

Announcements



- Homework 3 due tonight!
- HW 4 will be posted tonight. Start early.



Clustering

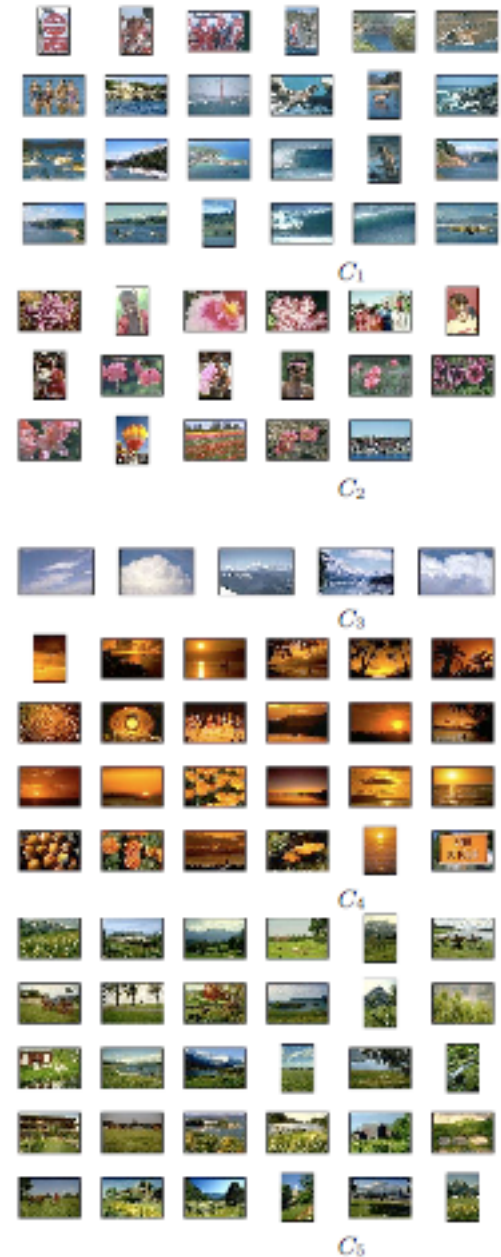
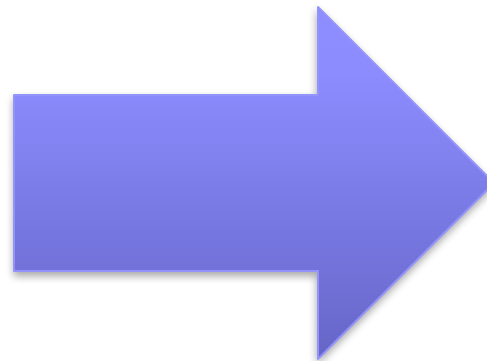
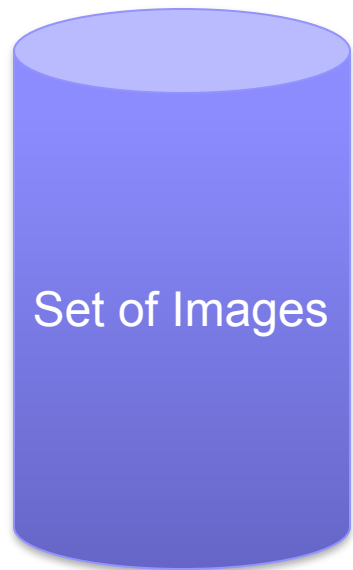
Machine Learning – CSE546

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November 21, 2016

Clustering images



Clustering web search results

The screenshot shows the Clusty search engine interface. At the top, there are navigation links for 'web', 'news', 'images', 'wikipedia', 'blogs', 'jobs', and 'more'. A search bar contains the word 'race', and there are buttons for 'Search' and 'advanced preferences'. Below the search bar, there are tabs for 'clusters', 'sources', and 'sites'. The 'clusters' tab is active, showing a list of clusters. The 'Human' cluster is selected, and it contains 8 documents. The documents are listed in a numbered order, each with a title, a brief description, and a URL. The first document 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'. The seventh is 'Dopefish.com'. The eighth document is not fully visible.

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 (2)
- 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 (3)
- Ethnicity And Race (7)
- Race for the Cure (3)
- 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 **rac**es, 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 - [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/backgrounden/usa/race - [cache] - Ask
- [Amazon.com: Race: The Reality Of Human Differences: Vincent Sarich ...](#)

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 - [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 - [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 - [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 - [cache] - Open Directory

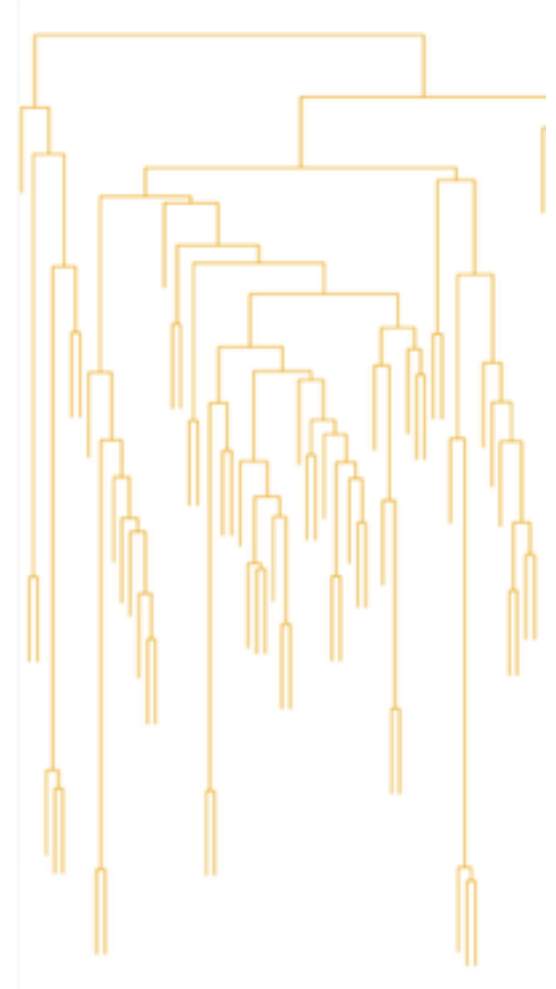
Hierarchical Clustering

Pick one:

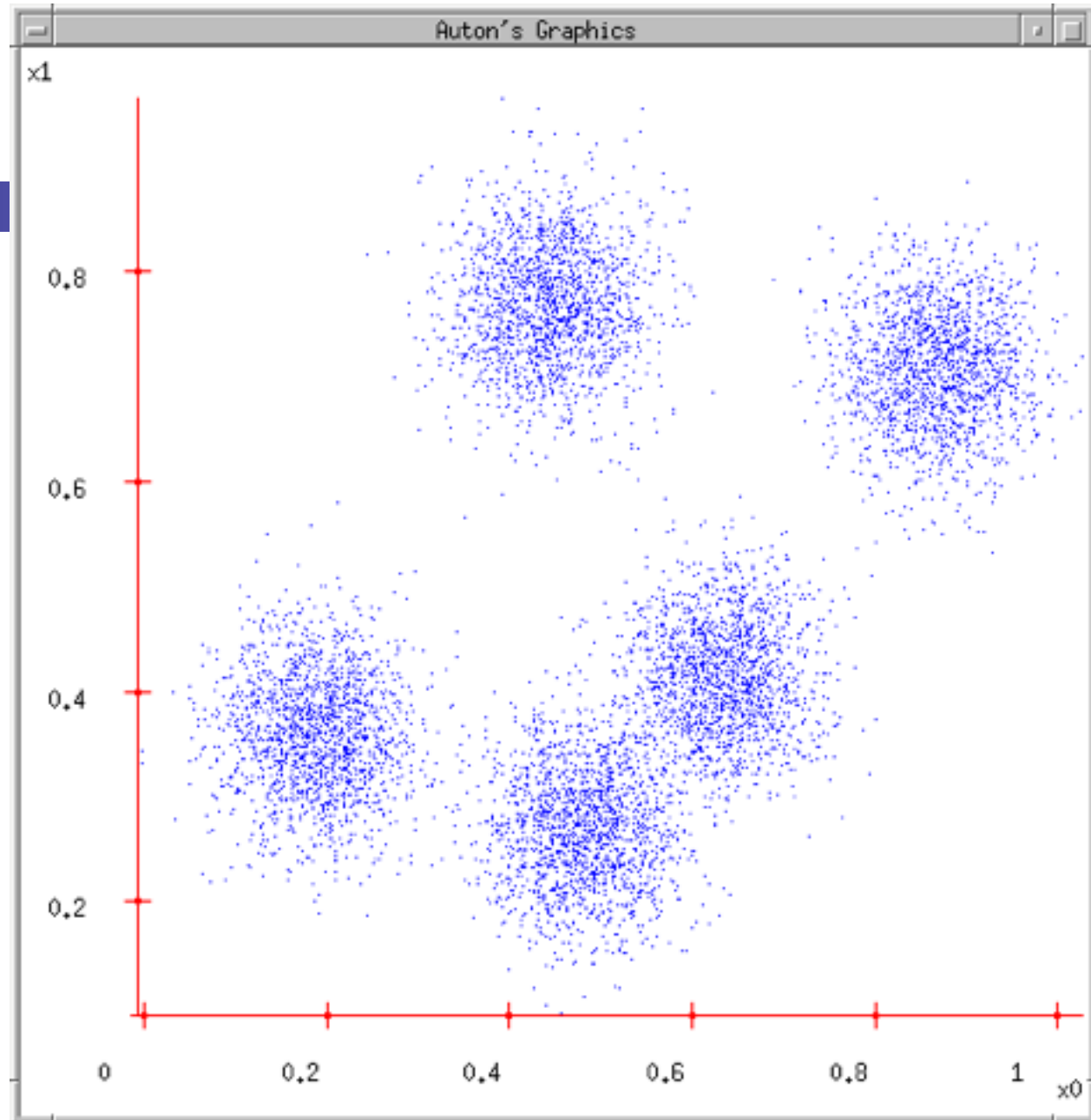
- Bottom up: start with every point as a cluster and merge
- Top down: start with a single cluster containing all points and split

Different rules for splitting/merging, no “right answer”

Gives apparently interpretable tree representation.
However, warning: even random data with no structure will produce a tree that “appears” to be structured.

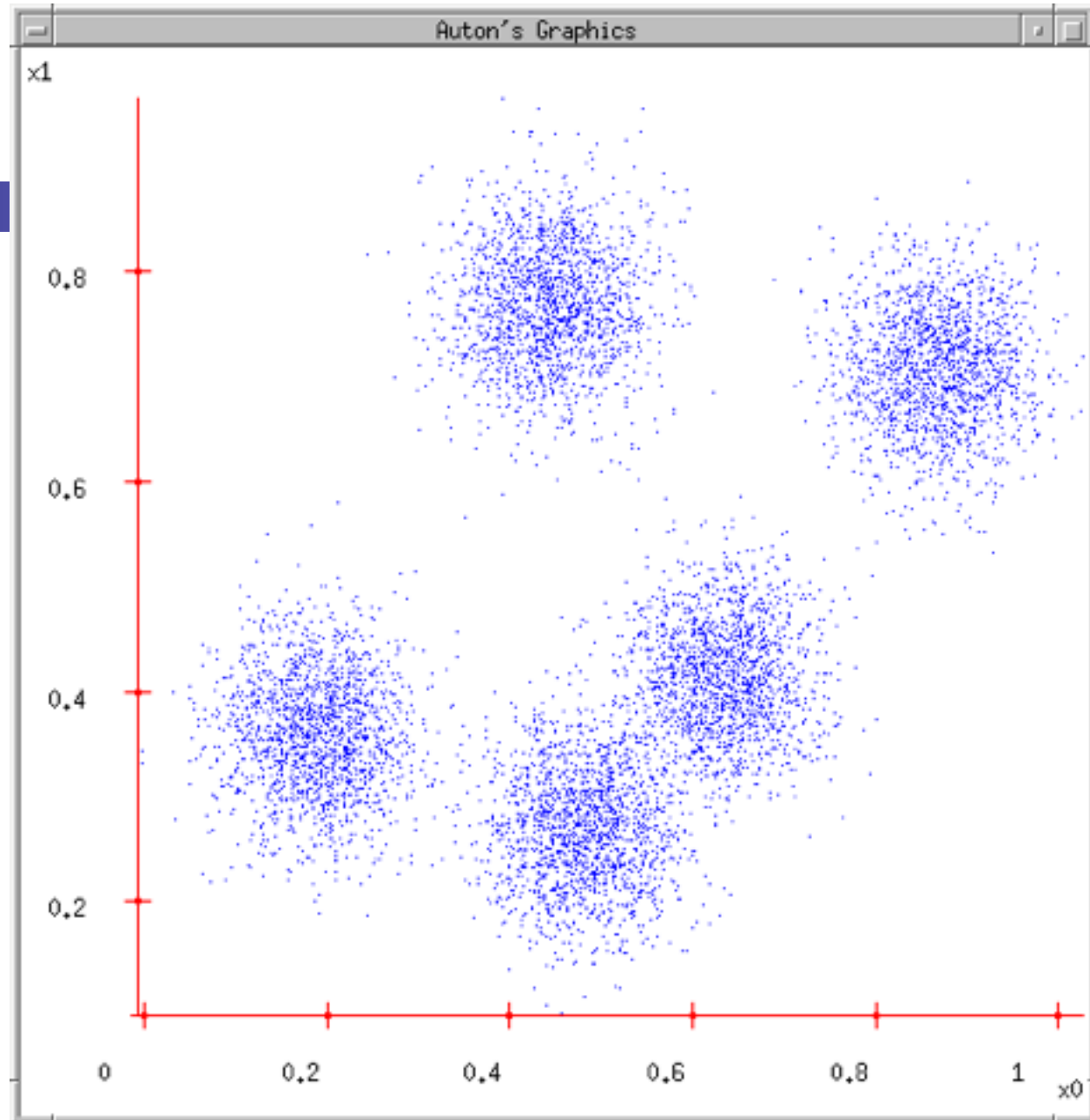


Some Data



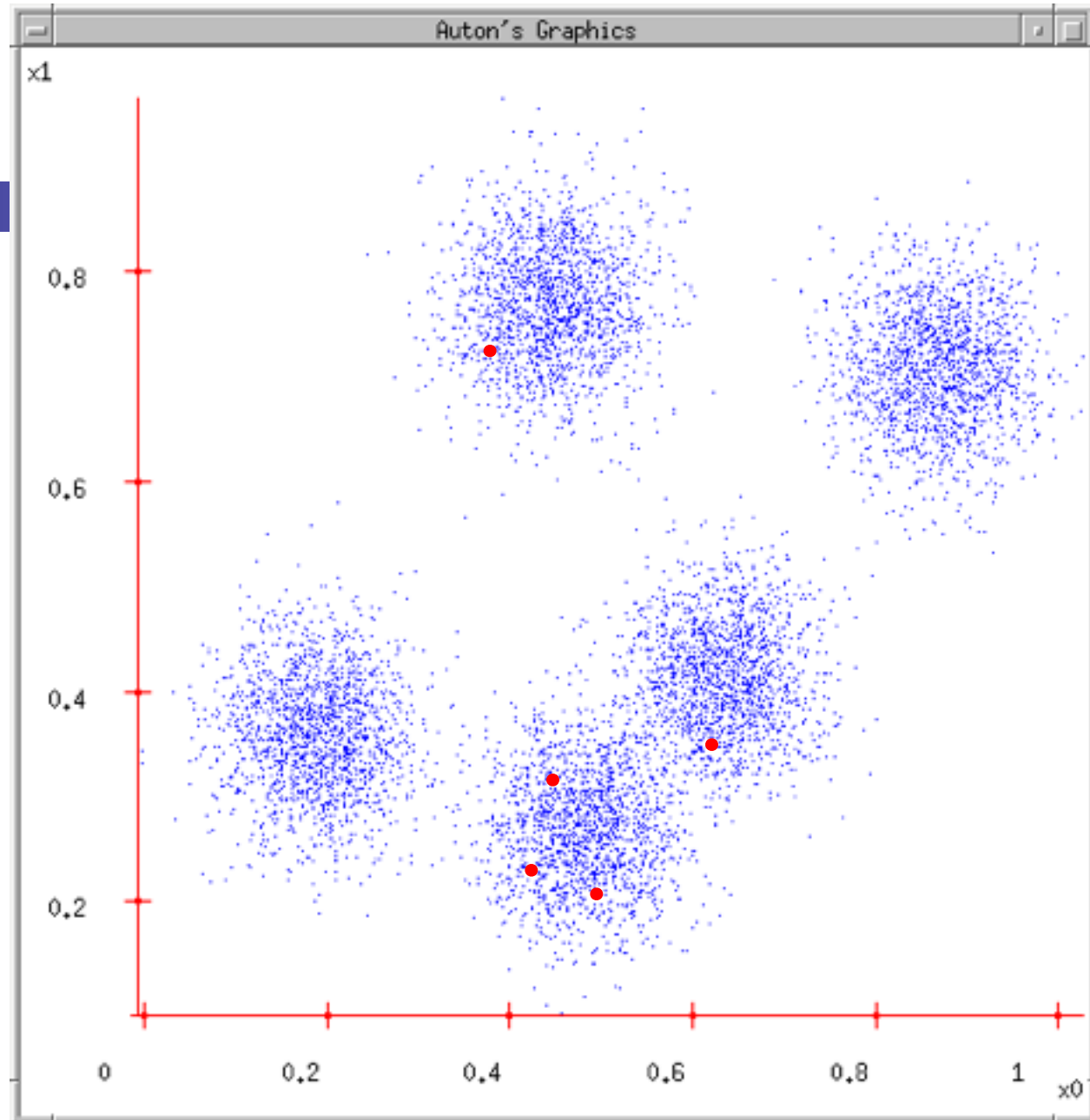
K-means

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



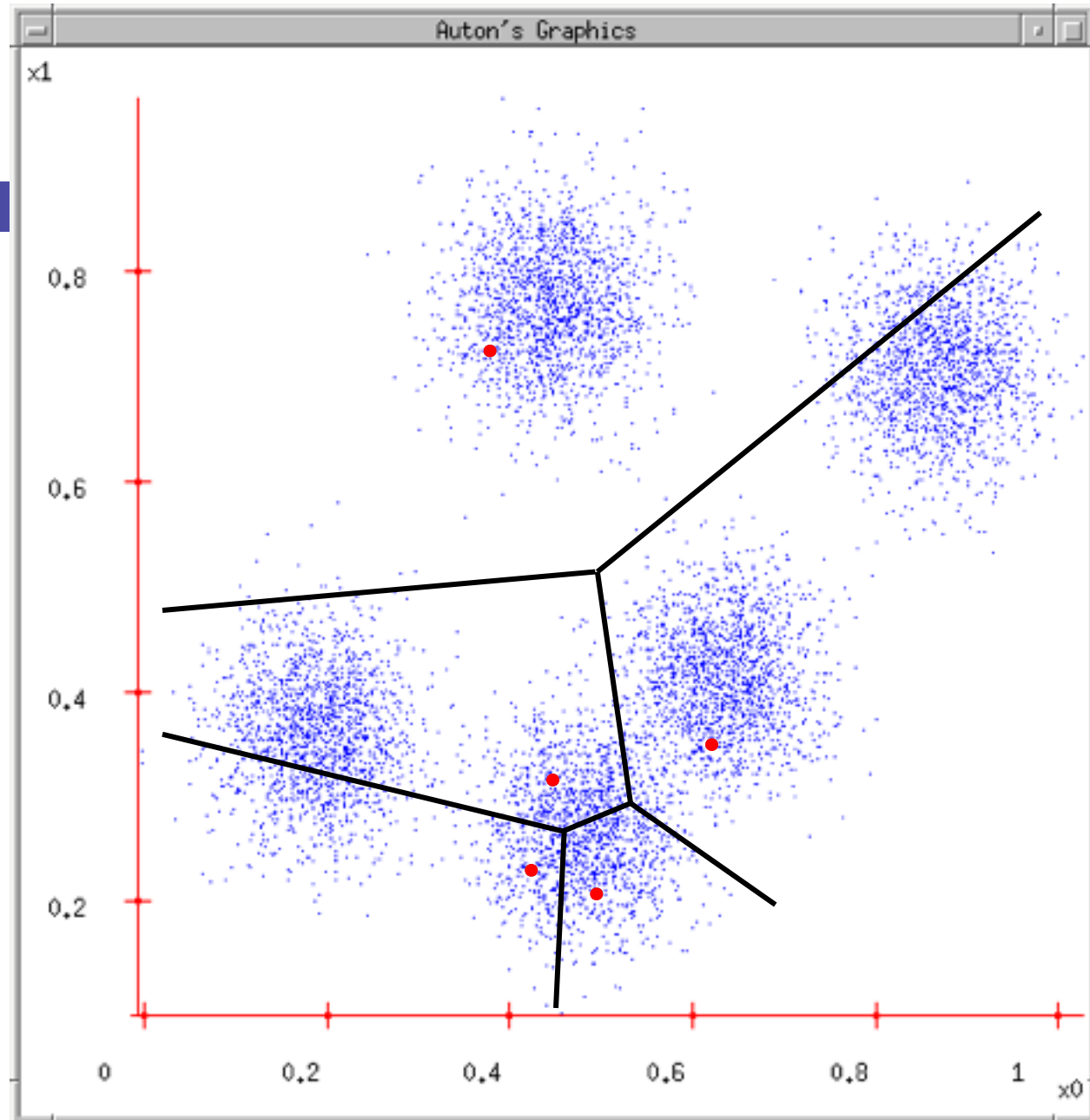
K-means

1. Ask user how many clusters they'd like.
(e.g. $k=5$)
2. Randomly guess k cluster Center locations



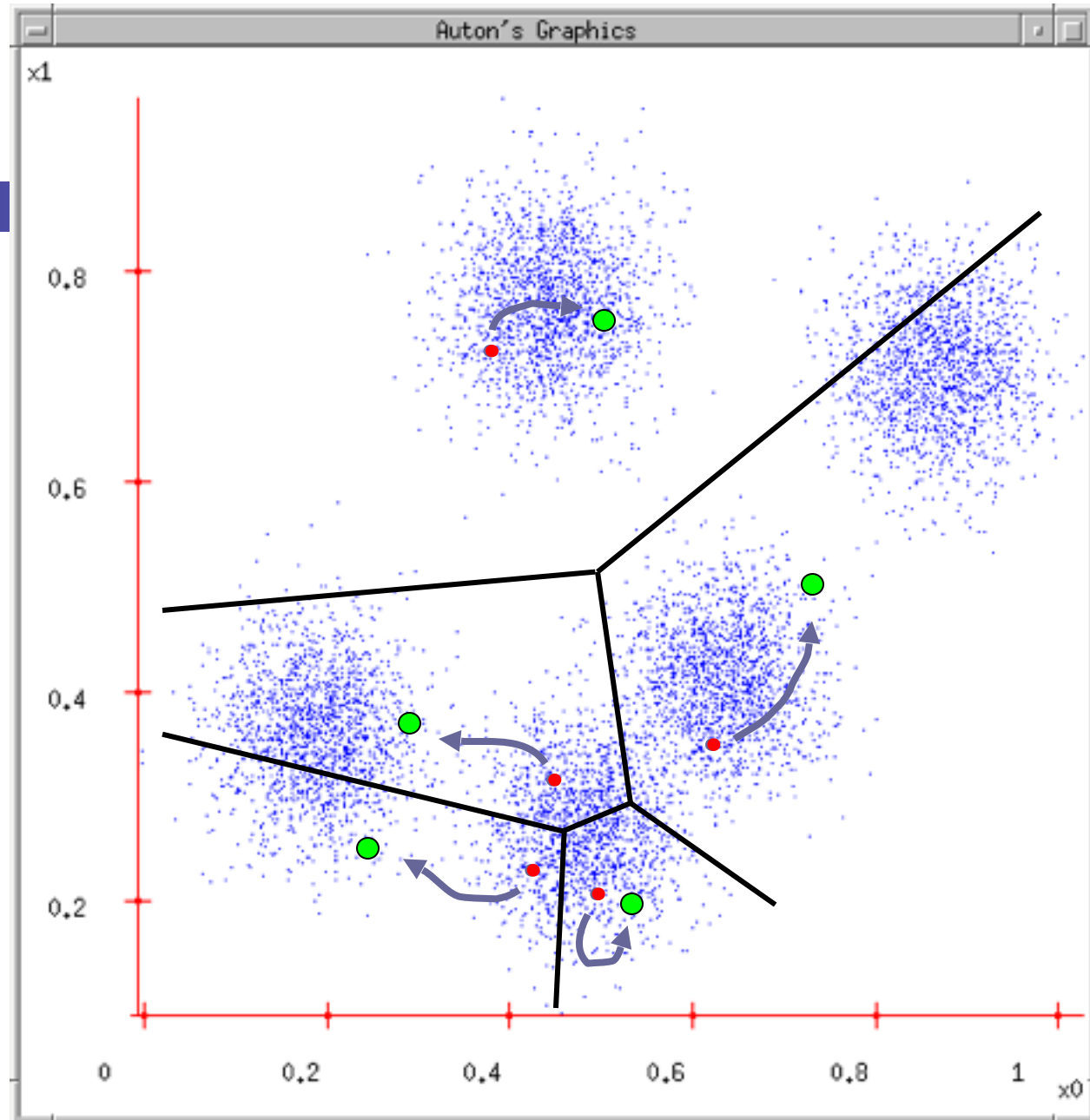
K-means

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



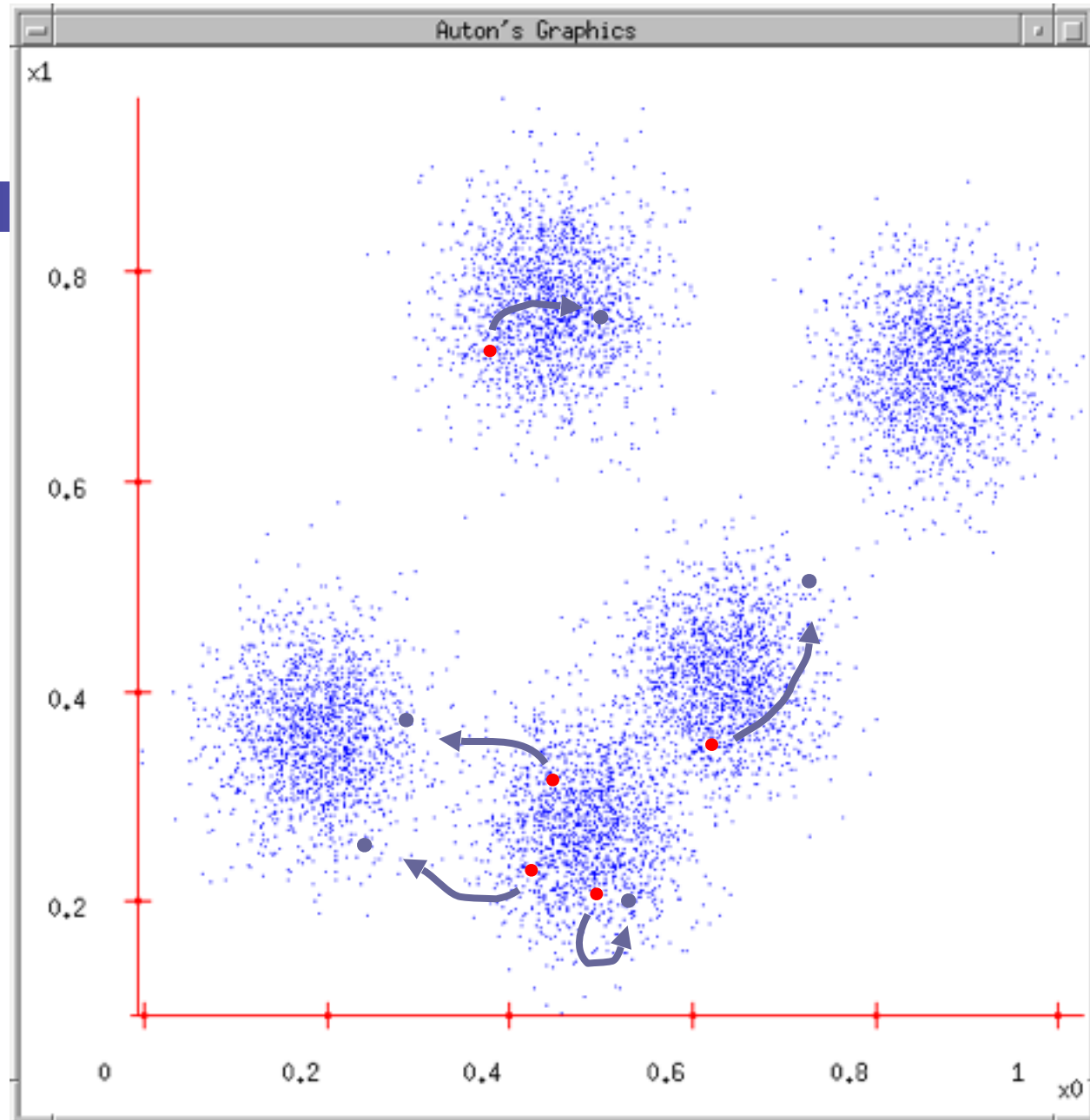
K-means

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



K-means

1. Ask user how many clusters they'd like.
(e.g. $k=5$)
2. Randomly guess k cluster Center locations
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:** μ_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!

What is K-means optimizing?

- Potential function $F(\mu, C)$ of centers μ and point allocations C :

- $$F(\mu, C) = \sum_{j=1}^{N_t} \|\mu_{C(j)} - x_j\|^2$$

- Optimal K-means:
 - $\min_{\mu} \min_C F(\mu, C)$

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 μ , 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 μ

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 1024×1024 grayscale image at 8 bits per pixel. The center image is the result of 2×2 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

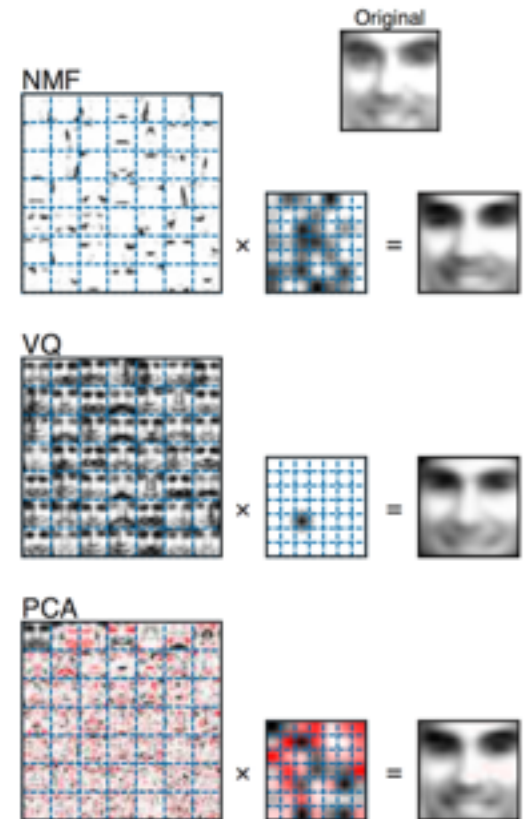
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Vector Quantization, Fisher Vectors

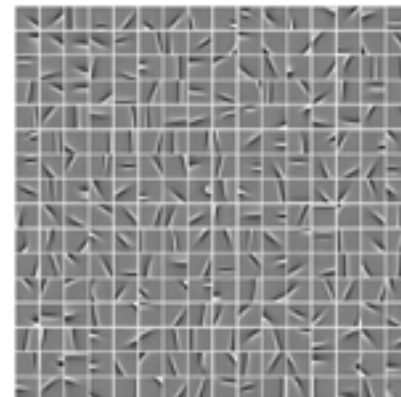
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Typical output of k-means on patches



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

Adjacency matrix: \mathbf{W}

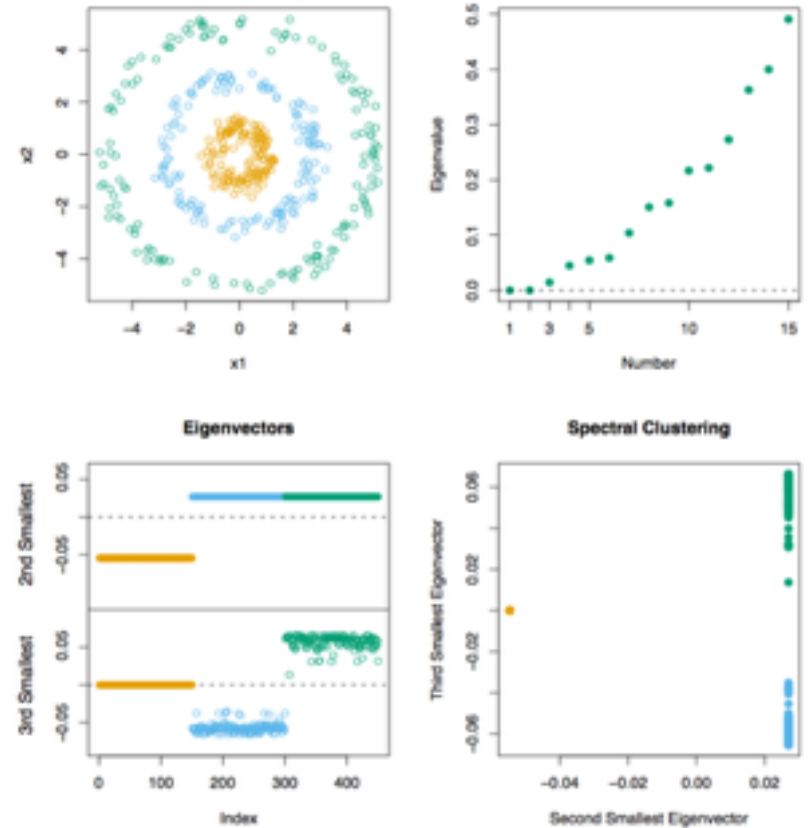
$\mathbf{W}_{i,j}$ = weight of edge (i,j)

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

Given feature vectors, could construct:

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

Popular to use the Laplacian \mathbf{L} or its normalized form $\tilde{\mathbf{L}} = \mathbf{I} - \mathbf{D}^{-1}\mathbf{W}$ as a regularizer for learning over graphs





Mixtures of Gaussians

Machine Learning – CSE546

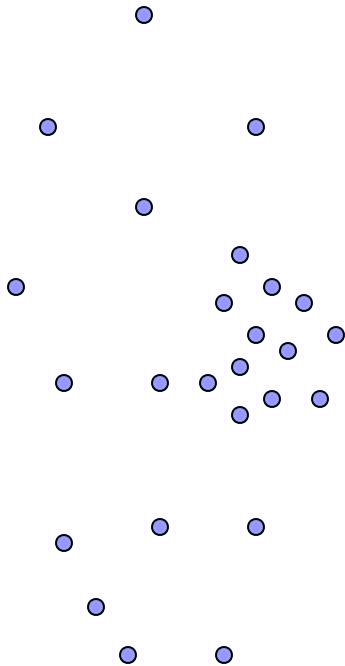
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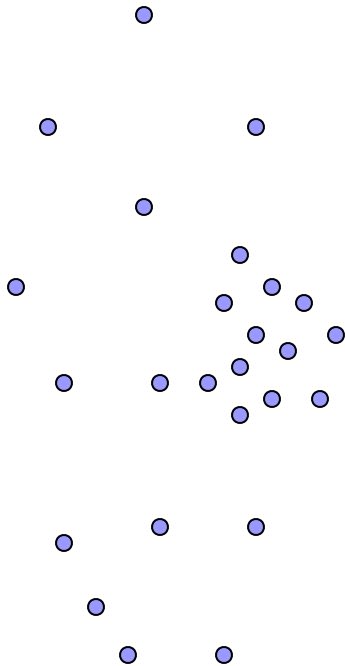
(One) bad case for k-means

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



(One) bad case for k-means

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



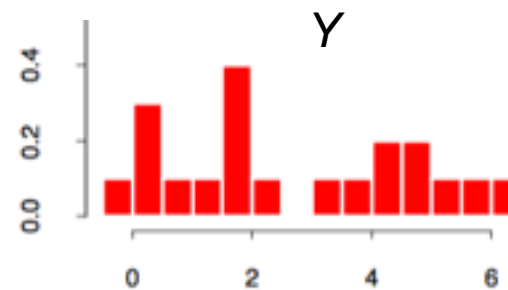
Mixture models

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

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

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

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



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

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

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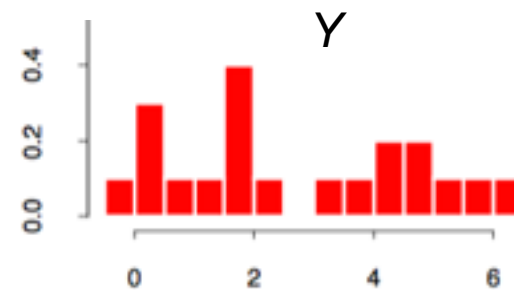
$$\Delta \in \{0, 1\} \text{ with } \Pr(\Delta = 1) = \pi$$

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

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

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

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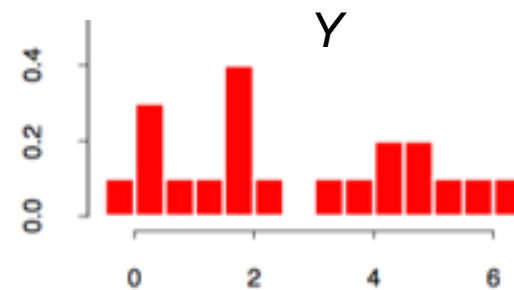
$$\Delta \in \{0, 1\} \text{ with } \Pr(\Delta = 1) = \pi$$

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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 θ ?



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

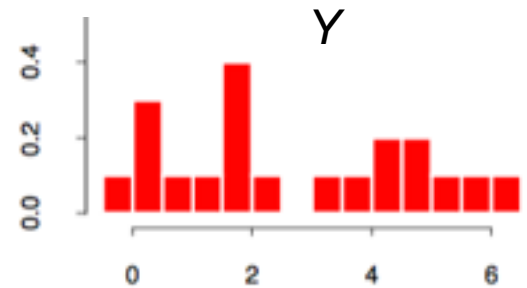
$\mathbf{\Delta} = \{\Delta_i\}_{i=1}^n$ is unobserved data

Mixture models

$$\begin{aligned} Y_1 &\sim N(\mu_1, \sigma_1^2), \\ Y_2 &\sim N(\mu_2, \sigma_2^2), \\ Y &= (1 - \Delta) \cdot Y_1 + \Delta \cdot Y_2, \end{aligned}$$

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

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



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

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

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 θ , how would we choose $\mathbf{\Delta}$?

Mixture models

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

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

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

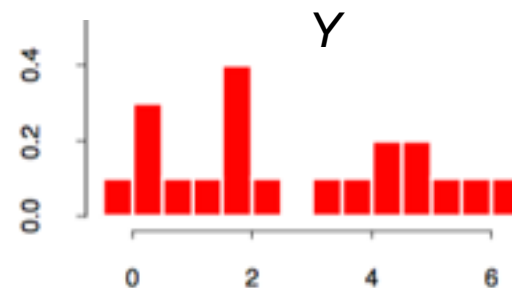
$$\Delta \in \{0, 1\} \text{ with } \Pr(\Delta = 1) = \pi$$

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

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

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

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

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

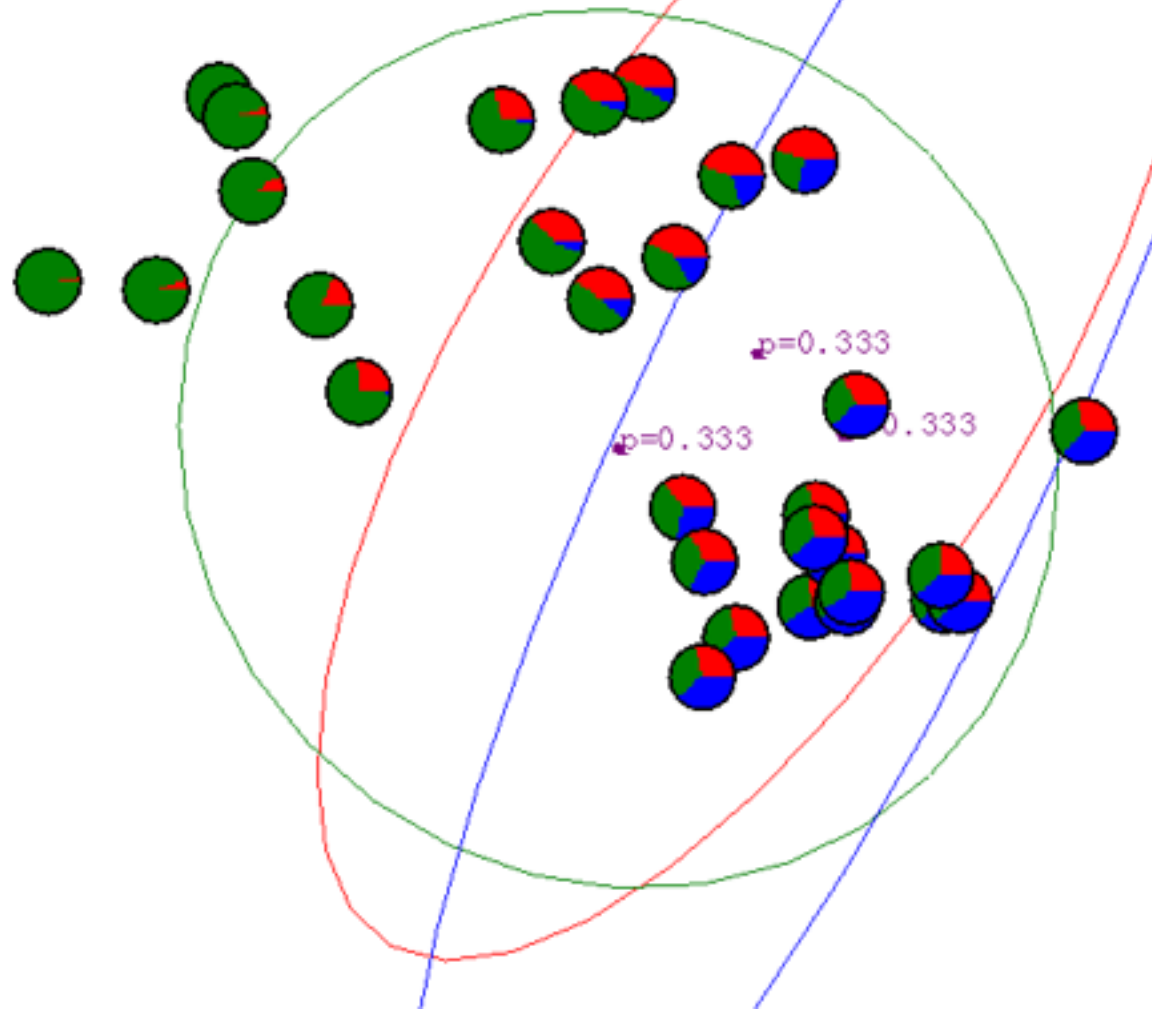
3. *Maximization Step*: compute the weighted means and variances:

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

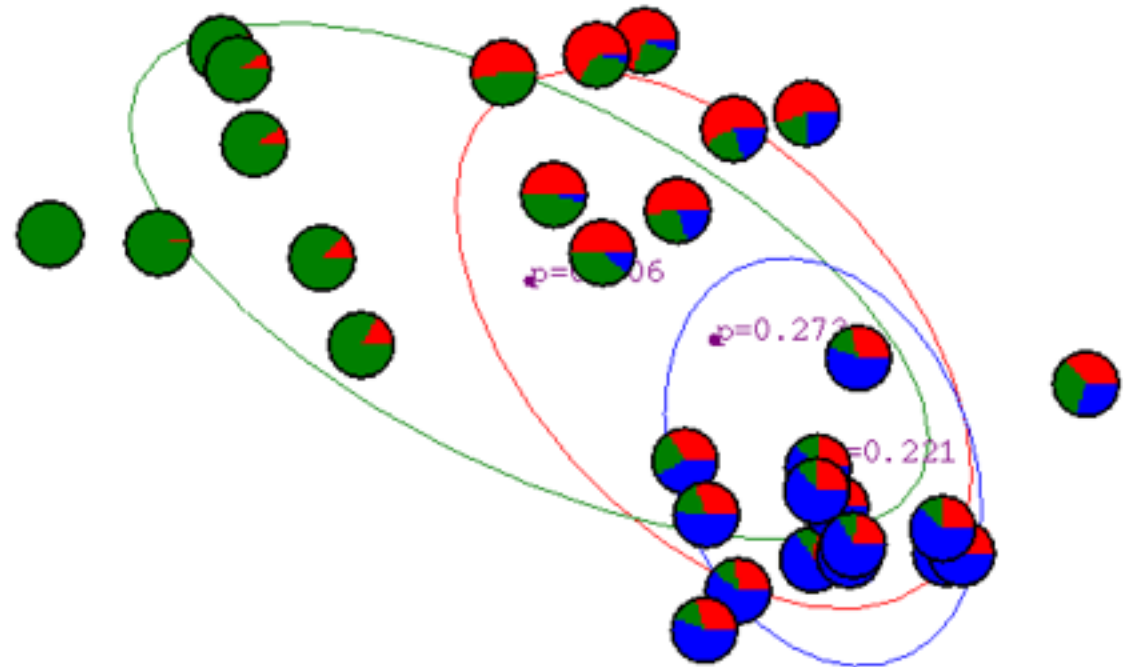
and the mixing probability $\hat{\pi} = \sum_{i=1}^N \hat{\gamma}_i / N$.

4. Iterate steps 2 and 3 until convergence.
-

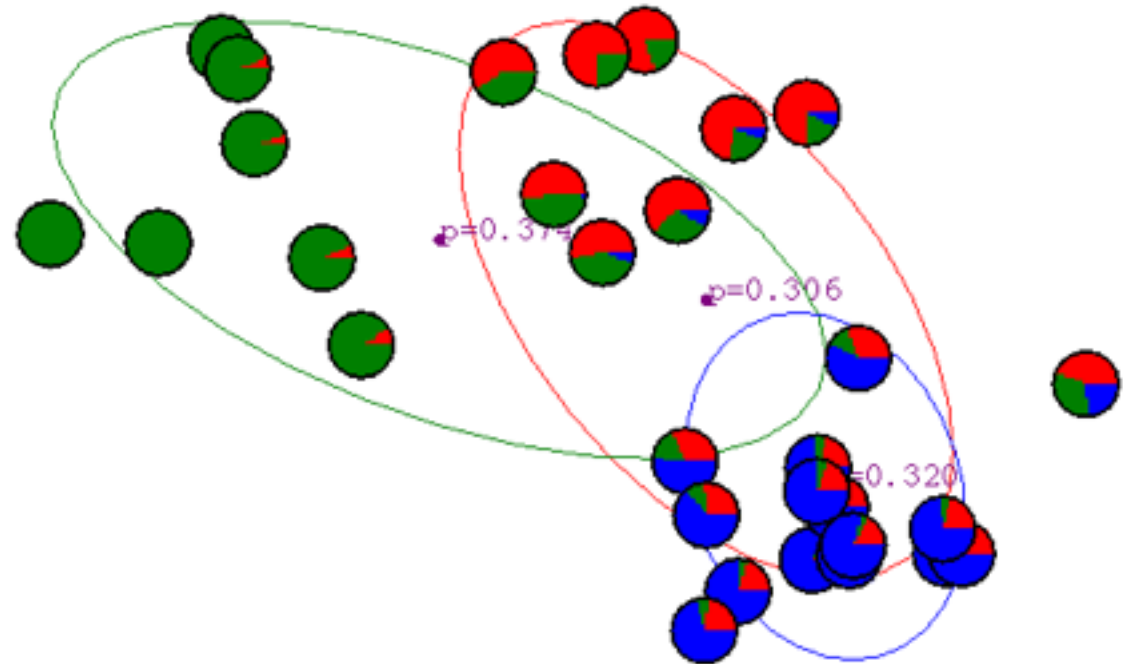
Gaussian Mixture Example: Start



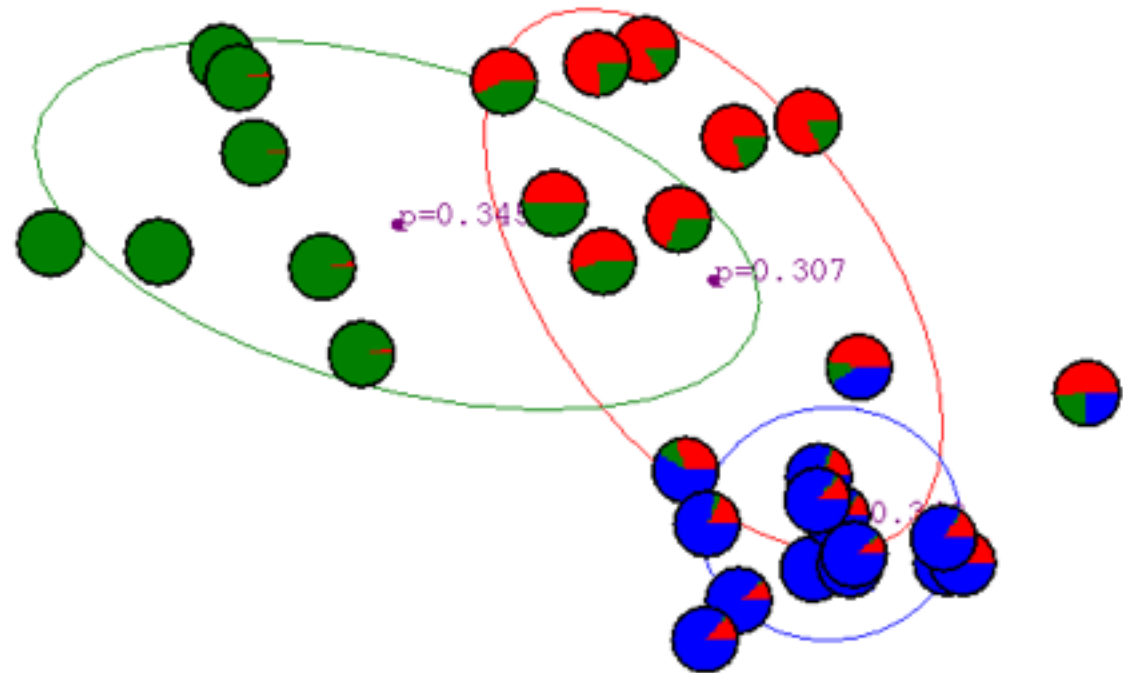
After first iteration



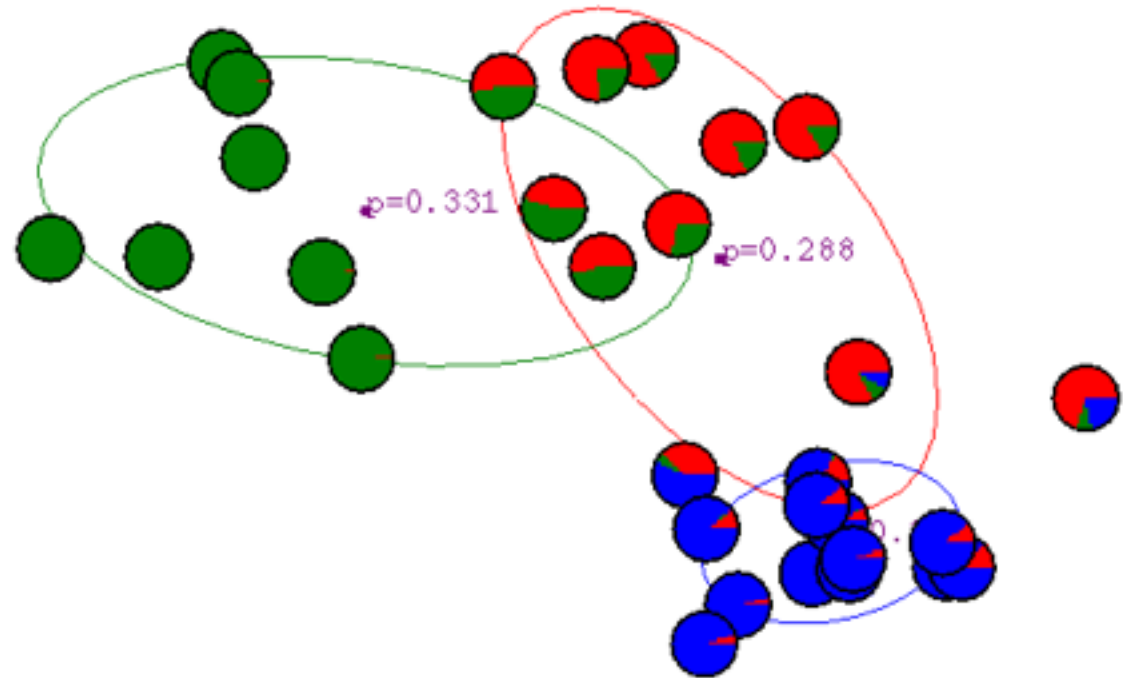
After 2nd iteration



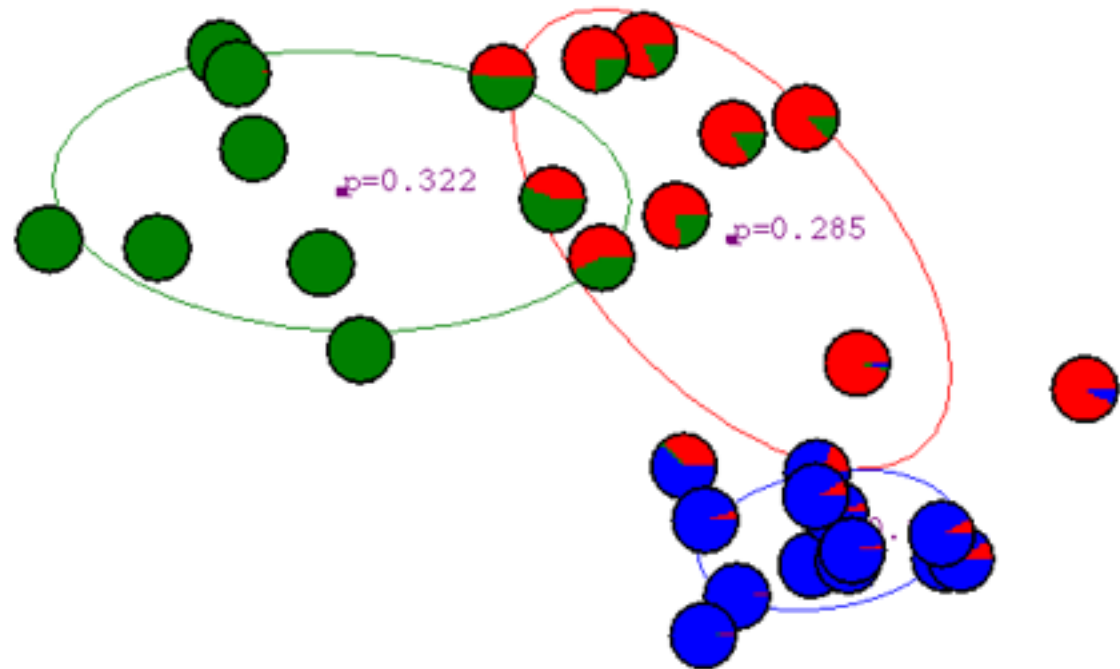
After 3rd iteration



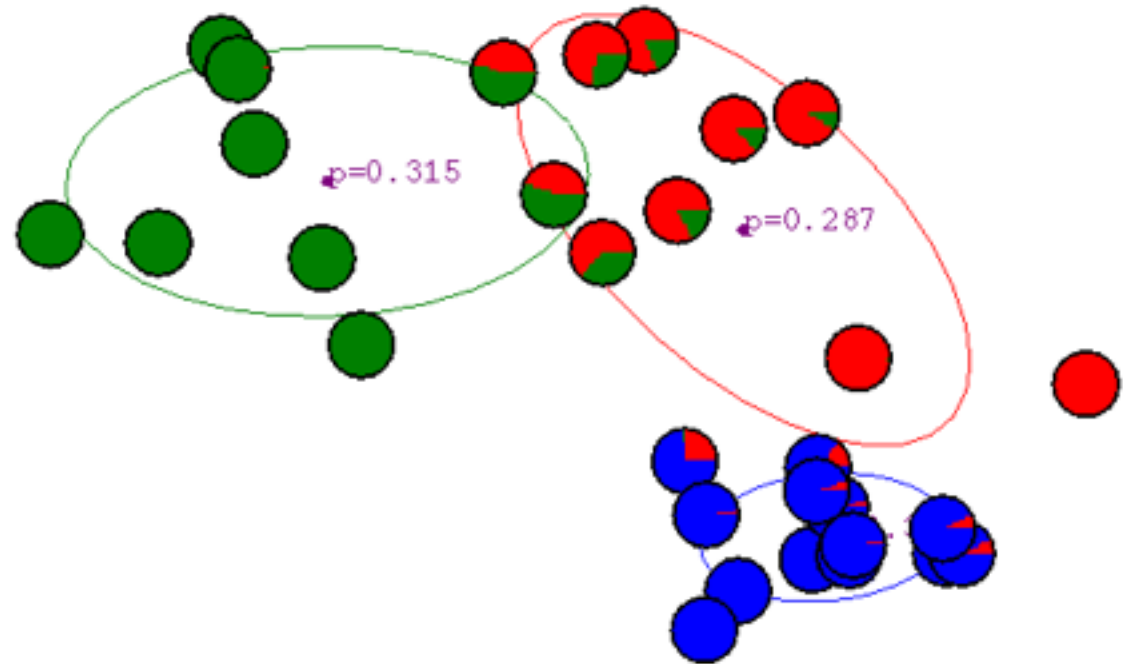
After 4th iteration



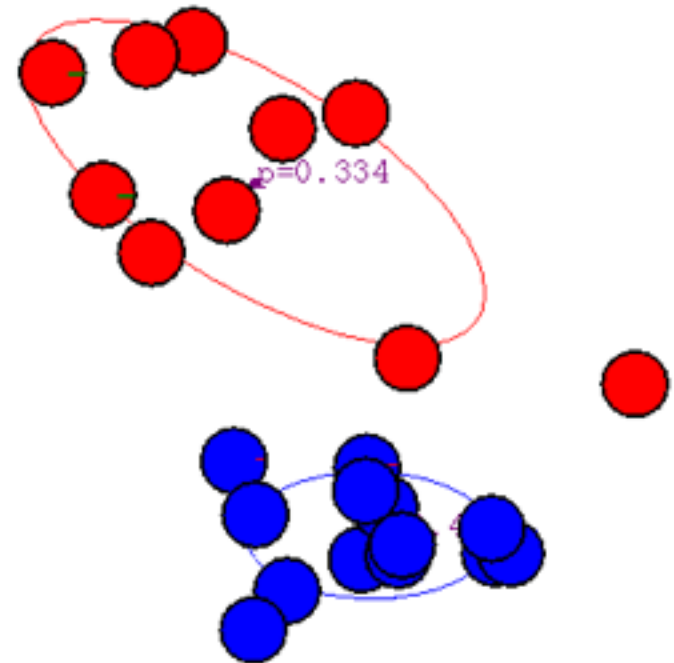
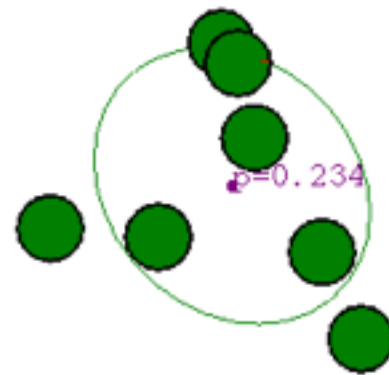
After 5th iteration



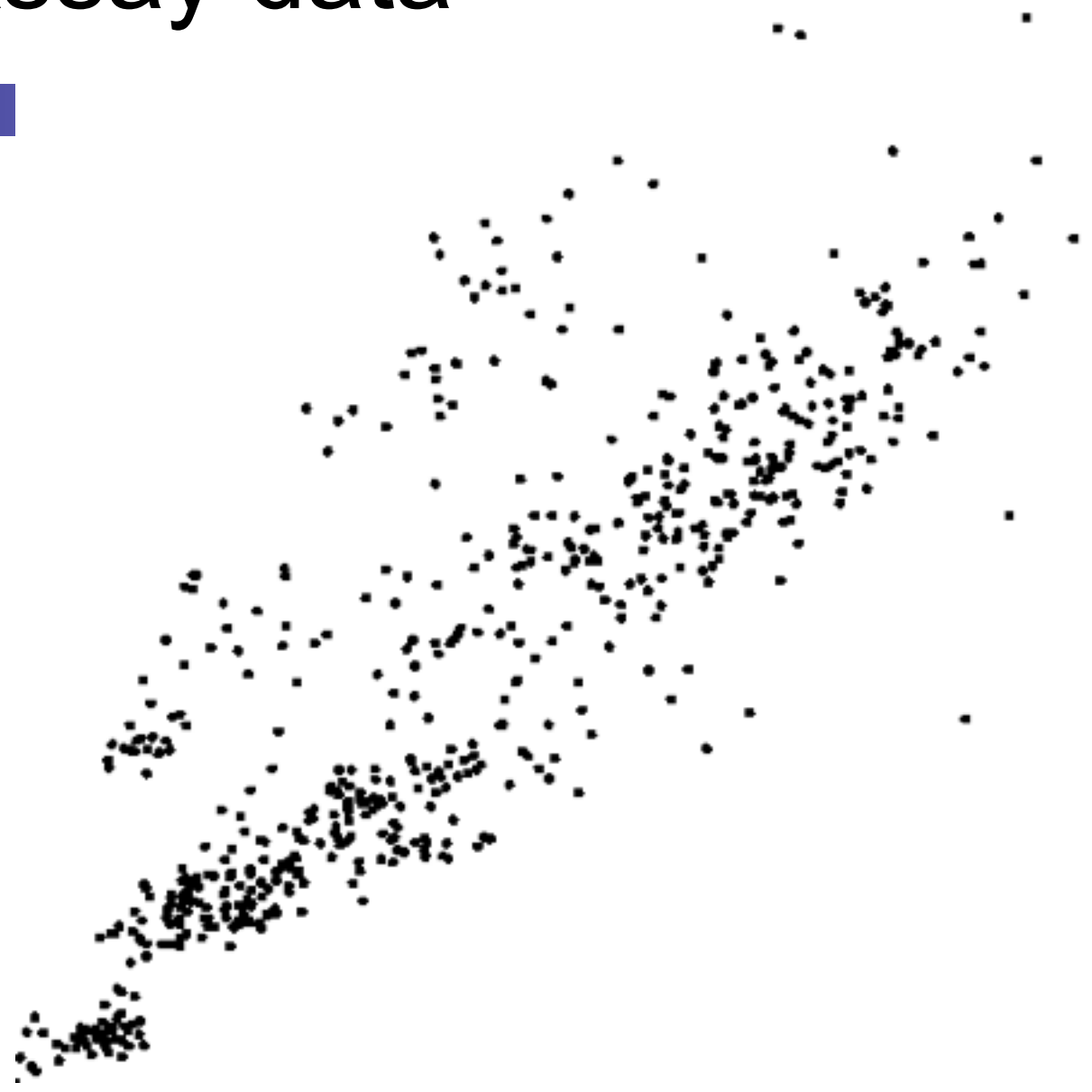
After 6th iteration



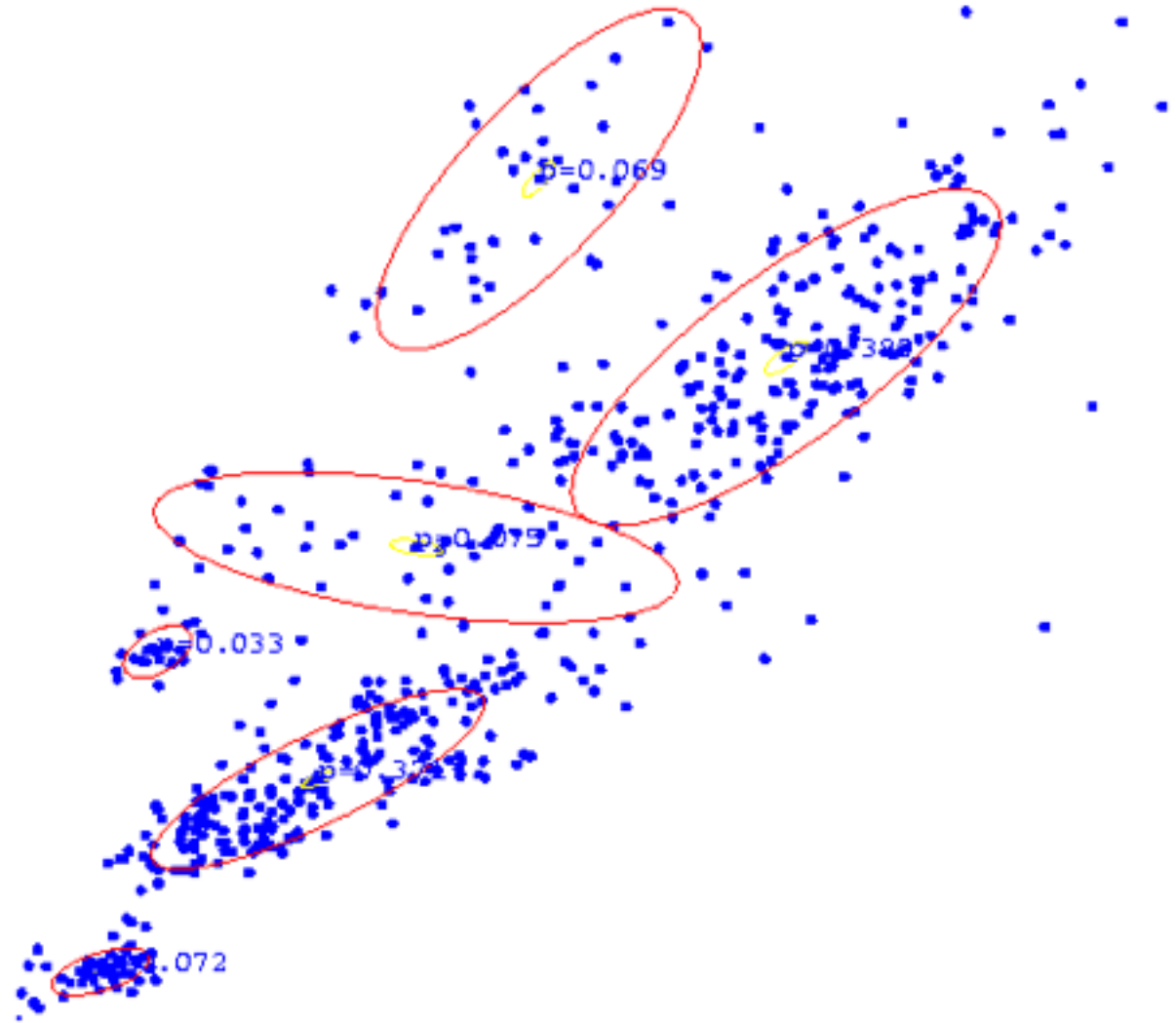
After 20th iteration




Some Bio Assay data

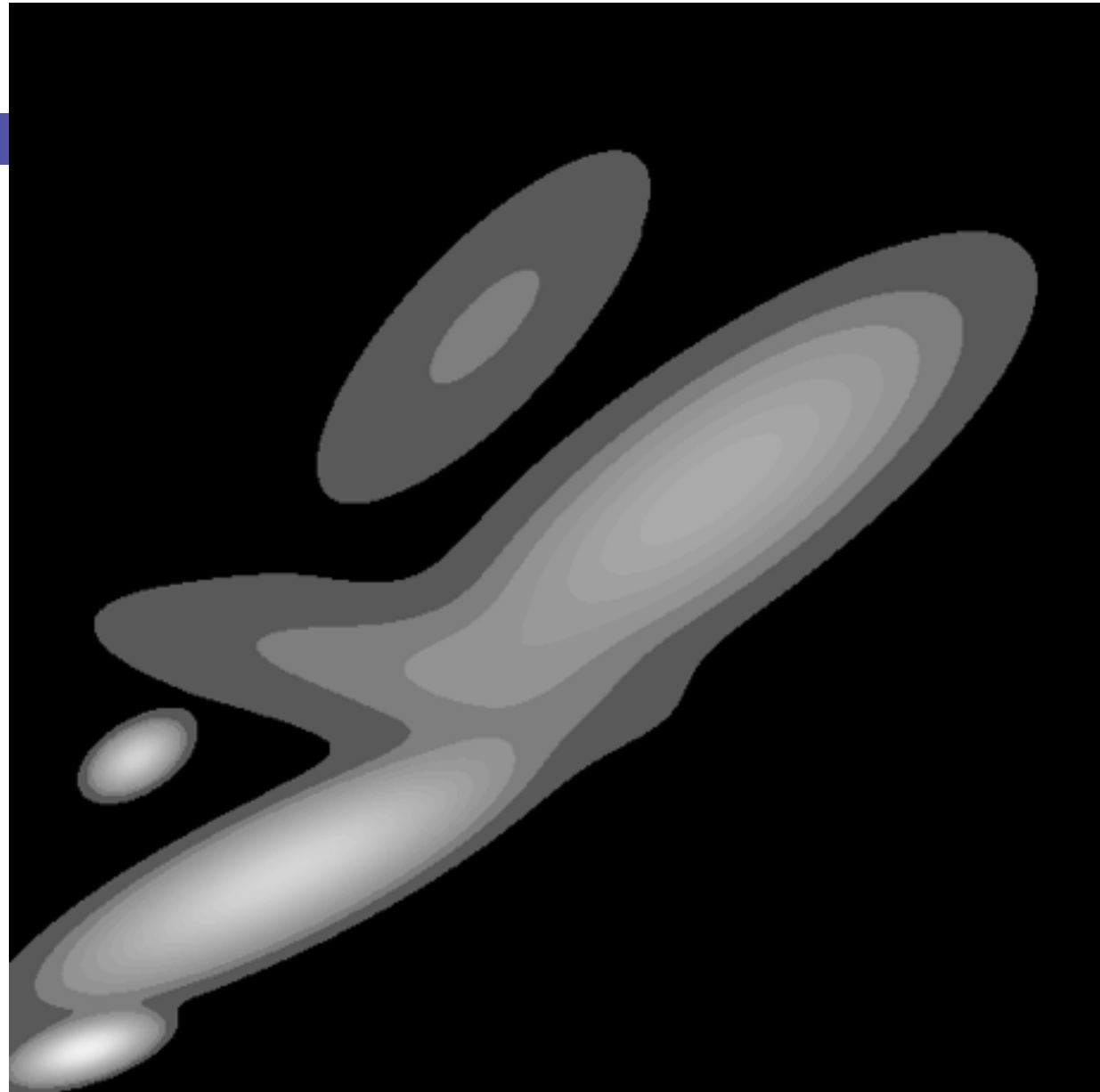


GMM clustering of the assay data





Resulting Density Estimator



Expectation Maximization Algorithm

The iterative gaussian mixture model (GMM) fitting algorithm is special case of EM:

Algorithm 8.2 *The EM Algorithm.*

1. Start with initial guesses for the parameters $\hat{\theta}^{(0)}$.
2. *Expectation Step*: at the j th step, compute

$$Q(\theta', \hat{\theta}^{(j)}) = E(\ell_0(\theta'; \mathbf{T}) | \mathbf{Z}, \hat{\theta}^{(j)}) \quad (8.43)$$

as a function of the dummy argument θ' .

3. *Maximization Step*: determine the new estimate $\hat{\theta}^{(j+1)}$ as the maximizer of $Q(\theta', \hat{\theta}^{(j)})$ over θ' .
 4. Iterate steps 2 and 3 until convergence.
-

\mathbf{Z} is observed data

Δ is unobserved data

$$\mathbf{T} = (\mathbf{Z}, \Delta)$$

Missing data example

$x_i \sim \mathcal{N}(\mu, \Sigma)$ but suppose some entries of x_i are *missing*

$$\ell(\theta | \mathbf{T}, \theta) = -\frac{1}{2} \log(2\pi |\Sigma|) + (x_i - \mu)^T \Sigma^{-1} (x - \mu)$$

\mathbf{Z} is observed data

Δ is unobserved data

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E Step: $\mathbb{E}[\ell(\theta'; \mathbf{T}) | \mathbf{Z}, \hat{\theta}^{(j)}]$

Natural choice for $\hat{\theta}^{(0)}$?

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Connection to matrix factorization?



Density Estimation

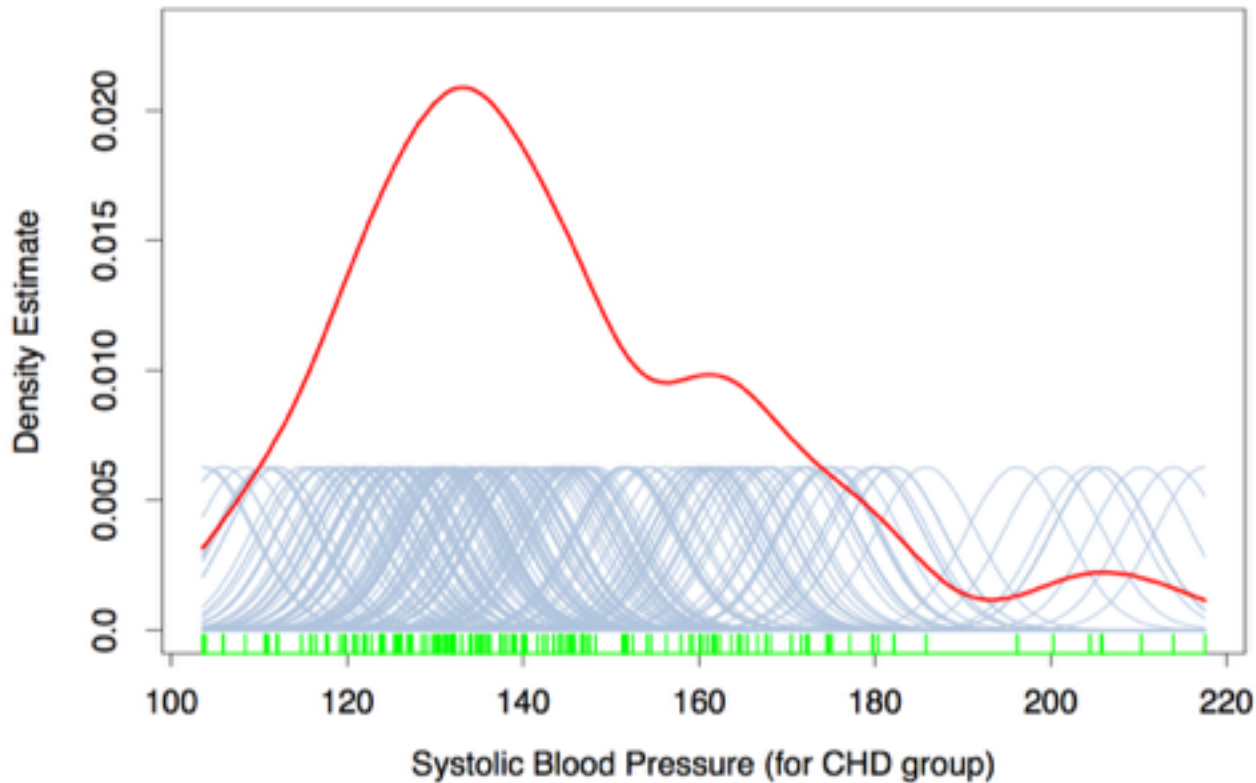
Machine Learning – CSE546

Kevin Jamieson

University of Washington

November 21, 2016

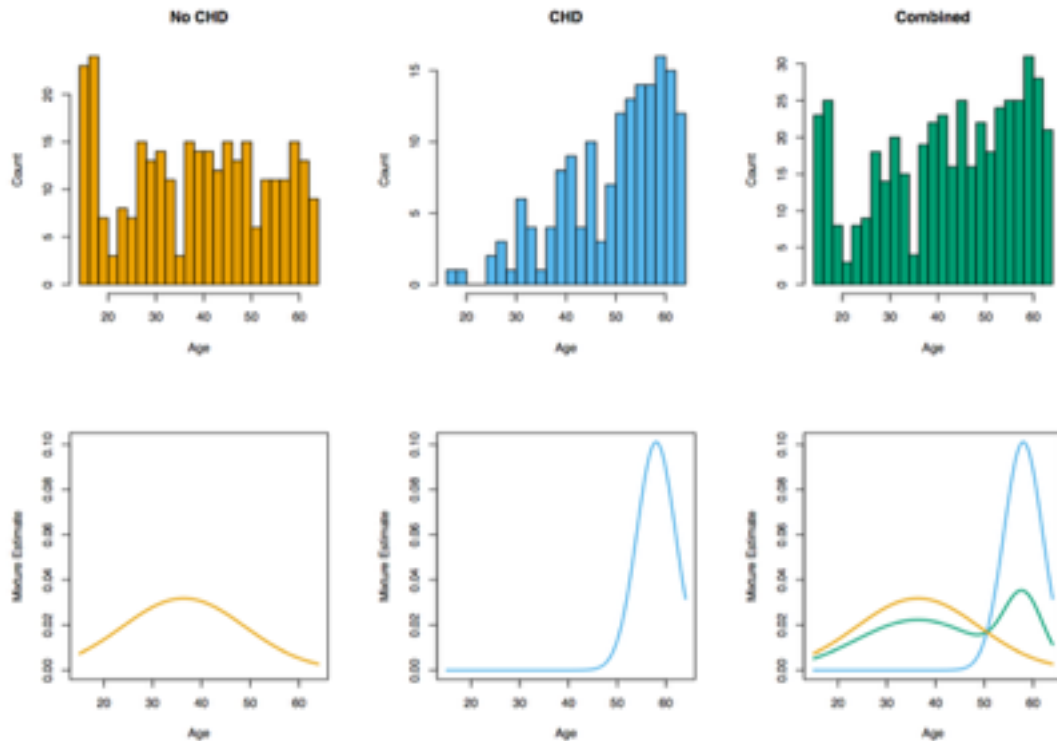
Kernel Density Estimation



$$f(x) = \sum_{m=1}^M \alpha_m \phi(x; \mu_m, \Sigma_m)$$

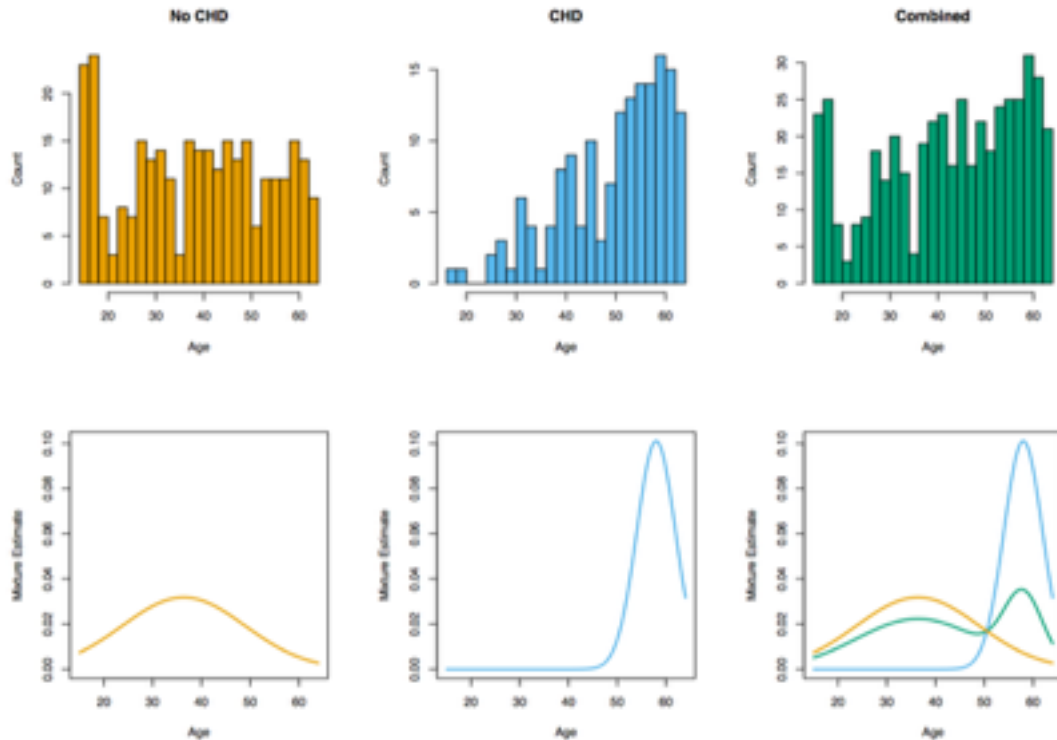
A very “lazy” GMM

Kernel Density Estimation



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Kernel Density Estimation



What is the Bayes optimal classification rule?

$$\hat{r}_{im} = \frac{\hat{\alpha}_m \phi(x_i; \hat{\mu}_m, \hat{\Sigma}_m)}{\sum_{k=1}^M \hat{\alpha}_k \phi(x_i; \hat{\mu}_k, \hat{\Sigma}_k)}$$

$$f(x) = \sum_{m=1}^M \alpha_m \phi(x; \mu_m, \Sigma_m)$$

Predict $\arg \max_m \hat{r}_{im}$

Generative vs Discriminative

