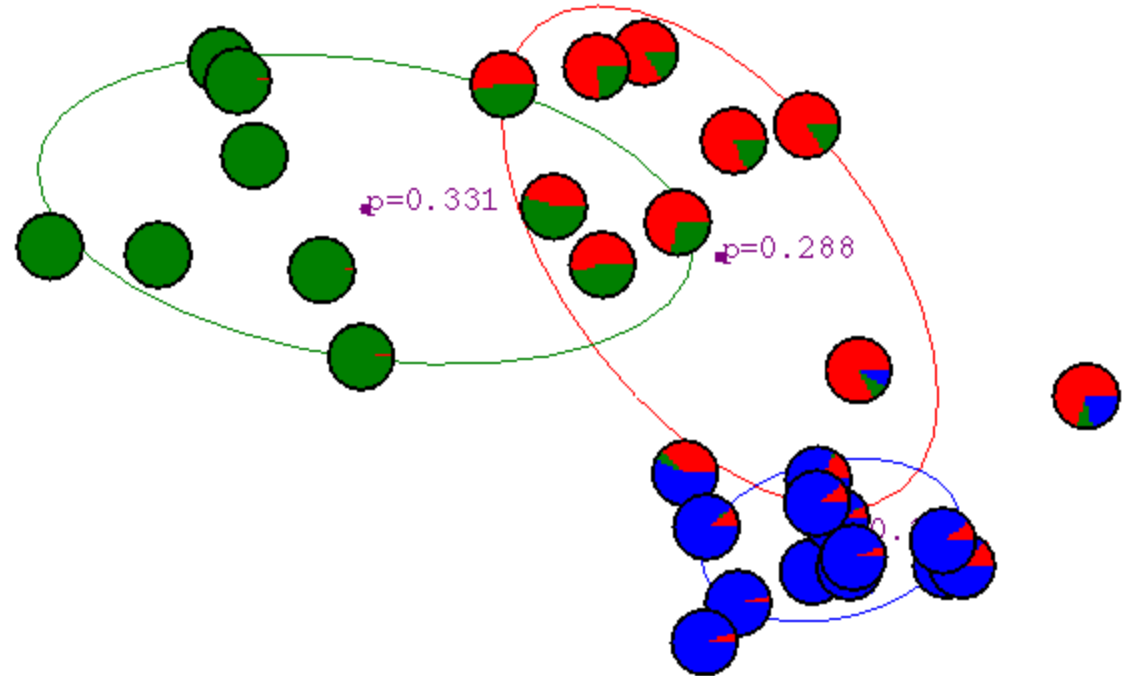




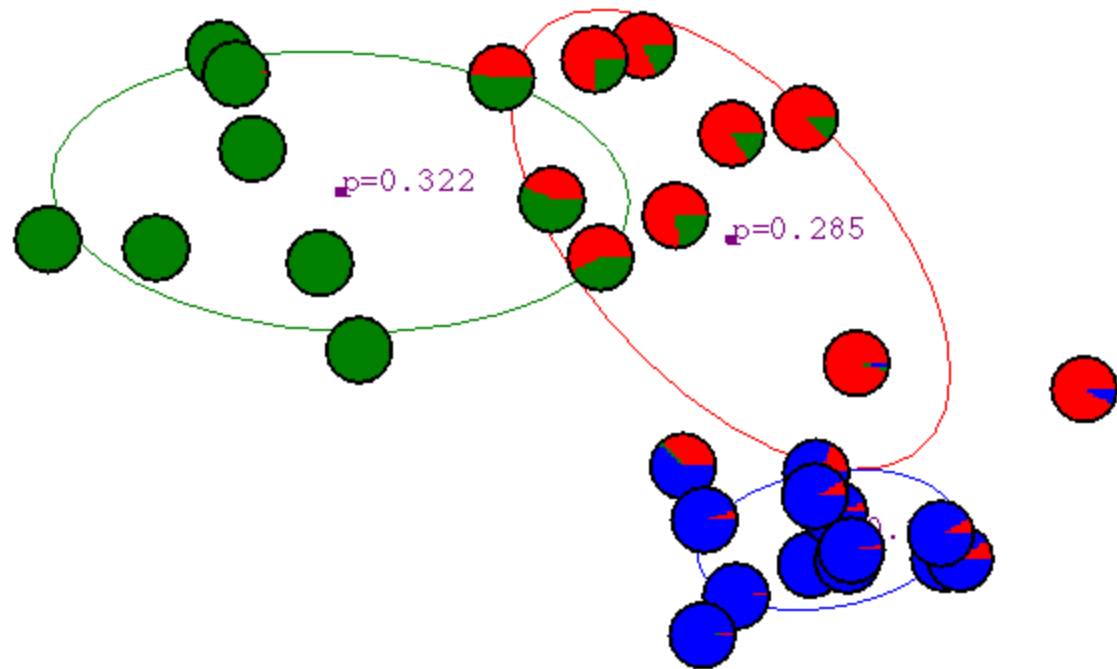
# After 3rd iteration



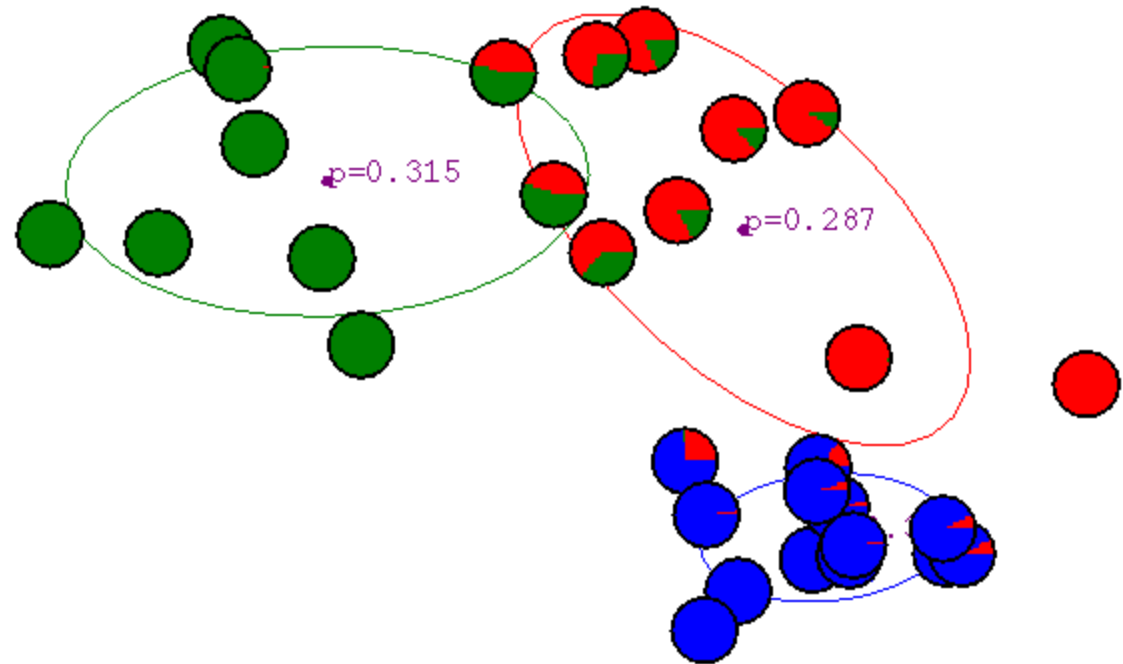
# After 4th iteration



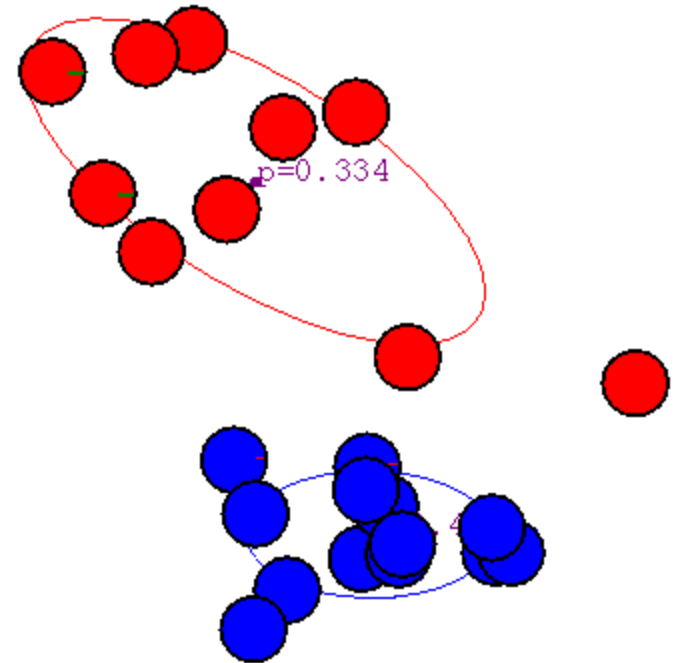
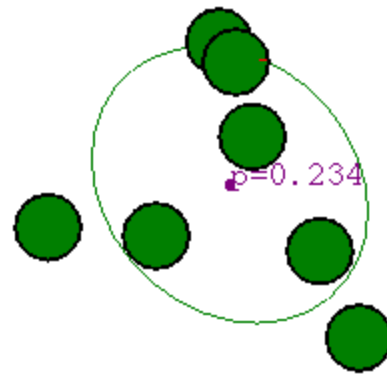
# After 5th iteration



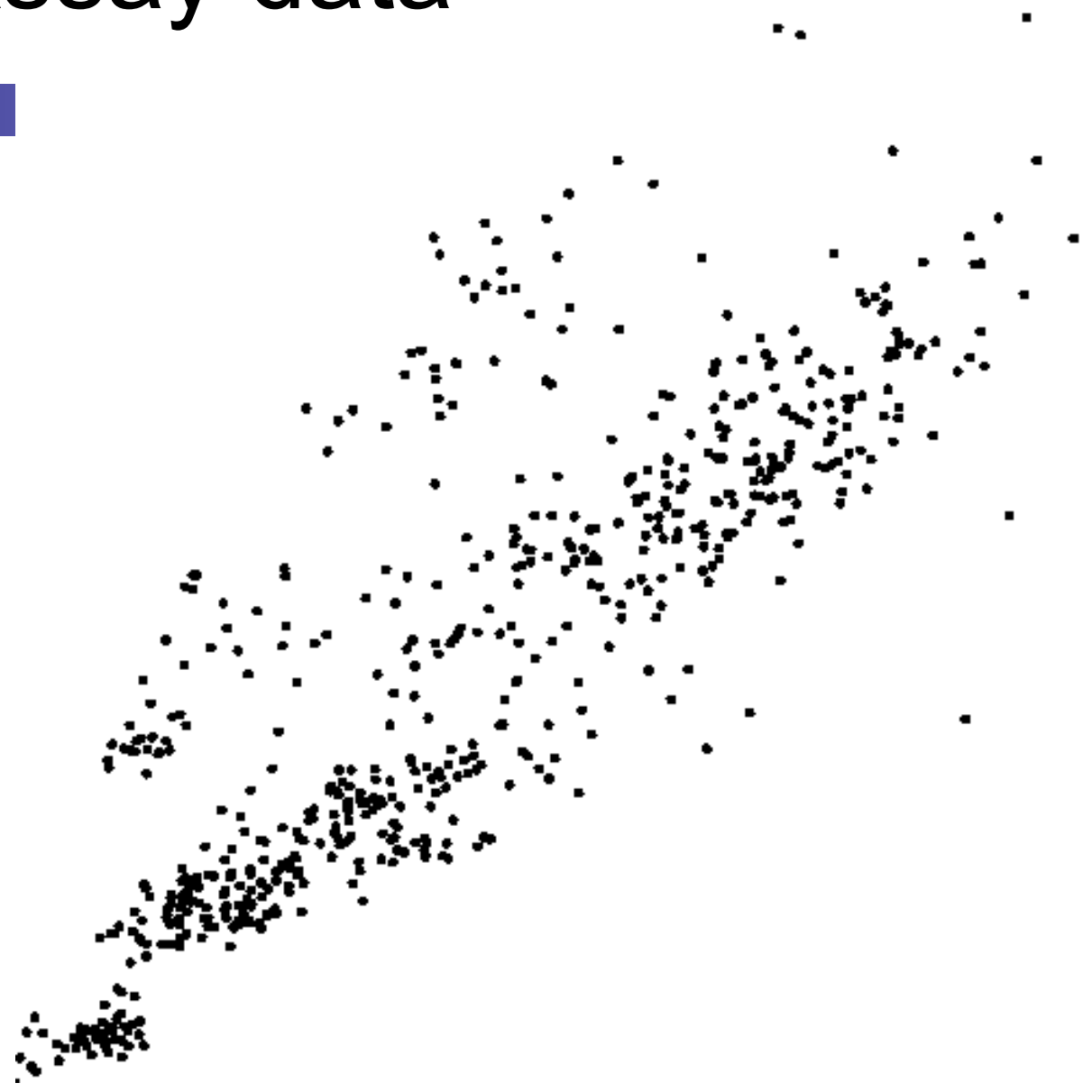
# After 6th iteration



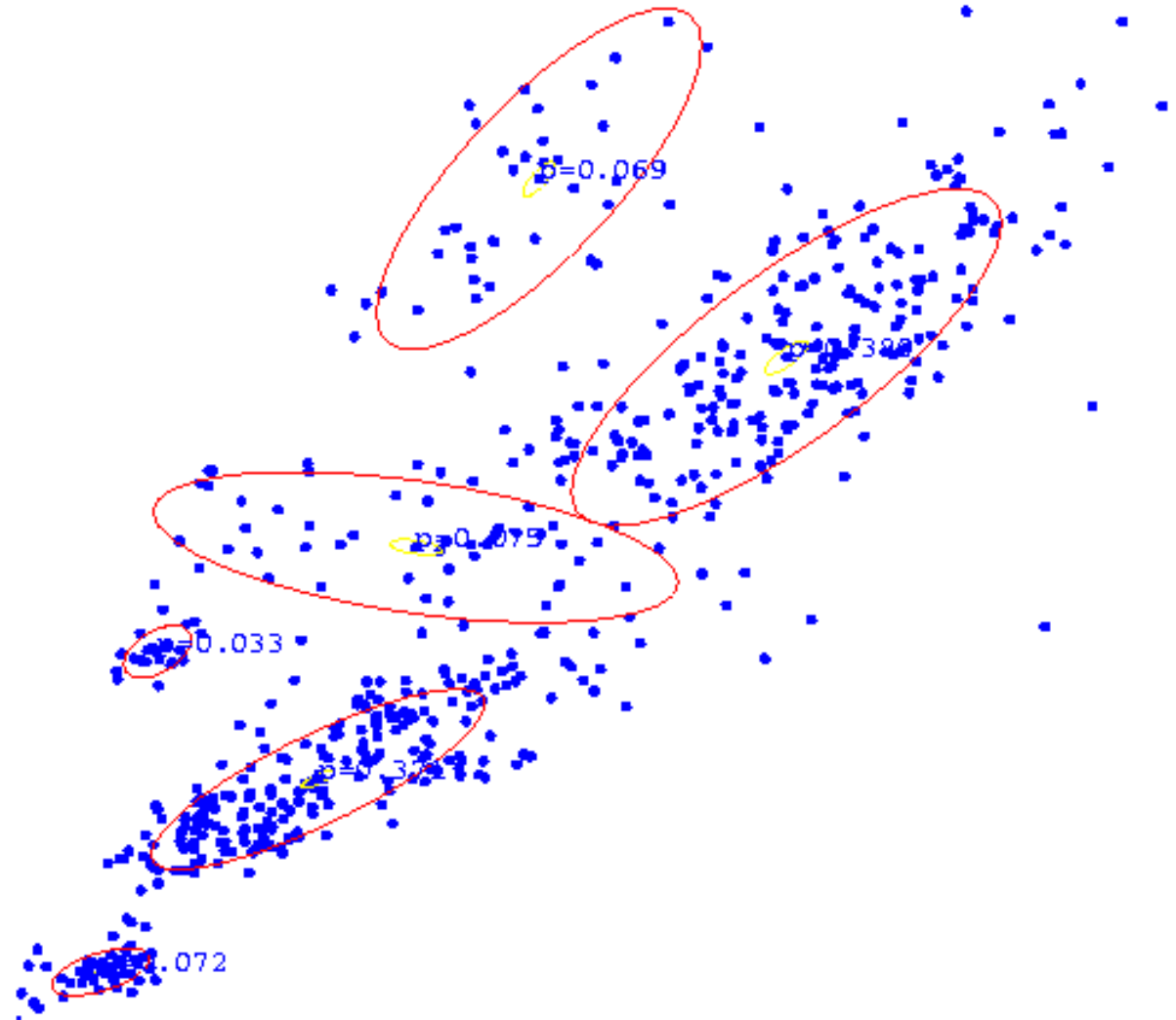
# After 20th iteration




# Some Bio Assay data



# GMM clustering of the assay data





# Resulting Density Estimator

