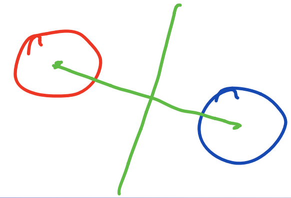
Practice

Milestone
- Appendix



- Fill in the missing plots:

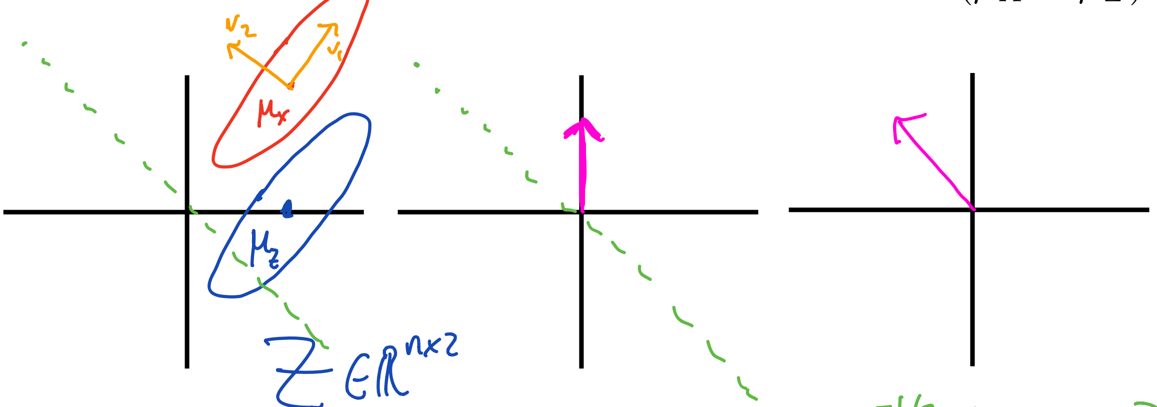
$$\Sigma = \mathbf{X}^T\mathbf{J}\mathbf{J}\mathbf{X} = \mathbf{Z}^T\mathbf{J}\mathbf{J}\mathbf{Z}$$

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

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

$X \in \mathbb{R}^{n \times 2}$

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



$$JX = US^{1/2}V^T$$

$$(JX)^T(JX)$$
$$= X^TJJ^TX$$
$$= VS^{1/2}S^{1/2}V^T$$
$$= VSV^T$$

$$\underbrace{VS^{-1/2}V^T(JX)^T}_{\substack{W \\ d \times n}} = VS^{-1/2}V^TVS^{1/2}U^T$$
$$= V \quad U^T$$

$WW^T = VU^TUV^T = VV^T$

Matrix Completion

Machine Learning – CSE546
Kevin Jamieson
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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, $\mathbf{U}^T\mathbf{U} = I$, $\mathbf{V}^T\mathbf{V} = I$.

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

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

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

$\mathbf{V}$ 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 $\text{diag}(\mathbf{S})$

Singular Value Decomposition (SVD)

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$$\mathbf{U} = [u_1, \ldots, u_r] \qquad \mathbf{V} = [v_1, \ldots, v_r] \qquad \mathbf{S} = \mathrm{diag}(s_1, \ldots, s_r)$$

$$\mathbf{A} = \sum_{k=1}^{r} u_k v_k^T s_k \qquad s_1 \geq s_2 \geq \cdots \geq s_r$$

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

Singular Value Decomposition (SVD)

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

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

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$$\mathbf{A} = \sum_{k=1}^{r} u_k v_k^T s_k \qquad\qquad s_1 \geq s_2 \geq \cdots \geq s_r$$

In general: $$\sum_{k=1}^{p} u_i v_i^T s_i = \arg \min_{\mathbf{Z}:\mathrm{rank}(\mathbf{Z})=p} \|\mathbf{Z} - \mathbf{A}\|_F^2$$

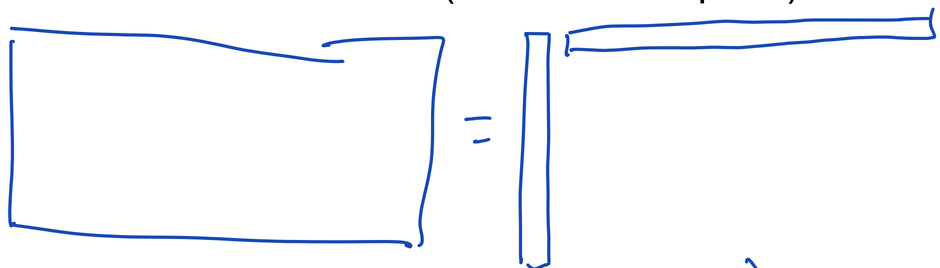
Matrix completion

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	
⋮						



$mn \gg d(m+n)$

$.0012\, mn \gg d(m+n) \implies$ learning is possible

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

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

user i gets assigned d $u_i \in \mathbb{R}^d$

movie j " " $v_j \in \mathbb{R}^d$

Predict user i will rate movie j as $u_i^T v_j$
$= (UV^T)_{i,j}$

$$\nabla_{u_i} \sum_{j:(i,j) \in S} (u_i^T v_j - s_{i,j})^2 = \sum_{j:(i,j) \in S} 2 v_j (u_i^T v_j - s_{i,j})$$

$$\rightarrow \left(\sum v_j v_j^T \right) u_i \quad 2 \sum v_j s_{i,j}$$

Matrix completion

n movies, m users, |*S*| ratings

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

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

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November 15, 2016

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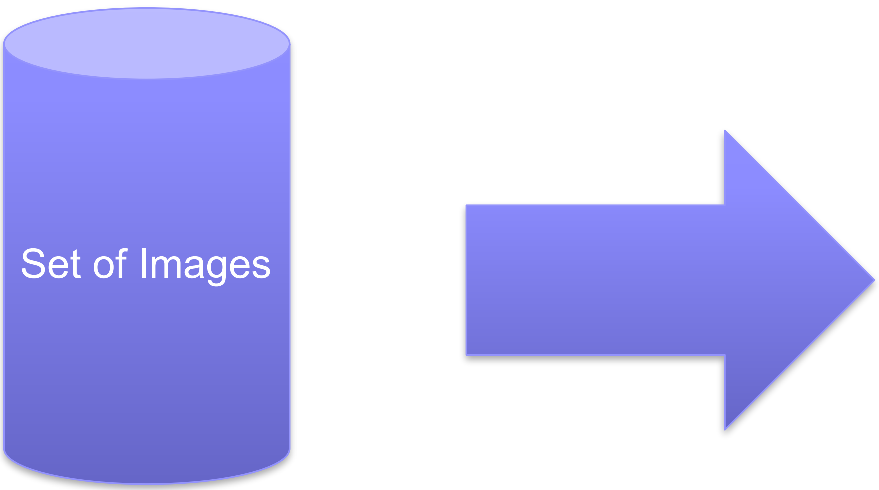
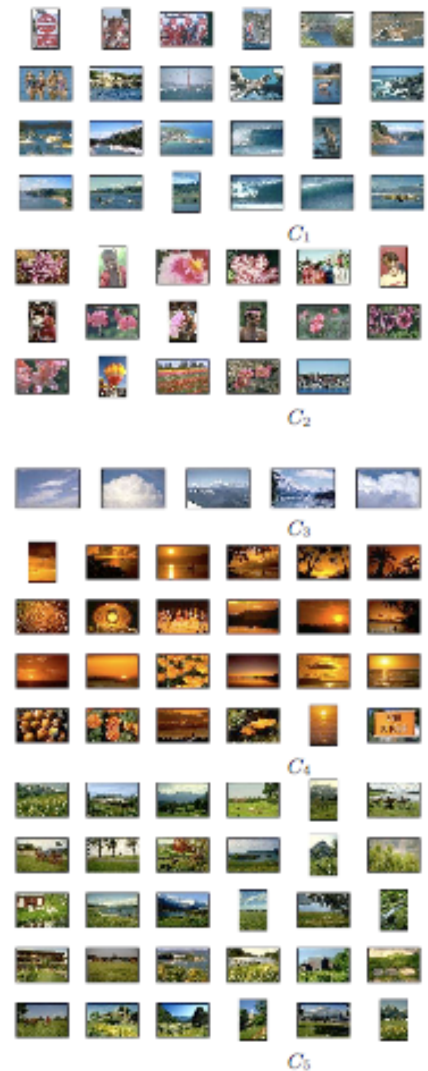
Clustering images





[Goldberger et al.]

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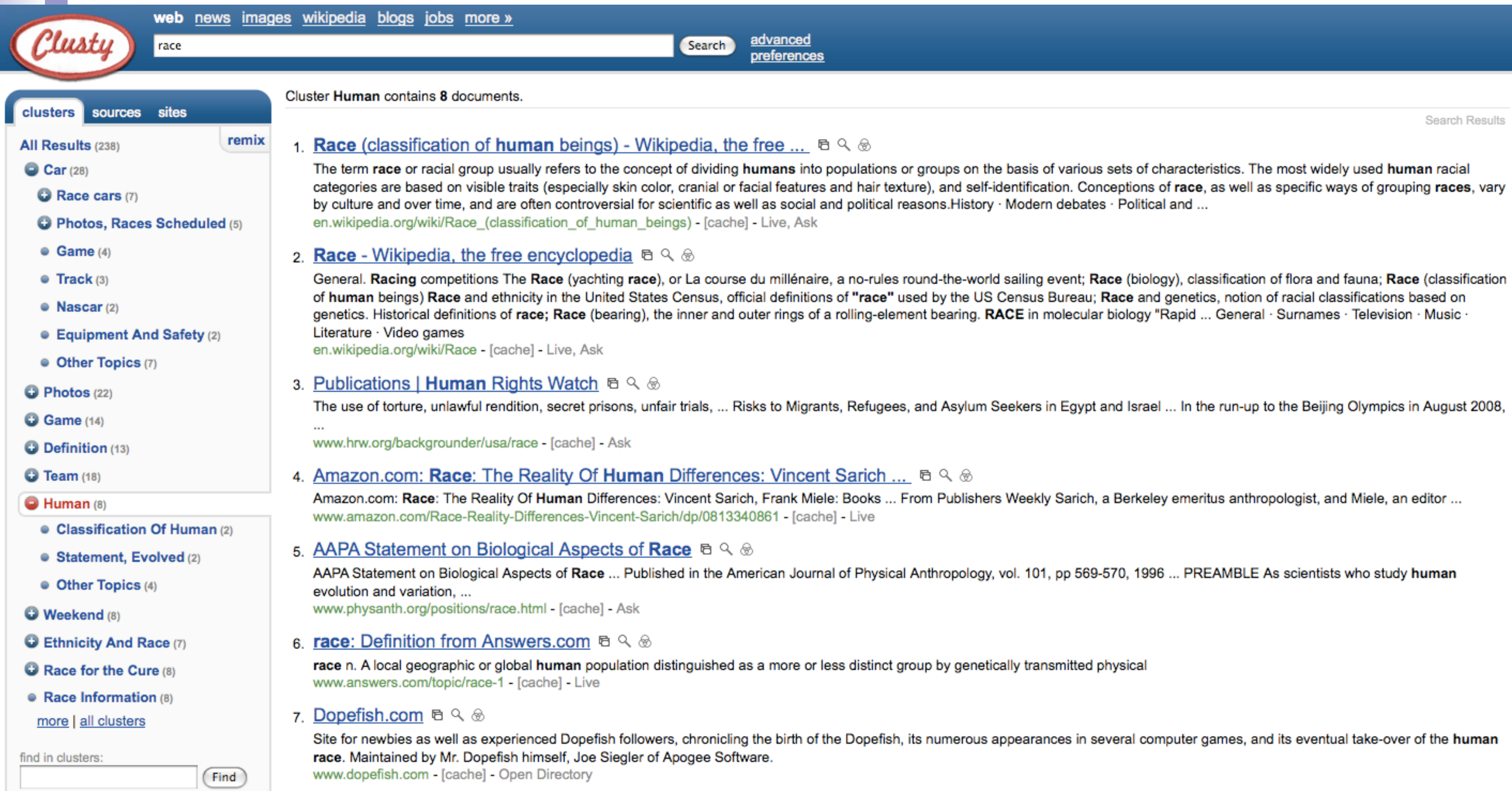
Clustering web search results



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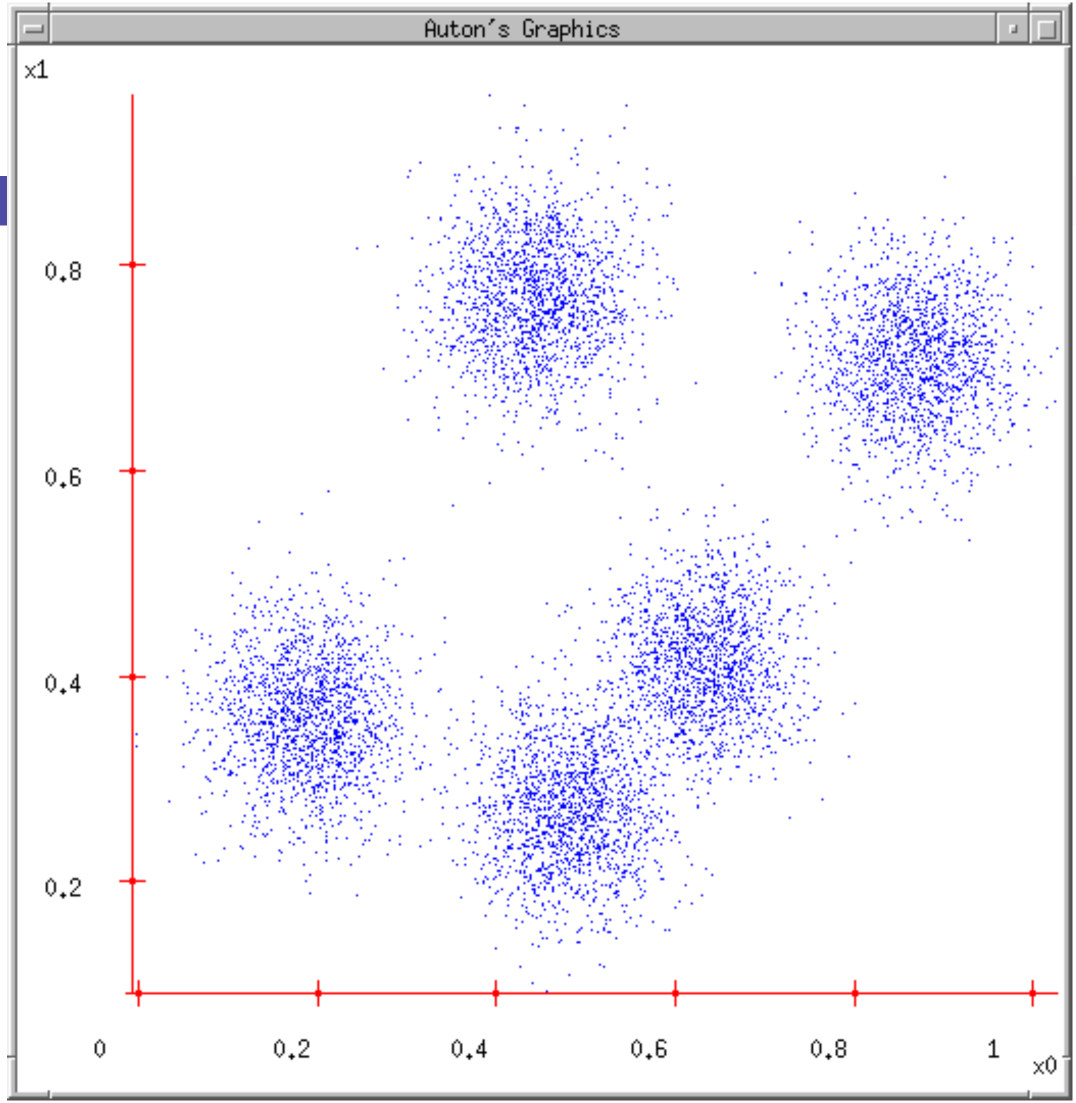
Some Data



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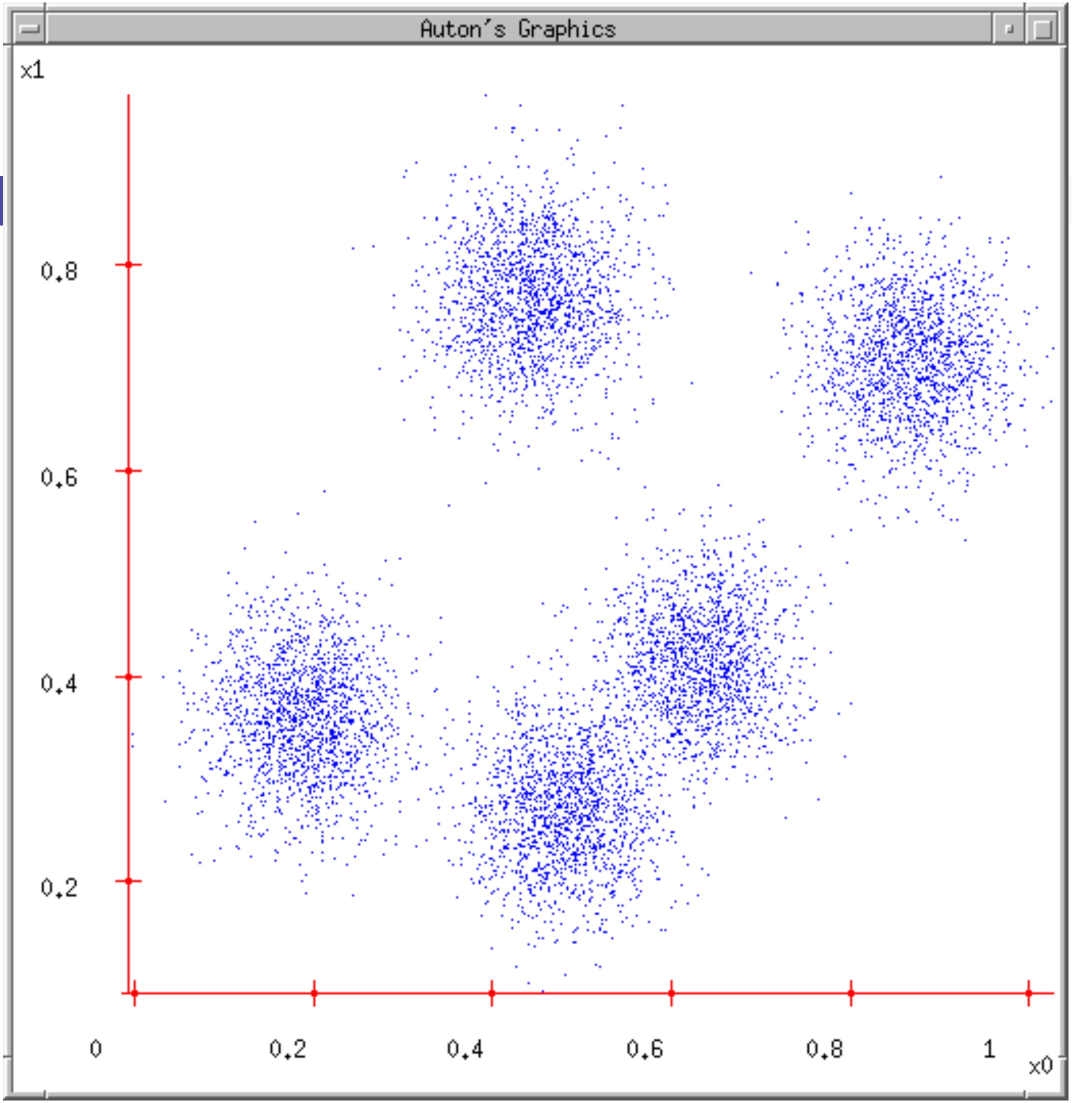
K-means

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



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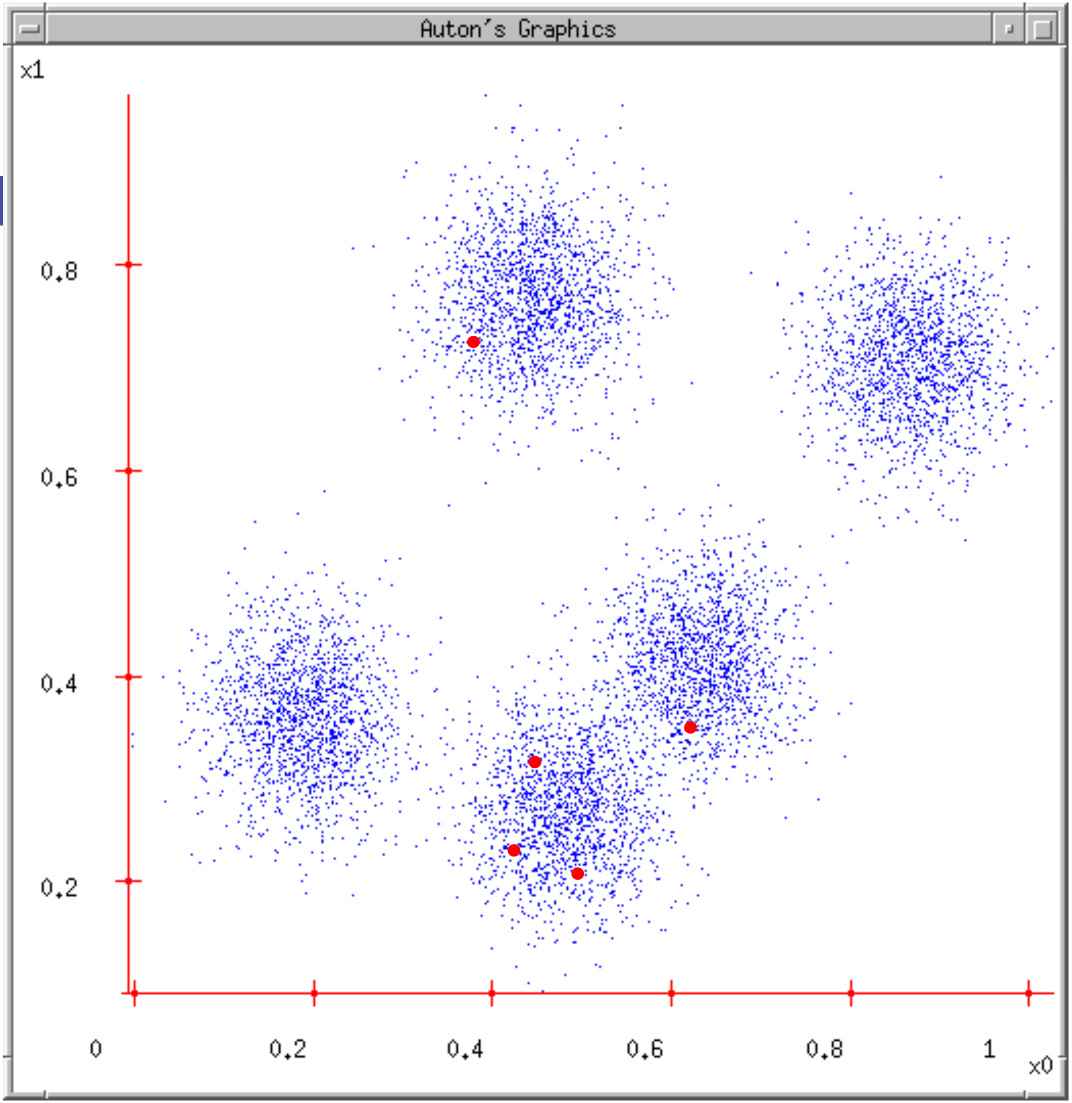
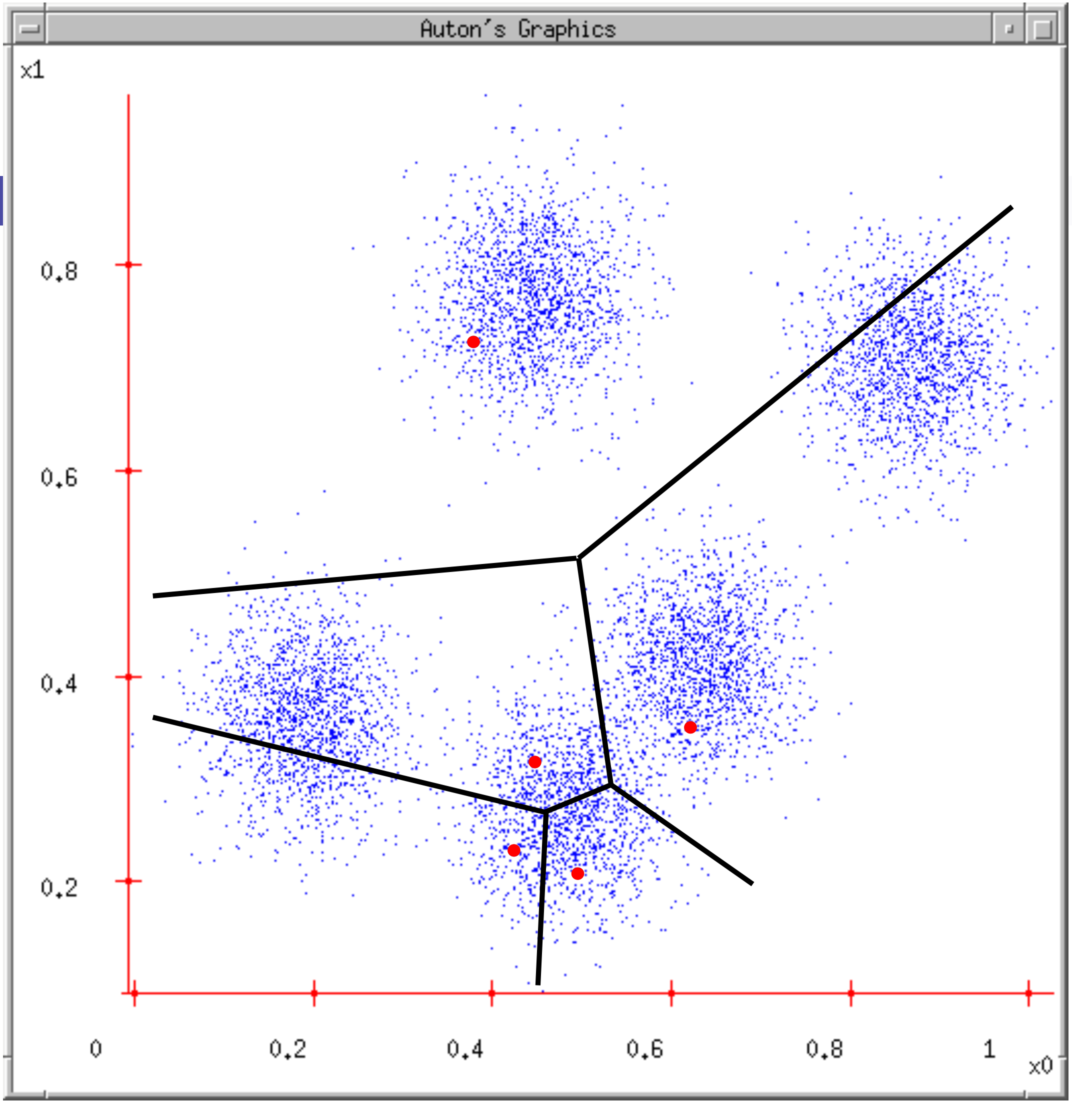


K-means

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)



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K-means

1. Ask user how many clusters they'd like. *(e.g. k=5)*
2. Randomly guess k cluster Center locations
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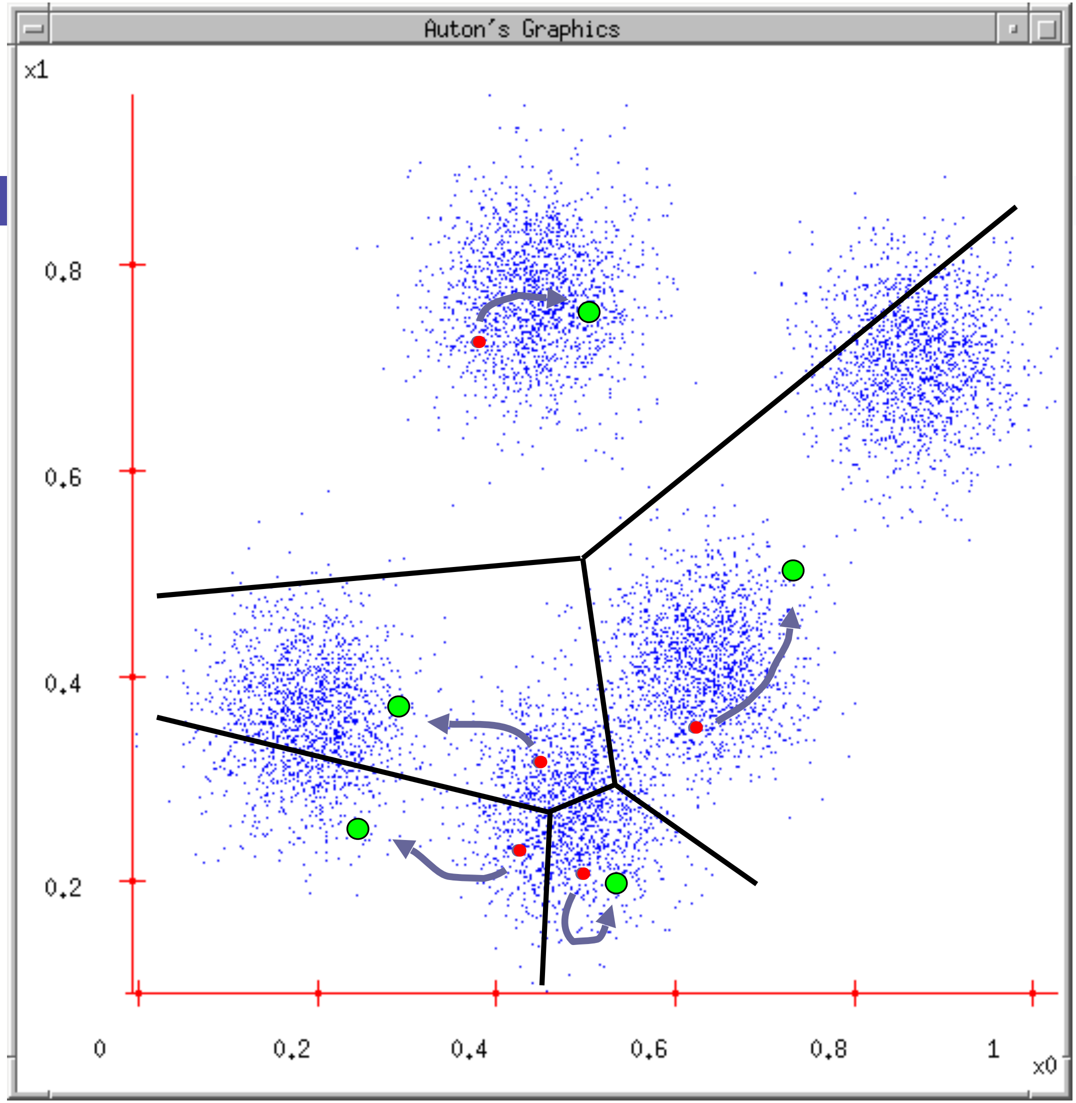
4. Each Center finds the centroid of the points it owns



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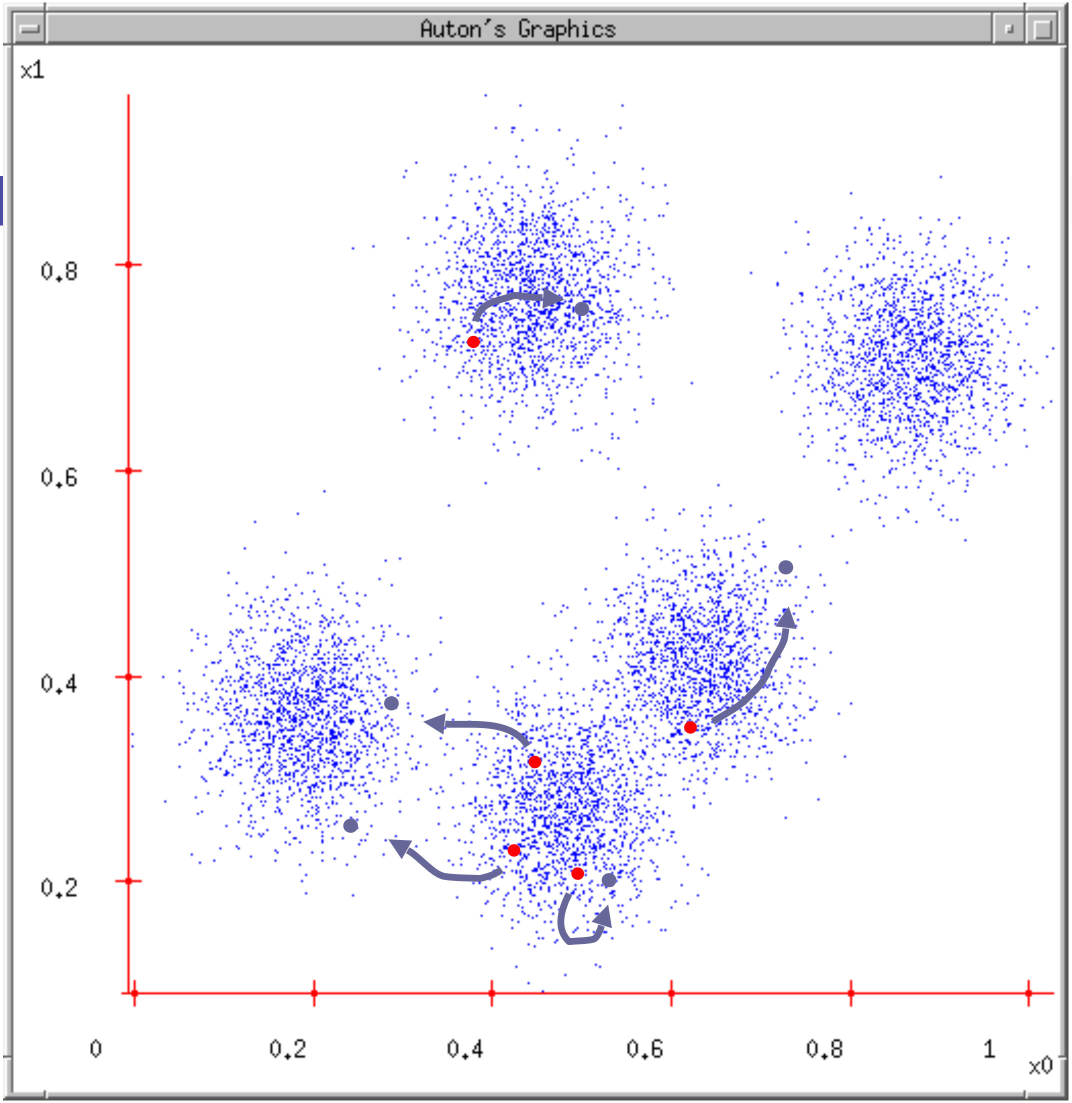
2. Randomly guess k cluster Center locations
3. Each datapoint finds out which Center it's closest to.
4. Each Center finds the centroid of the points it owns…
5. …and jumps there
6. …Repeat until terminated!



K-means

- Randomly initialize *k* centers
  - $\mu^{(0)} = \mu_1^{(0)}, \ldots, \mu_k^{(0)}$

- **Classify**: Assign each point $j \in \{1, \ldots N\}$ 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!

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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

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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

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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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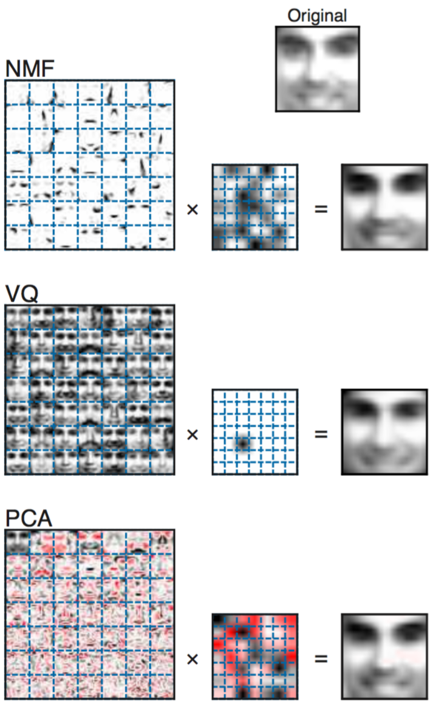

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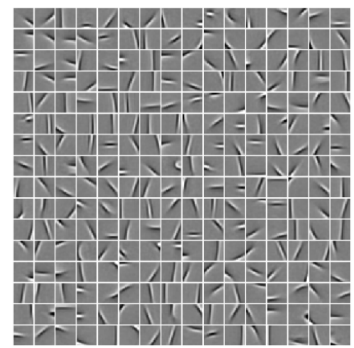
Typical output of k-means on patches



Similar reduced representation can be used as a feature vector

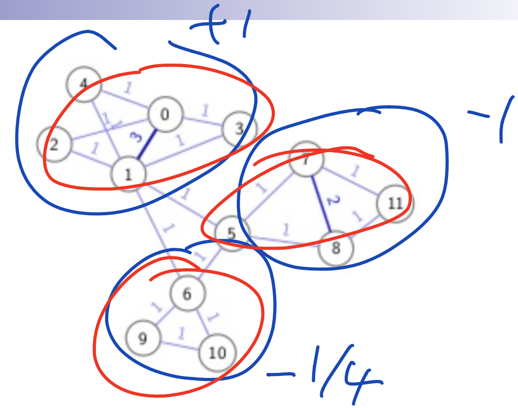
Coates, Ng, *Learning Feature Representations with K-means,* 2012

Spectral Clustering

Adjacency matrix: $\mathbf{W}$

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

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



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

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

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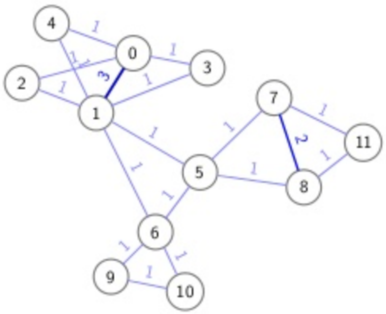

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$$\mathbf{f}^T\mathbf{L}\mathbf{f} = \sum_{i=1}^{N} g_i f_i^2 - \sum_{i=1}^{N}\sum_{i'=1}^{N} f_i f_{i'} w_{ii'}$$

$$= \frac{1}{2}\sum_{i=1}^{N}\sum_{i'=1}^{N} w_{ii'}(f_i - f_{i'})^2.$$

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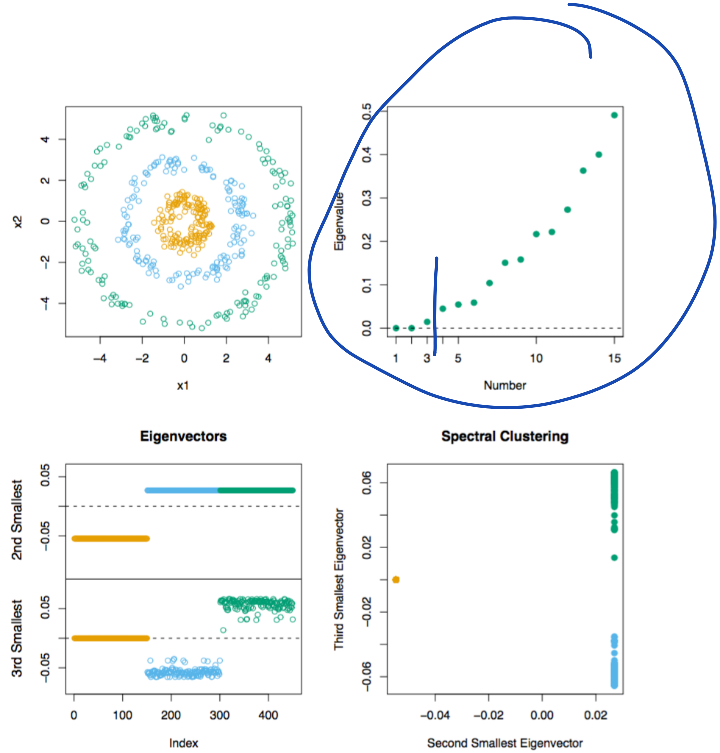
$i \neq j \quad D_{ij} = 0$

Given feature vectors, could construct:
- (k=10)-nearest neighbor graph with weights in {0,1}



Mixtures of Gaussians

Machine Learning – CSE546
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November 15, 2016

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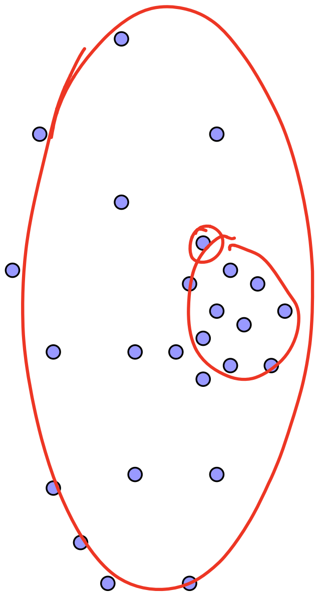
(One) bad case for k-means



- Clusters may overlap
- Some clusters may be "wider" than others

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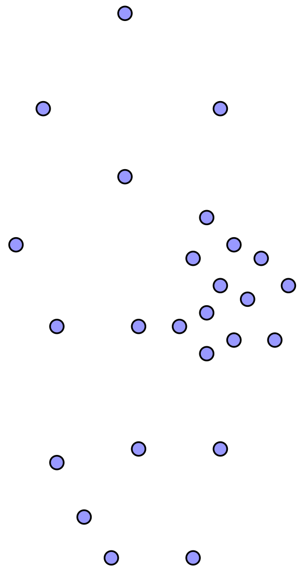

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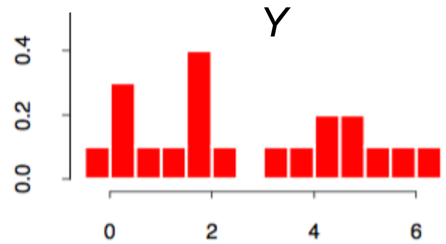
Mixture models

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

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



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

$$\phi_{(\mu,\sigma^2)}(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

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

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

$$\hat{\theta}_{MLE} = \arg\max_\theta \ell(\theta; Z)$$

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Mixture models

$$
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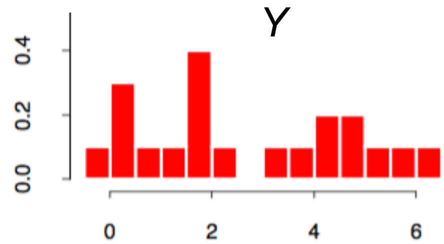
\end{aligned}
$$

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

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



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

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

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

$$\ell(\theta; y_i, \Delta_i = 0) = \log\left((1-\pi)\frac{1}{\sqrt{2\pi\sigma_1^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma_1^2}\right)\right)$$

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

$$\sum \ell(\theta; \Delta_i, y_i)$$

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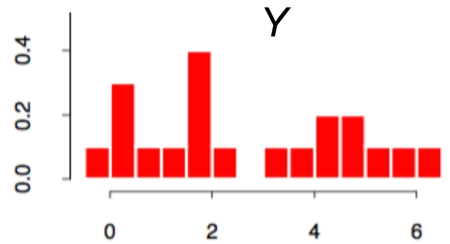

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If we knew Δ, how would we choose θ?

compute $\hat{\mu}_1$ $\hat{\mu}_2$ $\hat{\sigma}_1$ $\hat{\sigma}_2$

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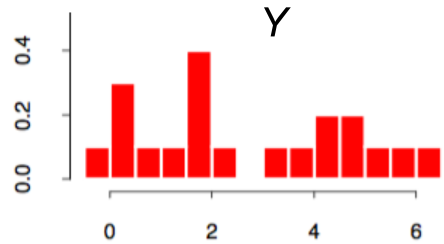

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$$\ell(\theta; \mathbf{Z}, \mathbf{\Delta}) = \sum_{i=1}^n (1-\Delta_i)\log[(1-\pi)\phi_{\theta_1}(y_i)] + \Delta_i \log(\pi\phi_{\theta_2}(y_i)]$$

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

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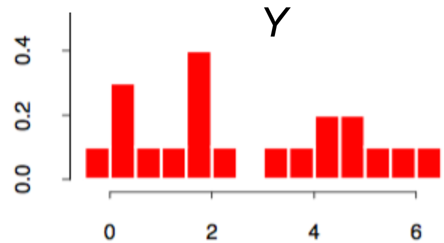
Mixture models

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

$\Delta \in \{0,1\}$ 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

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

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

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

$$\gamma_i(\theta) = \mathbb{E}[\Delta_i|\theta, \mathbf{Z}] = \frac{\pi\, \phi_{\mu_2,\sigma_2}(y_i)}{\pi\, \phi_{\mu_2}(y_i) + (1-\pi)\, \phi_{\mu_1}(y_i)}$$

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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

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

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

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

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

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

4. Iterate steps 2 and 3 until convergence.

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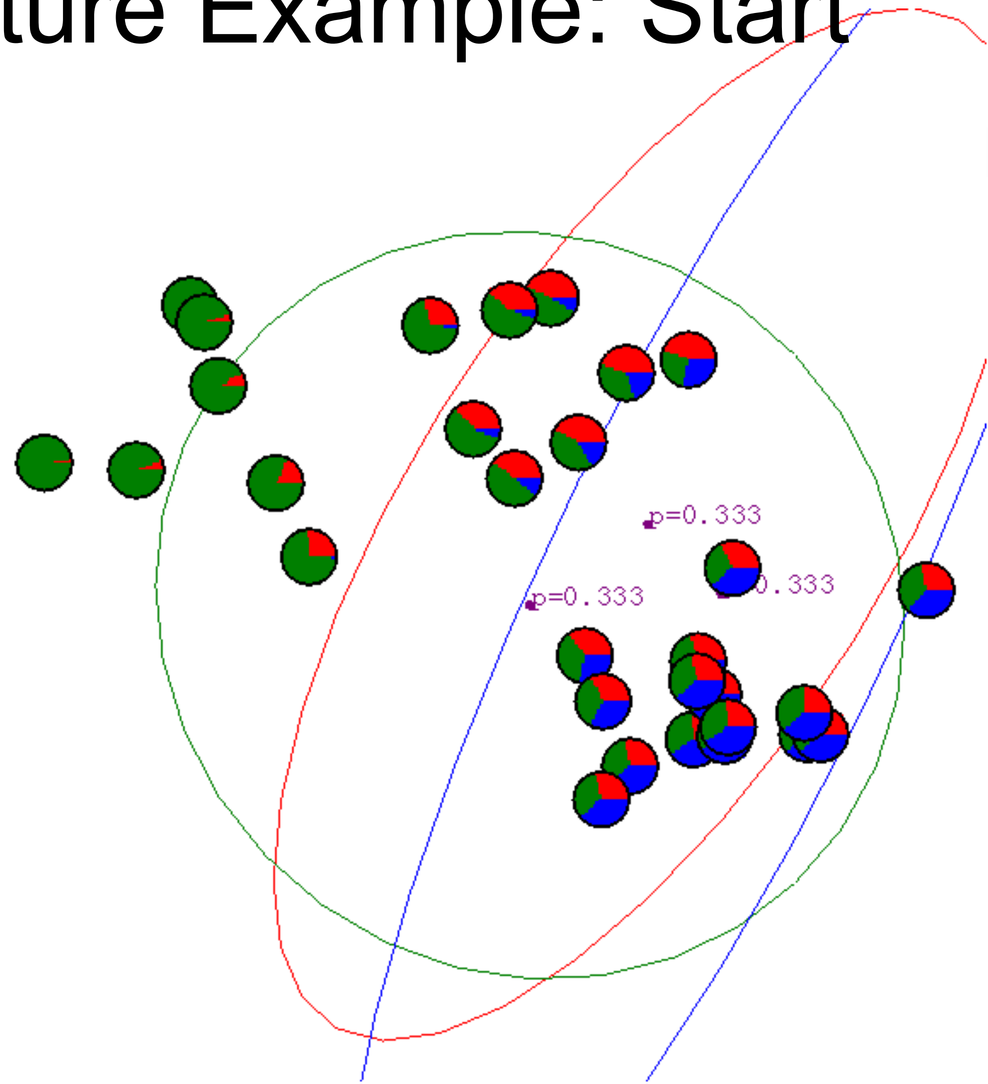
Gaussian Mixture Example: Start



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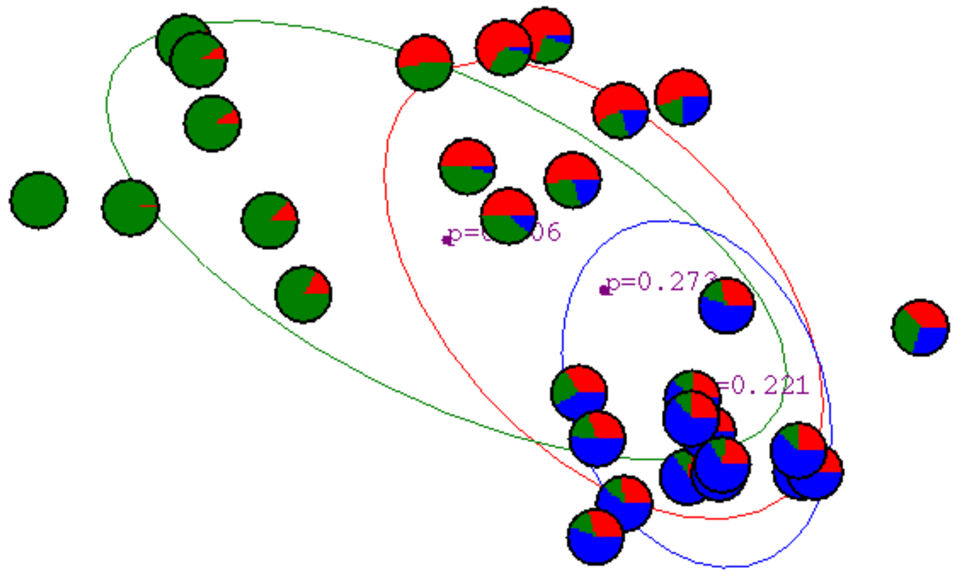
After first iteration



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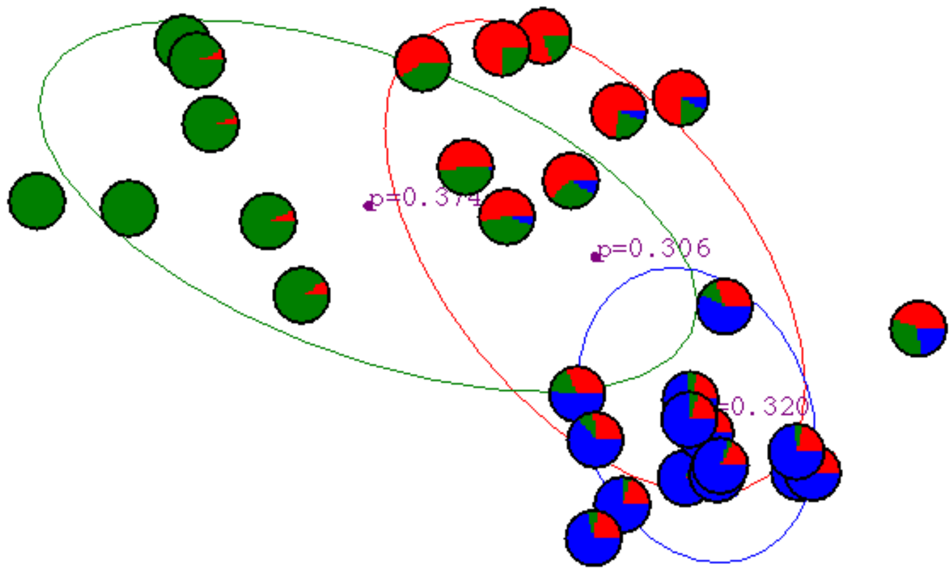
After 2nd iteration



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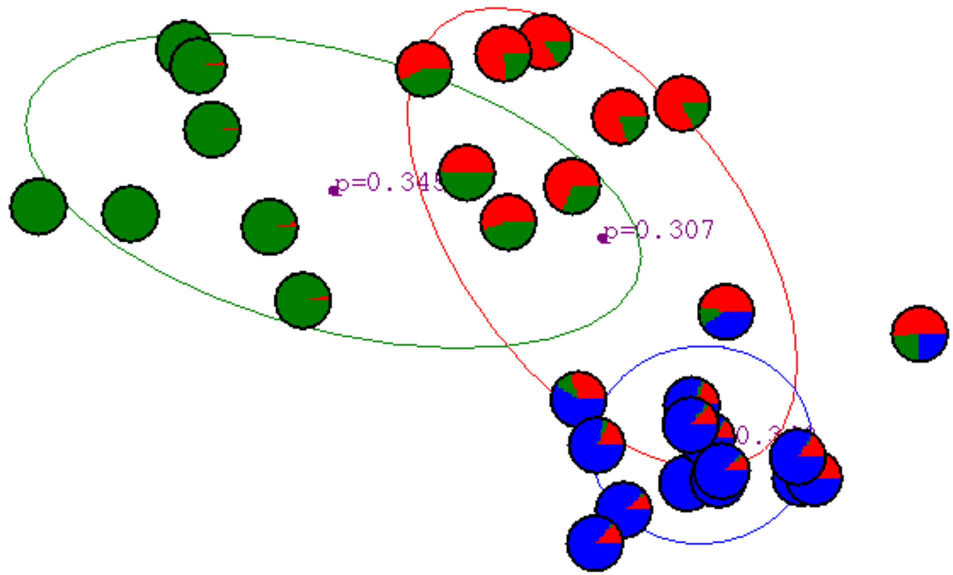
After 3rd iteration



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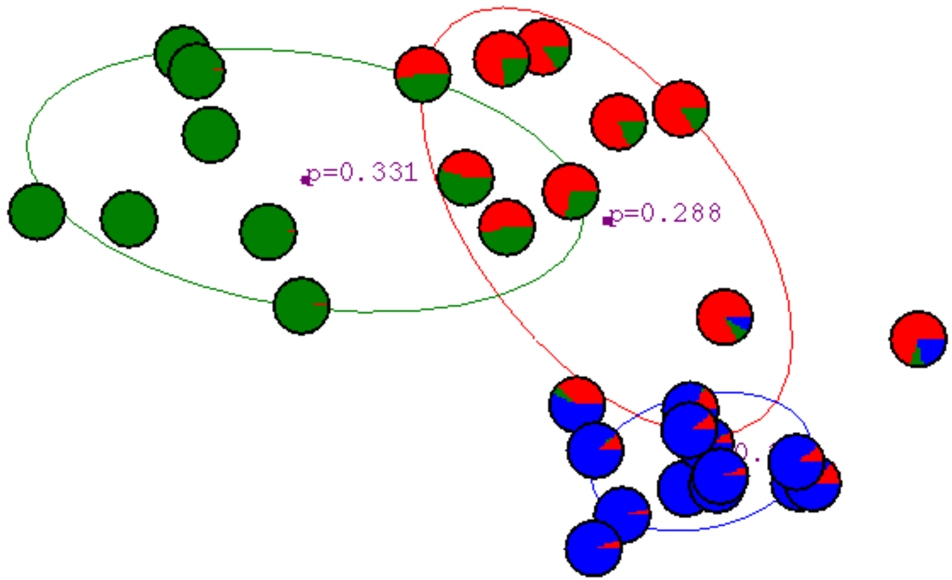
After 4th iteration



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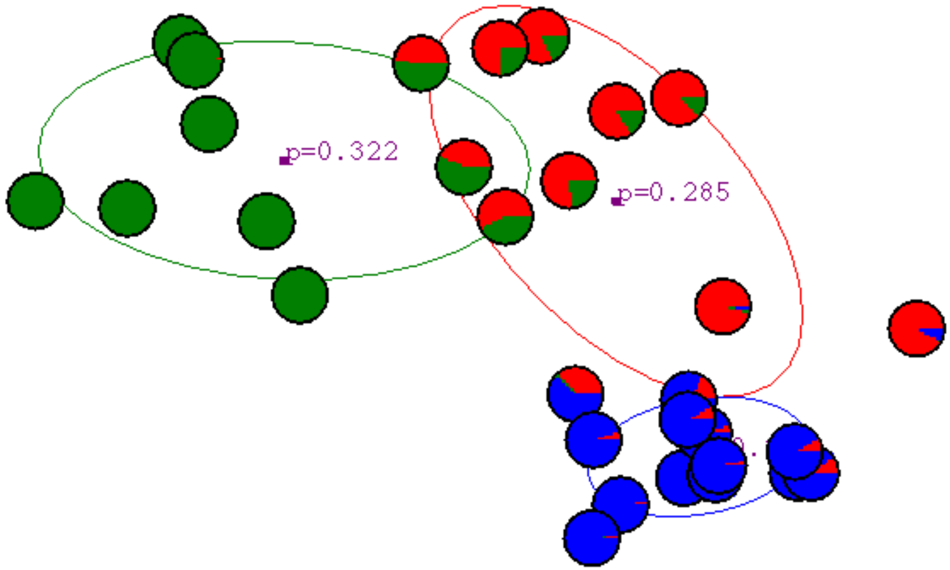
After 5th iteration



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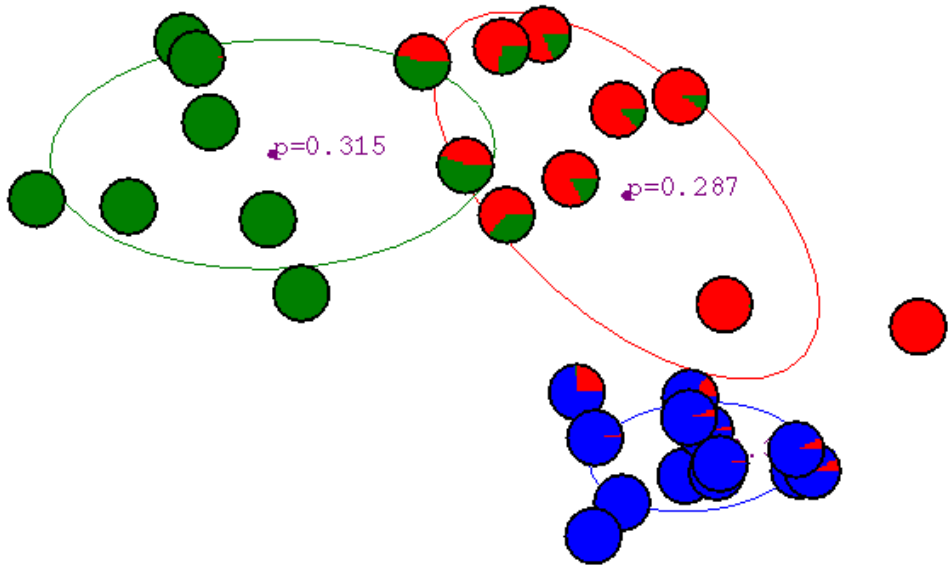
After 6th iteration



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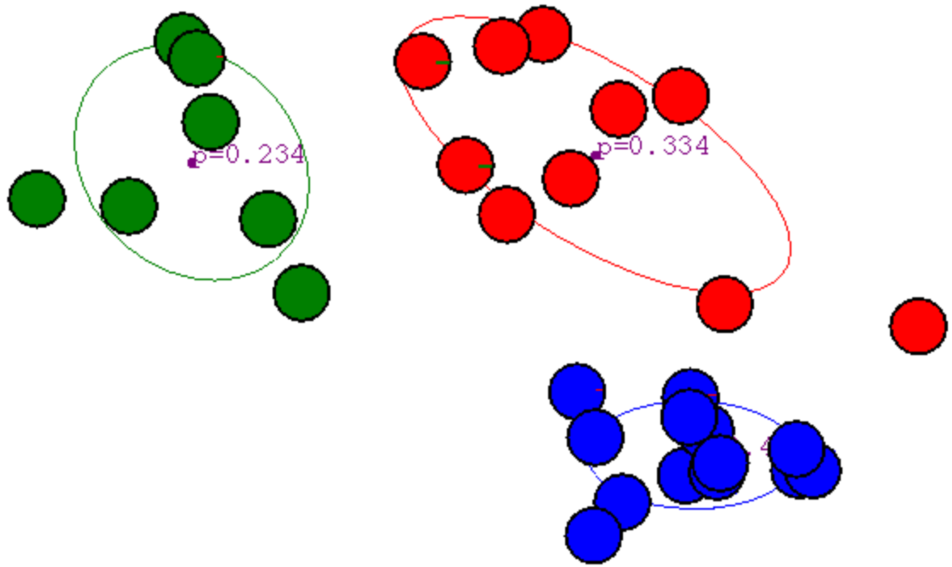
After 20th iteration



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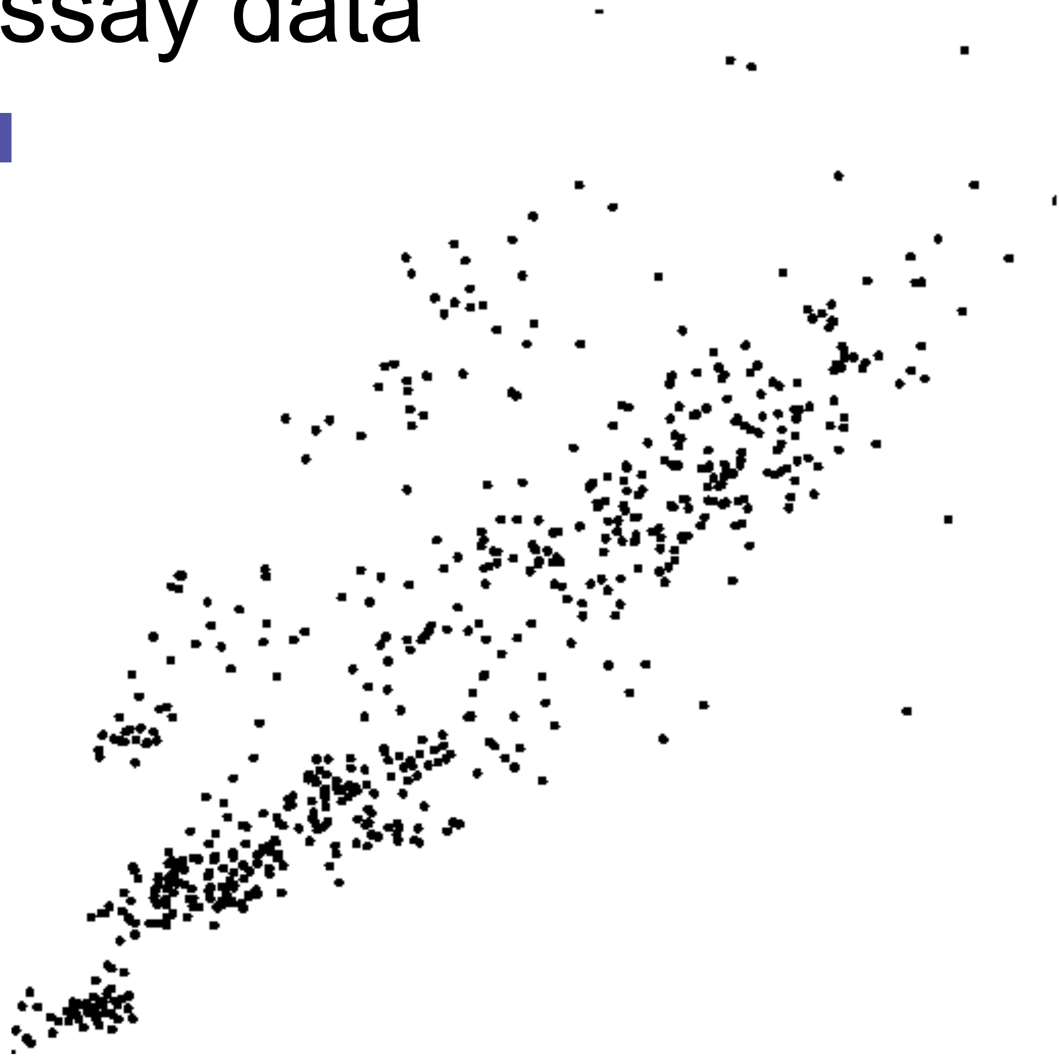
Some Bio Assay data



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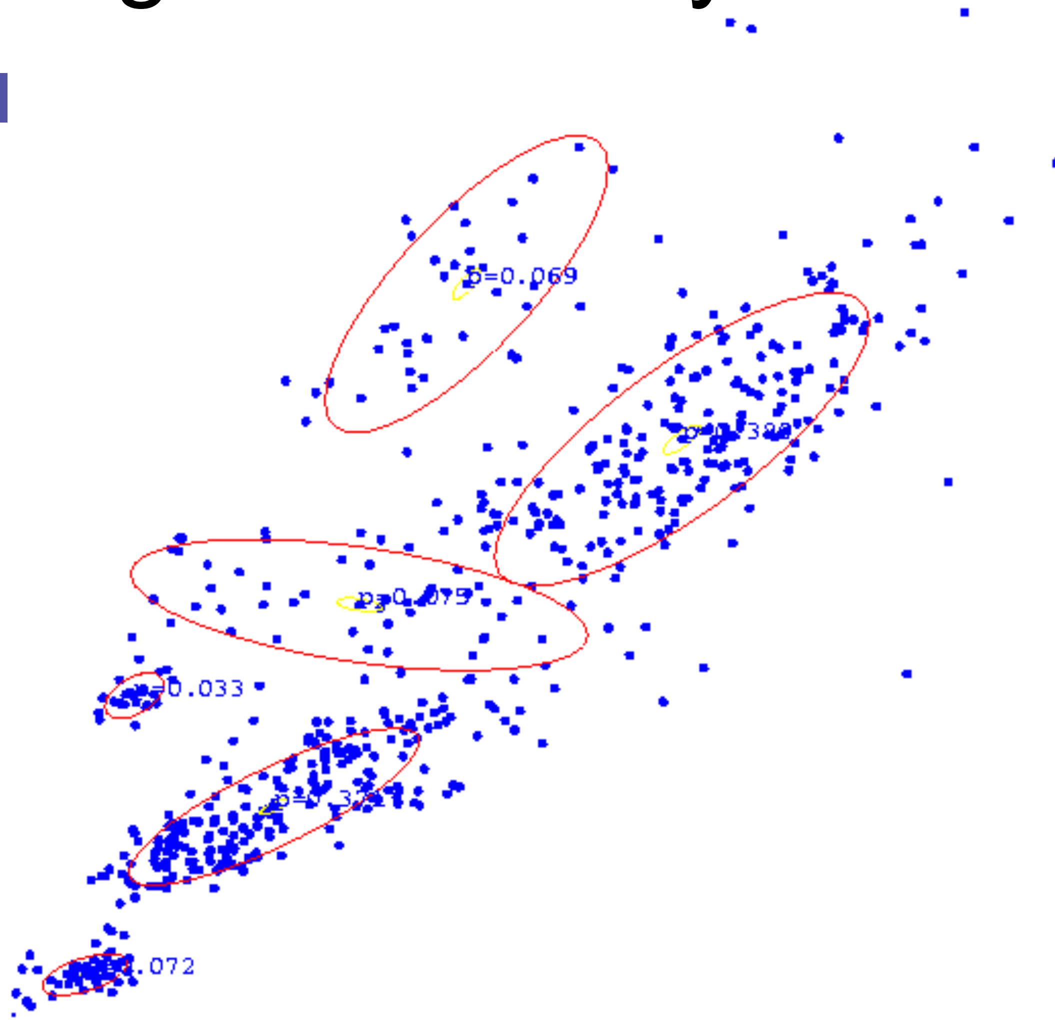
GMM clustering of the assay data



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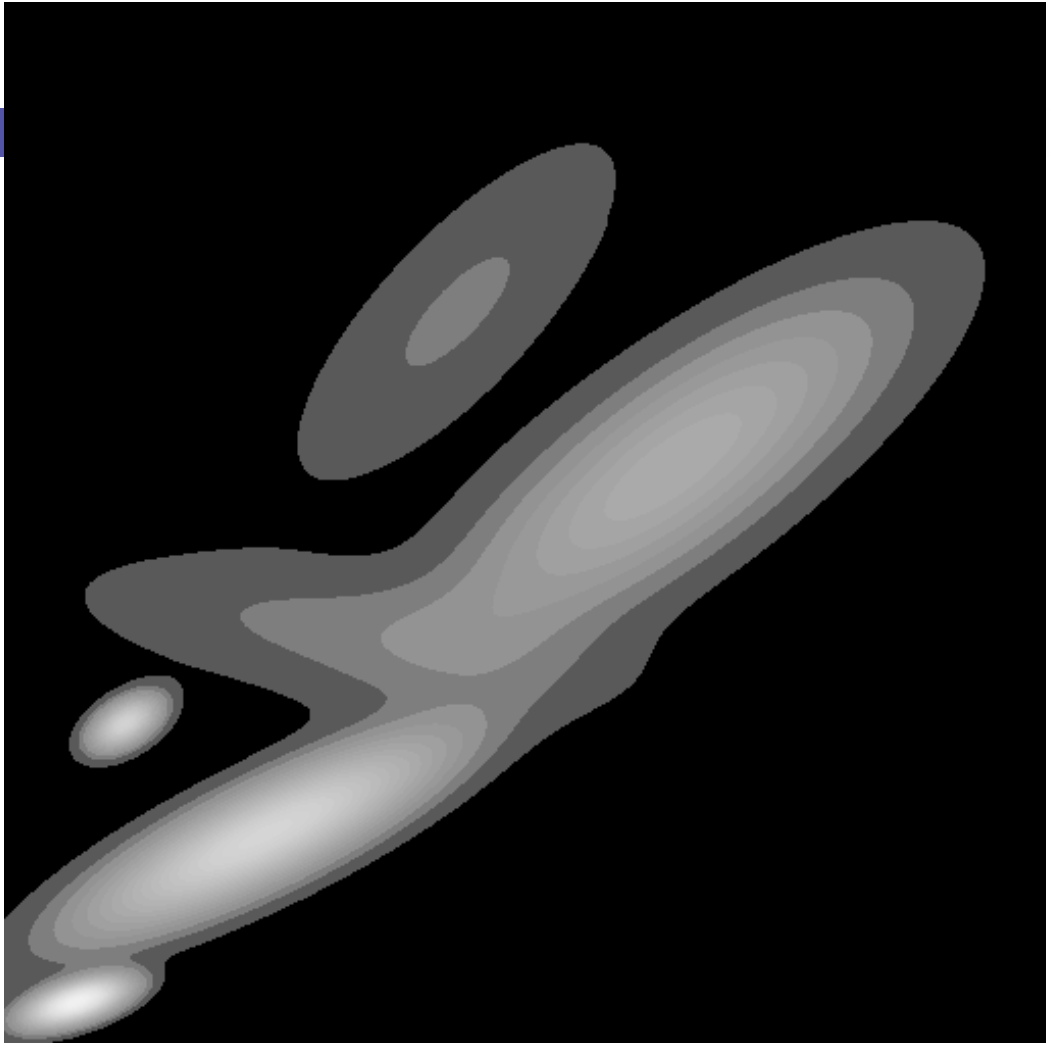
Resulting Density Estimator



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