Practice

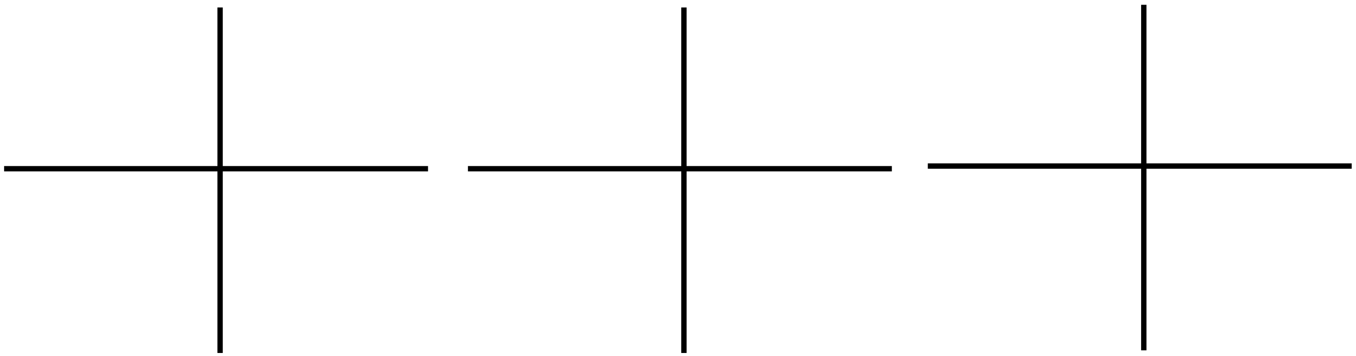
- Fill in the missing plots:

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

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

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

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



Matrix Completion

Machine Learning – CSE546

Kevin Jamieson
University of Washington

November 15, 2016

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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, $\mathbf{U}^T\mathbf{U} = I$, $\mathbf{V}^T\mathbf{V} = I$.

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

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

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

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

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

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

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

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

Singular Value Decomposition (SVD)

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

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

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

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

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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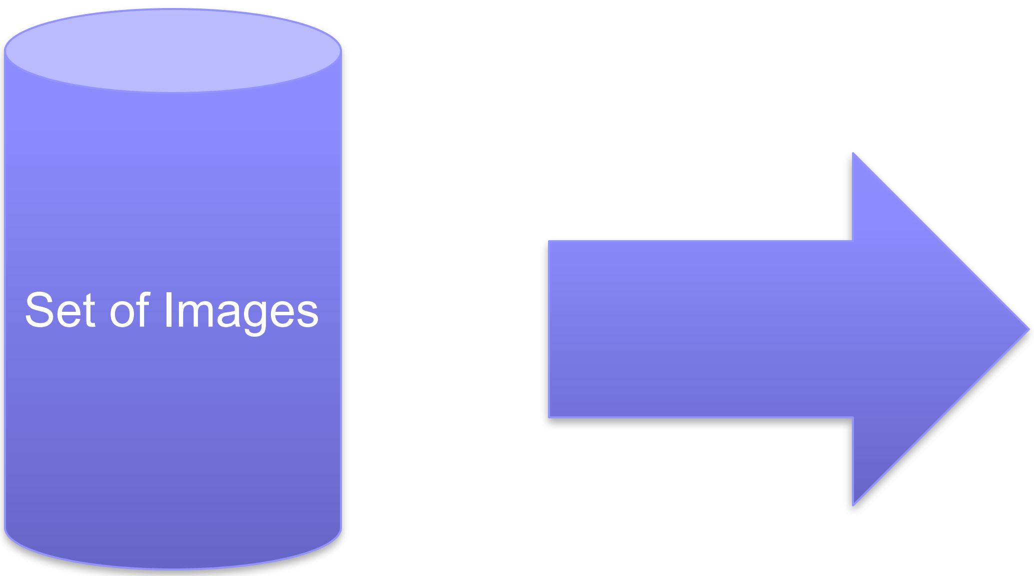
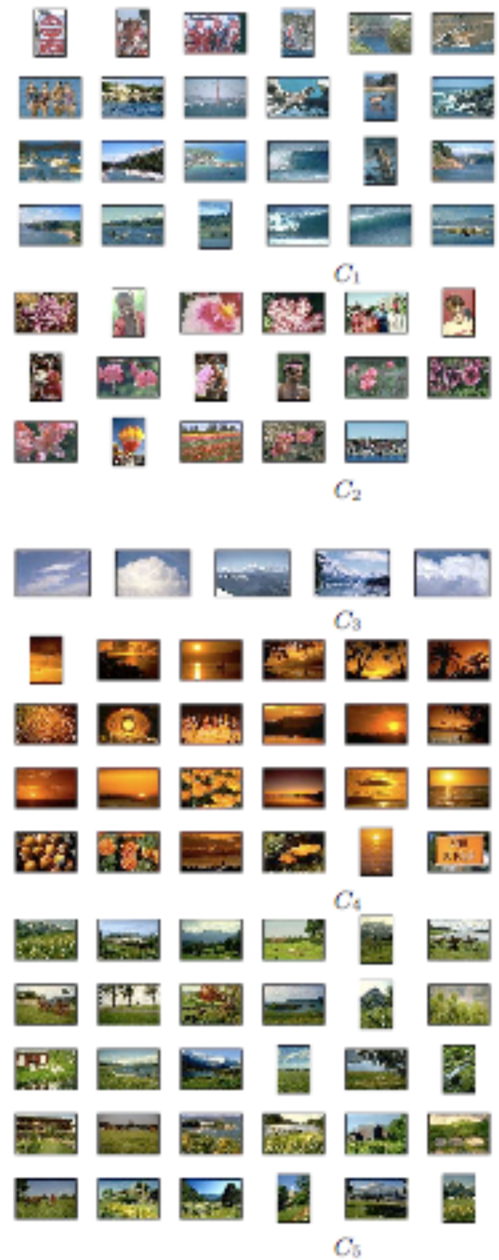
Clustering images





[Goldberger et al.]

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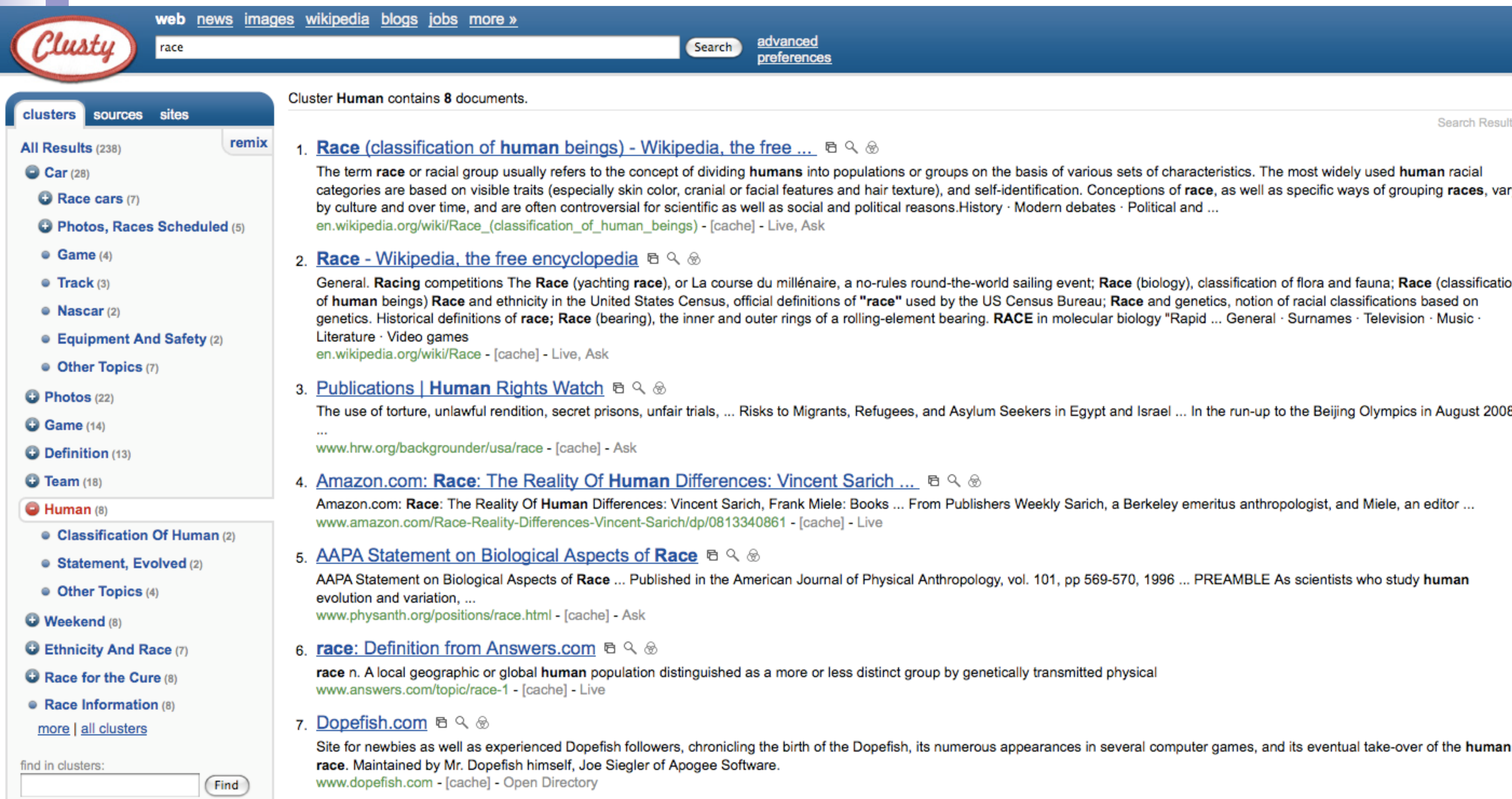
Clustering web search results



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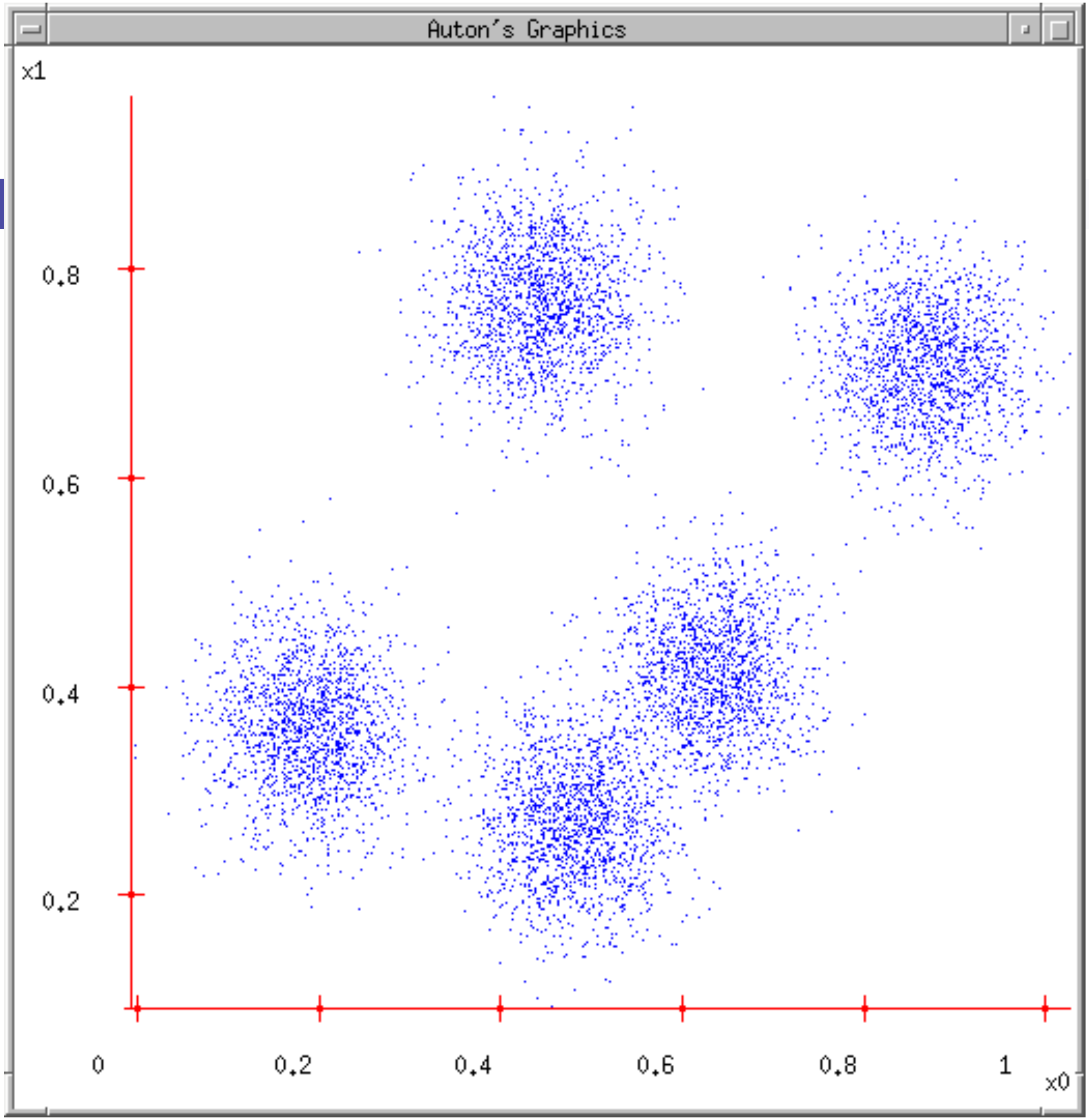
Some Data



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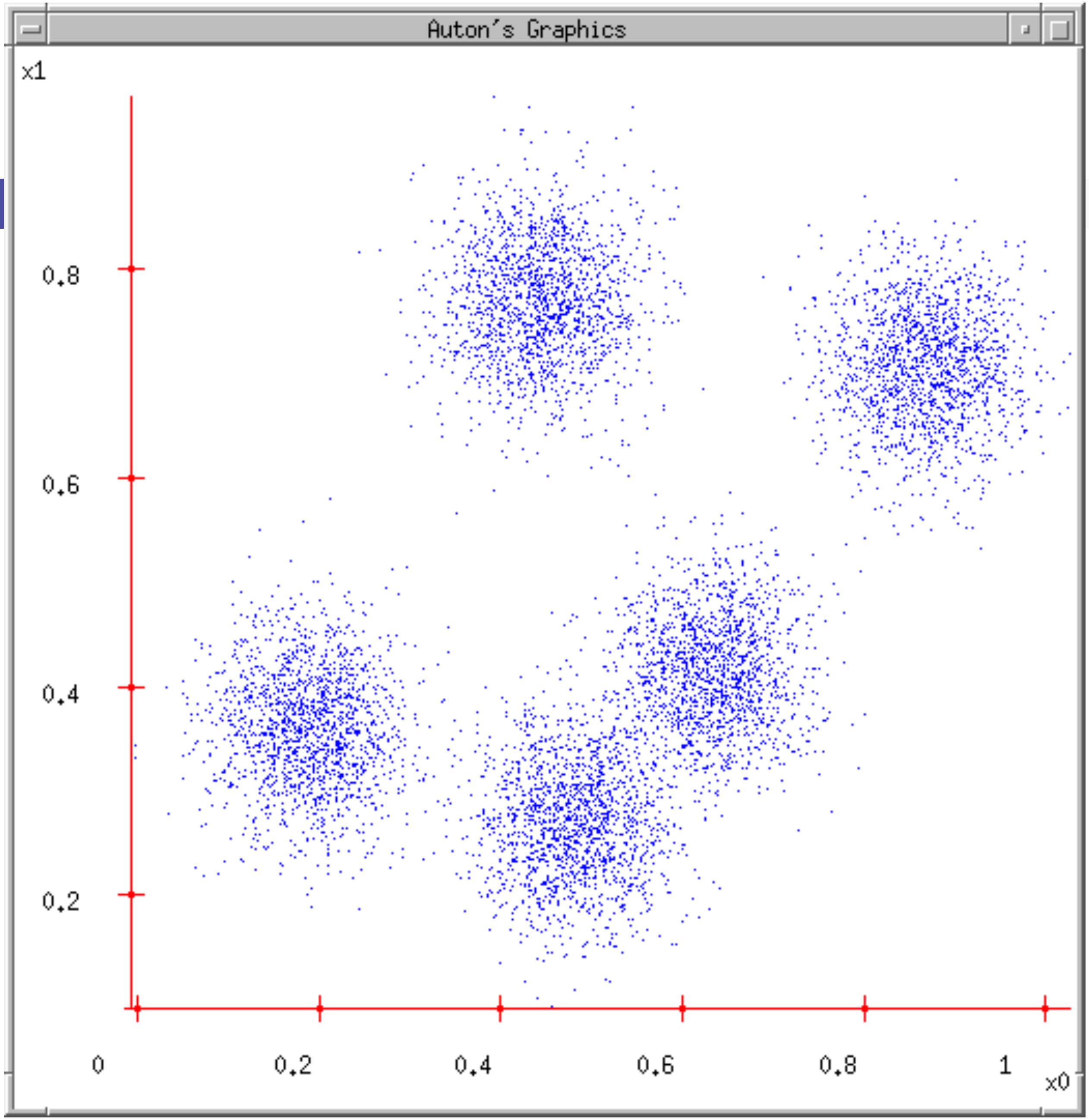
K-means

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



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K-means

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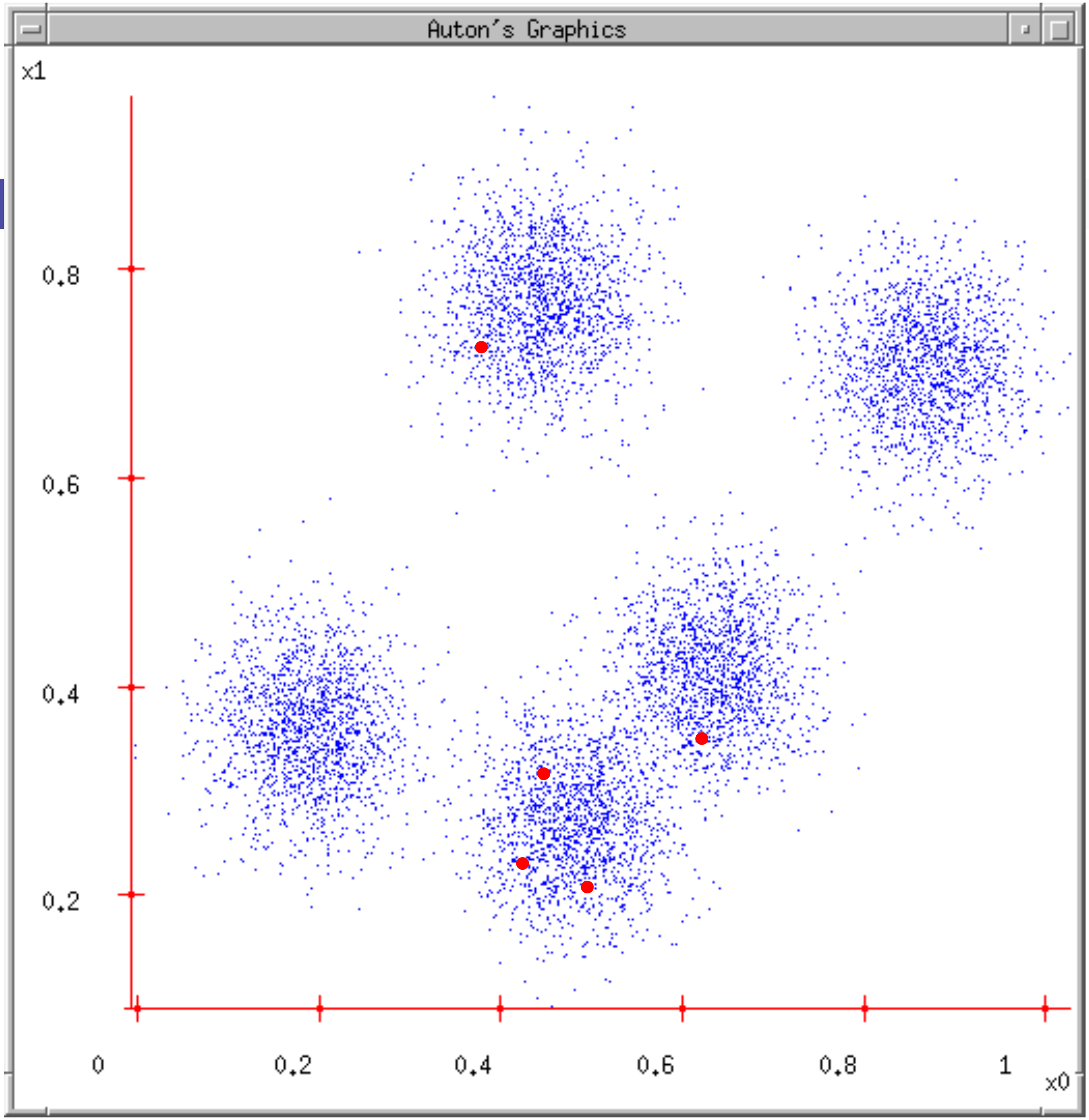

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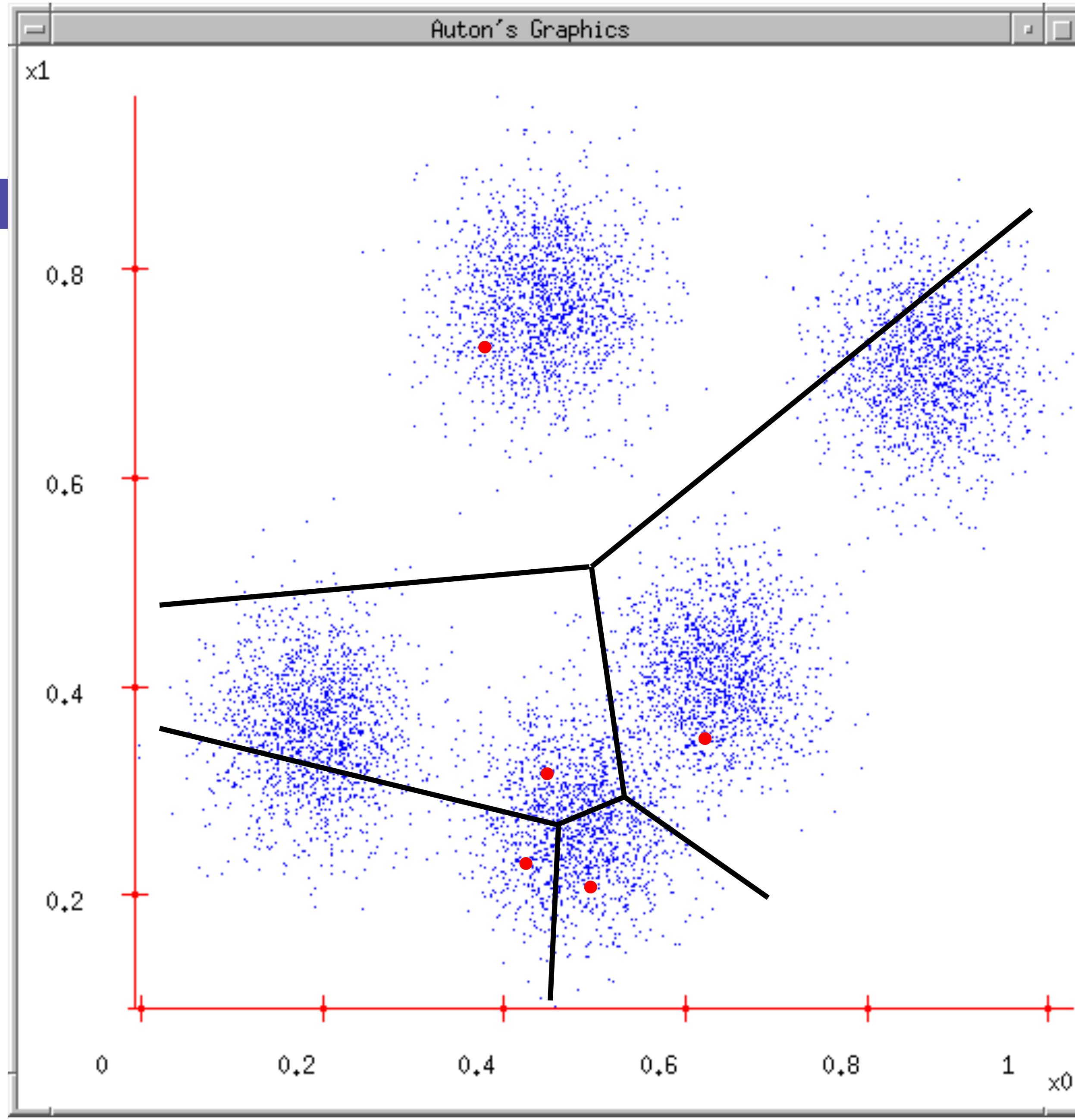
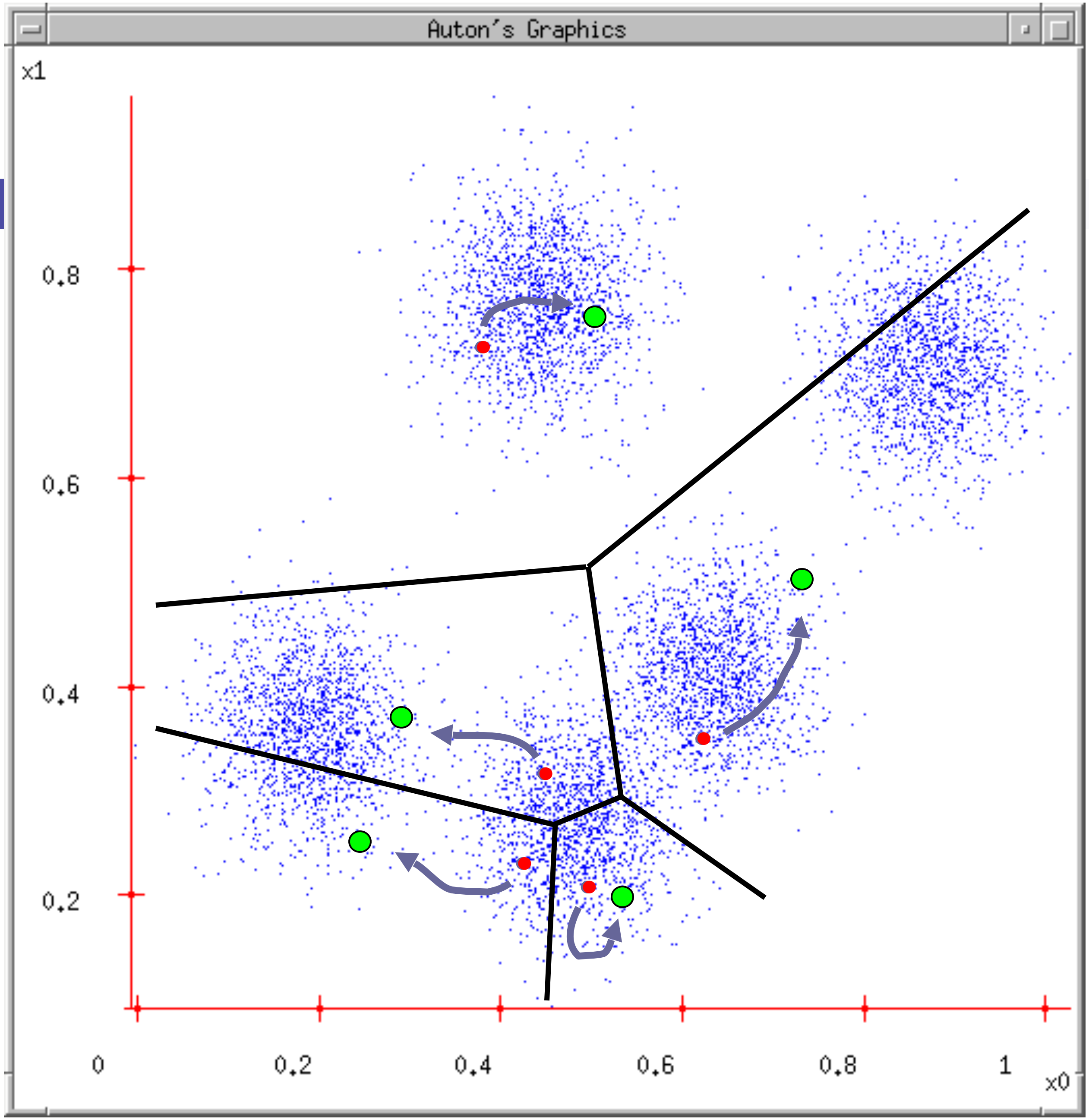
K-means

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)



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



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2. Randomly guess k cluster Center locations
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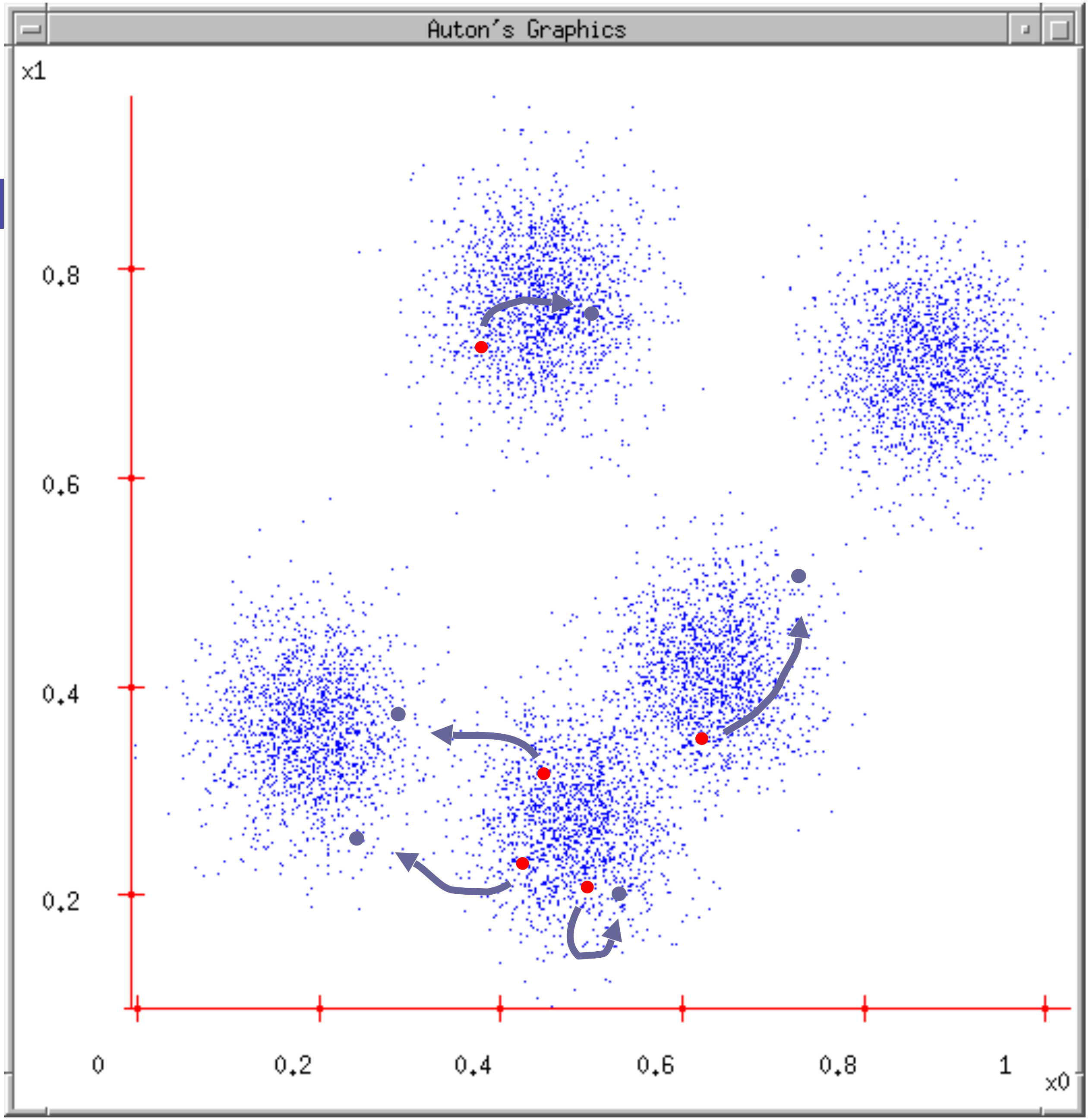
4. Each Center finds the centroid of the points it owns…
5. …and jumps there
6. …Repeat until terminated!



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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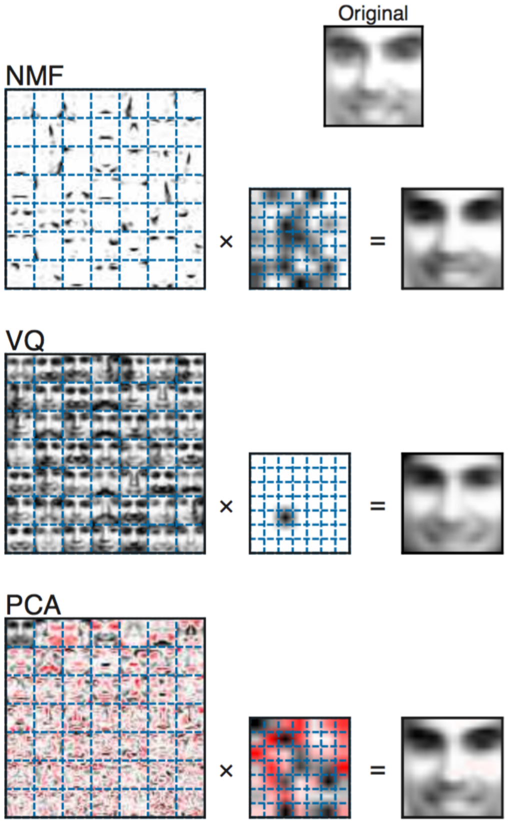

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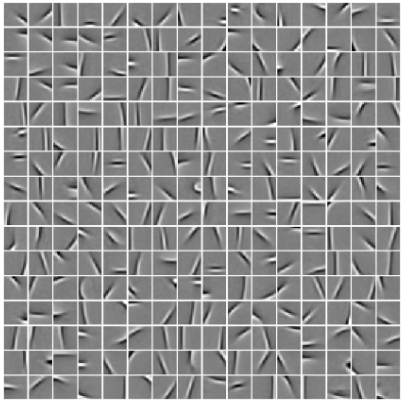
Typical output of k-means on patches

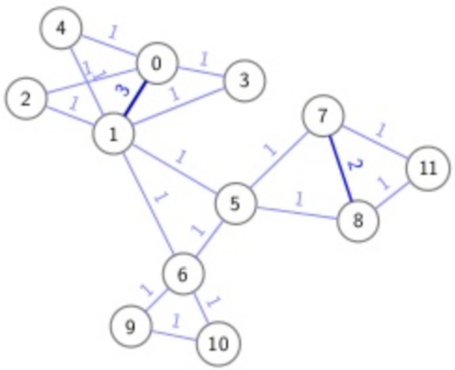


Similar reduced representation can be used as a feature vector

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

Spectral Clustering

Adjacency matrix: $\mathbf{W}$



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

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

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: $\mathbf{W}$

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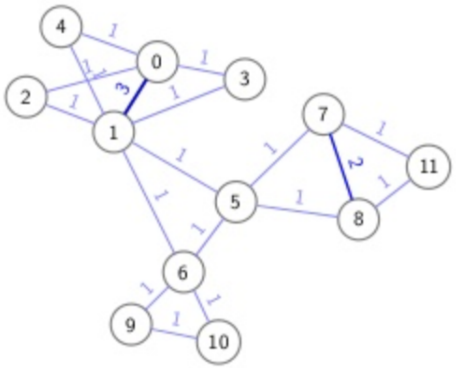
$$\mathbf{D}_{i,i} = \sum_{j=1}^{n} \mathbf{W}_{i,j} \qquad \mathbf{L} = \mathbf{D} - \mathbf{W}$$



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

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

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

Spectral Clustering

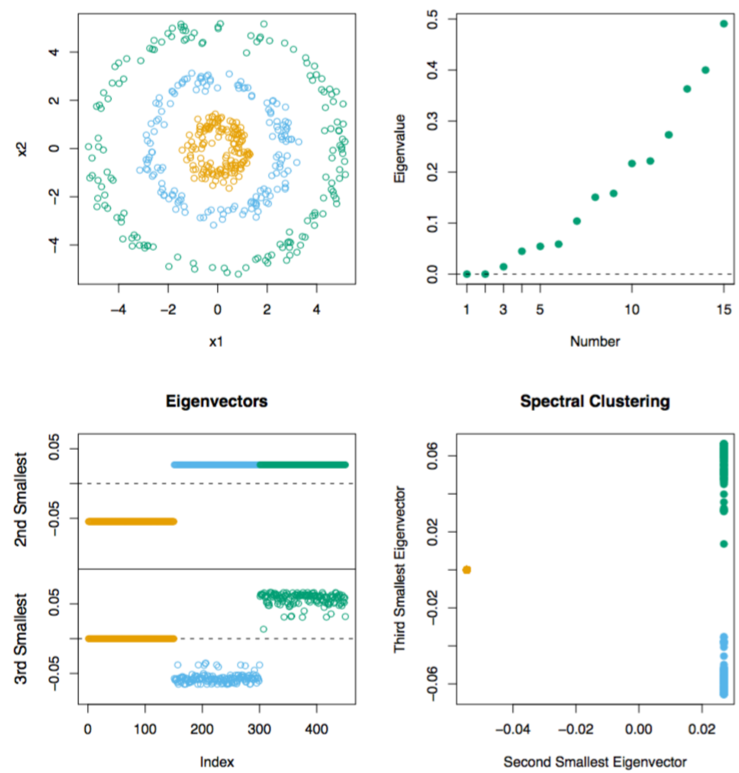
Adjacency matrix: $\mathbf{W}$

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

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

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

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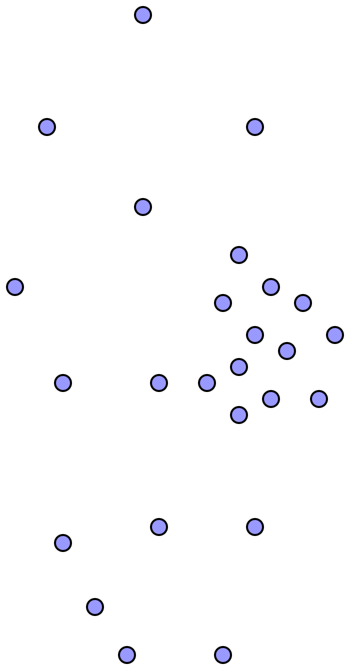
(One) bad case for k-means



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

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(One) bad case for k-means

- Clusters may overlap
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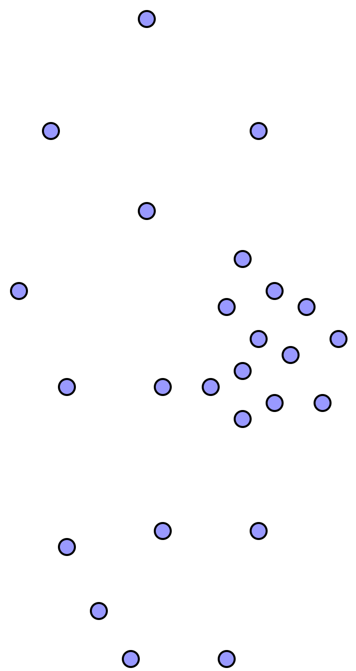

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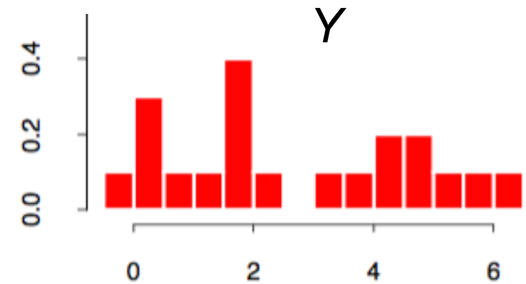
Mixture models

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

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



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

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

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

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Mixture models

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\begin{aligned}
Y_1 &\sim N(\mu_1, \sigma_1^2), \\
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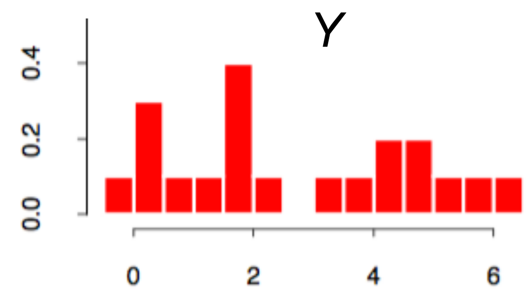
$\Delta \in \{0, 1\}$ with $\Pr(\Delta = 1) = \pi$

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



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

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

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

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Mixture models

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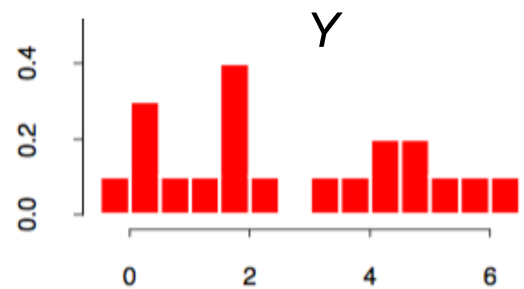

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If we knew Δ, how would we choose θ?

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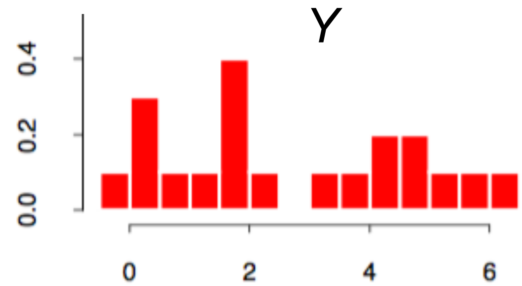

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$$

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

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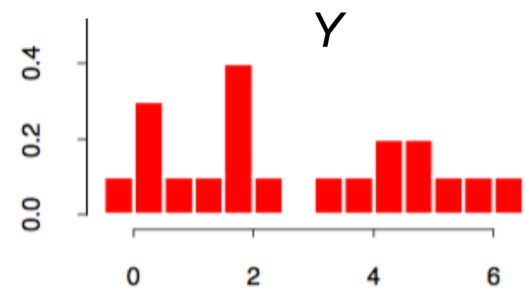

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$$\gamma_i(\theta) = \mathbb{E}[\Delta_i | \theta, \mathbf{Z}] =$$

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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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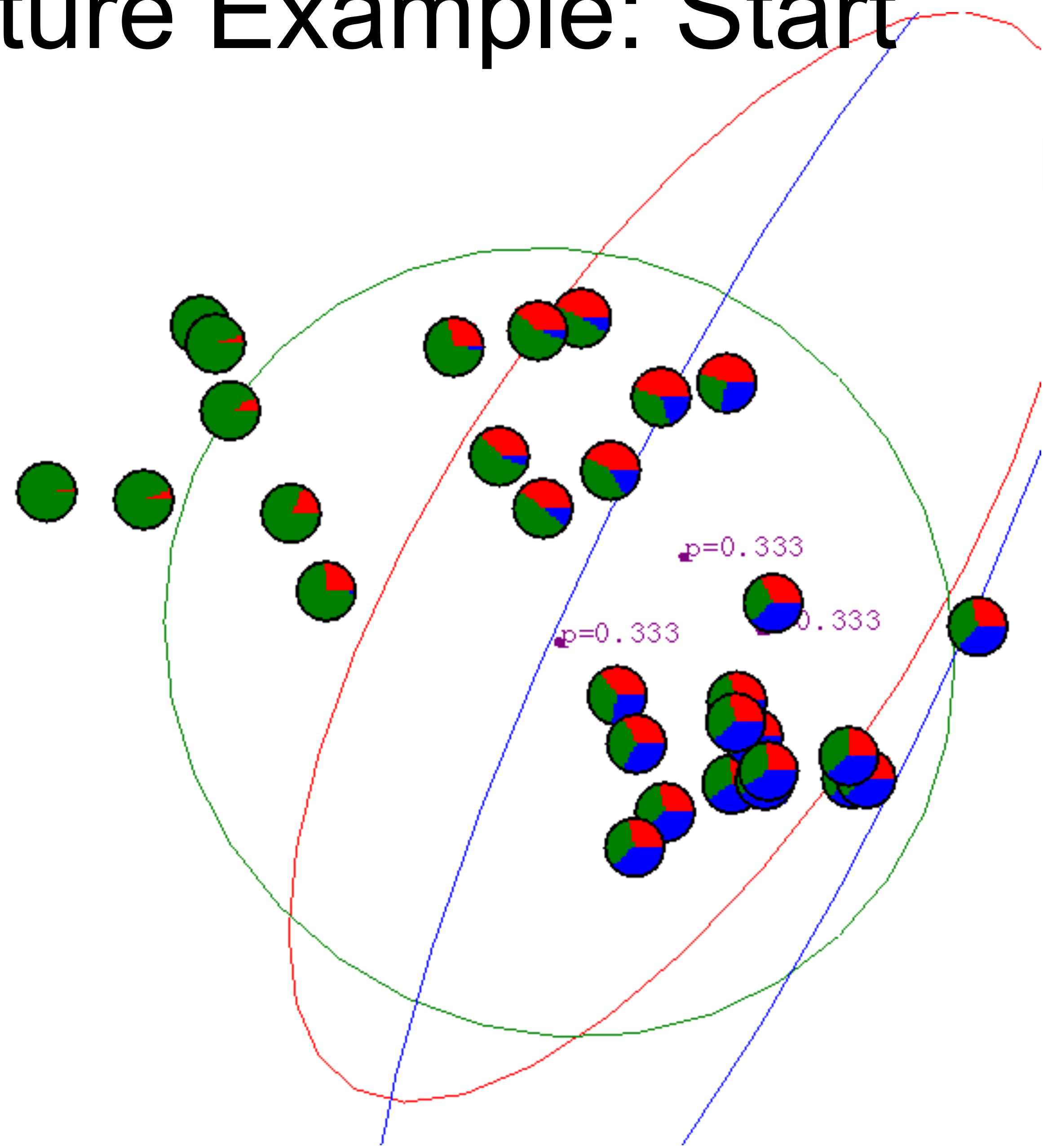
Gaussian Mixture Example: Start



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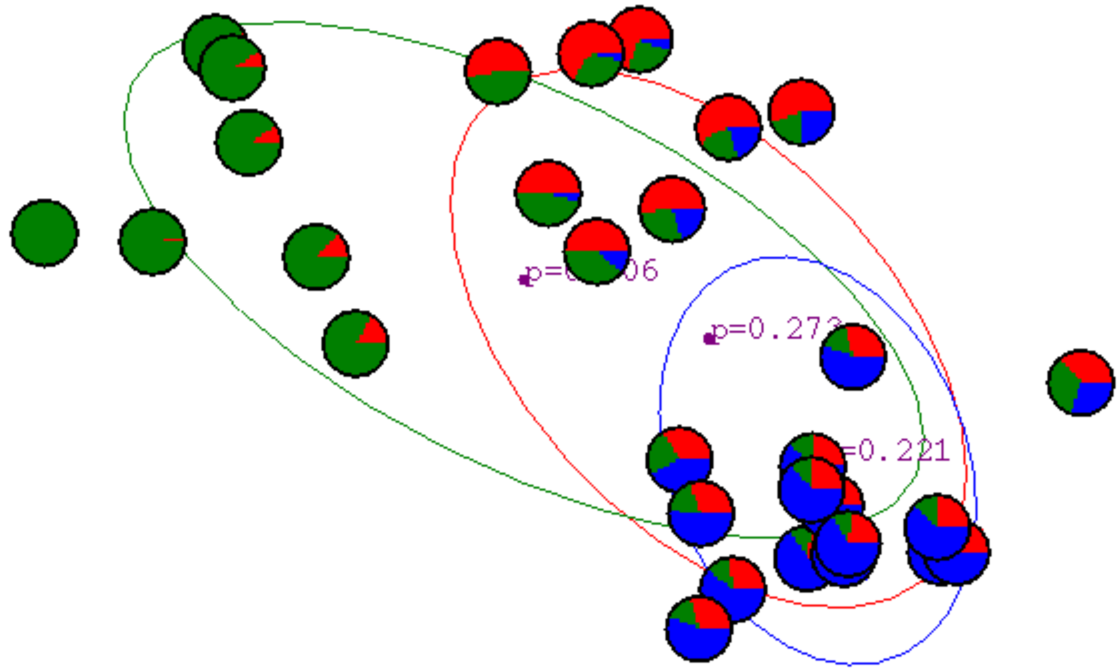
After first iteration



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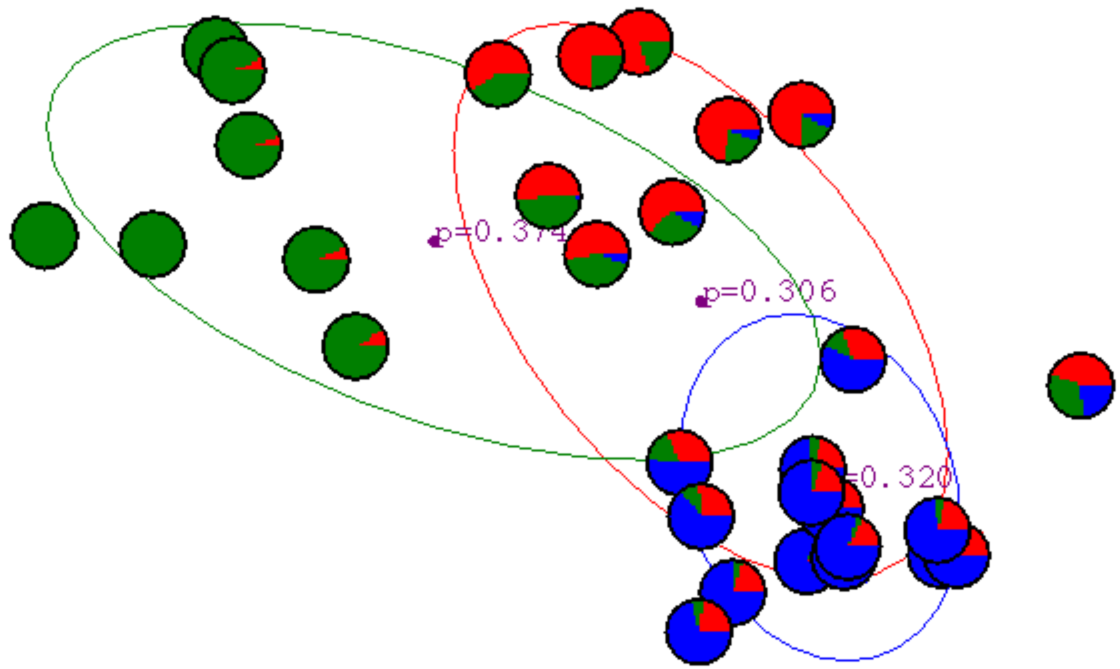
After 2nd iteration



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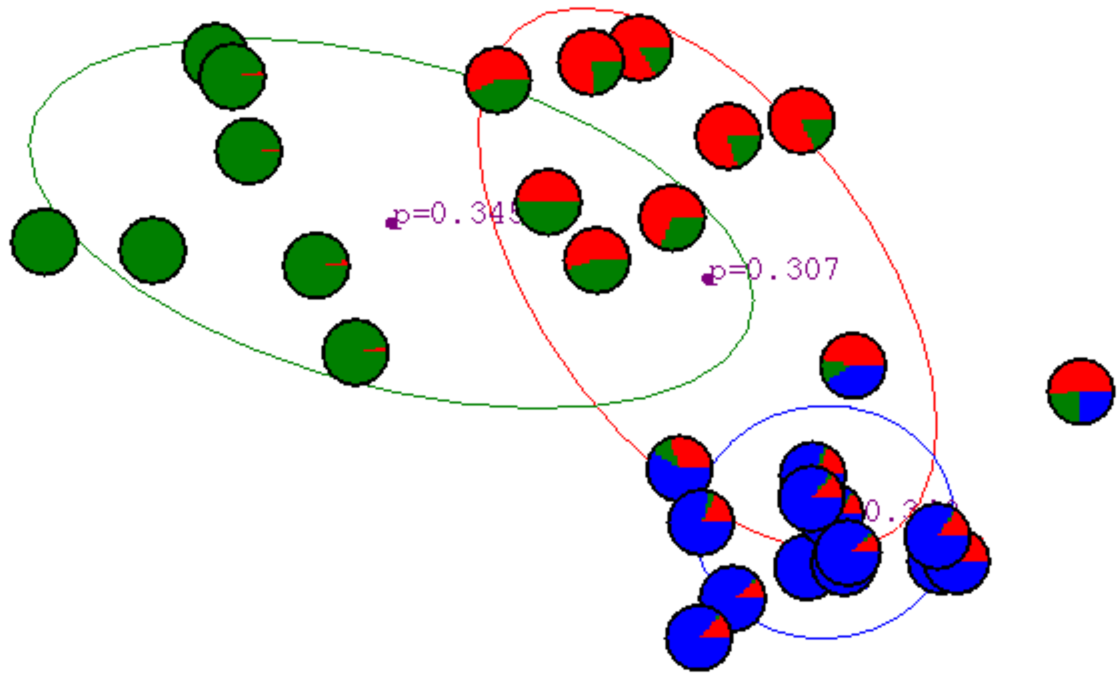
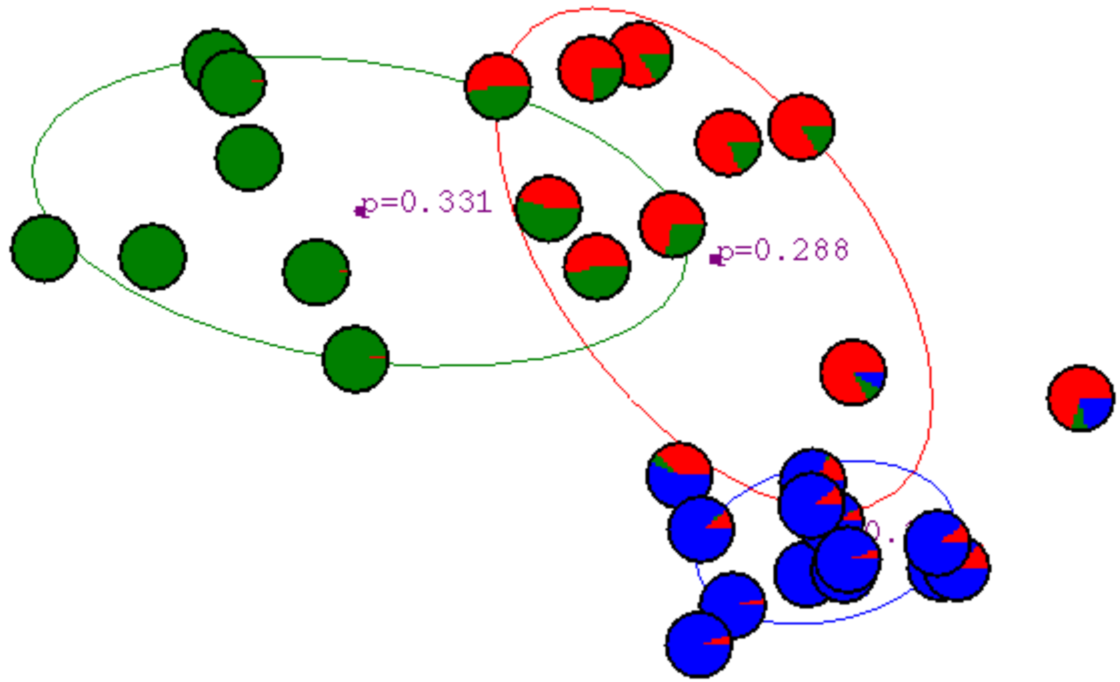
After 3rd iteration



After 4th iteration



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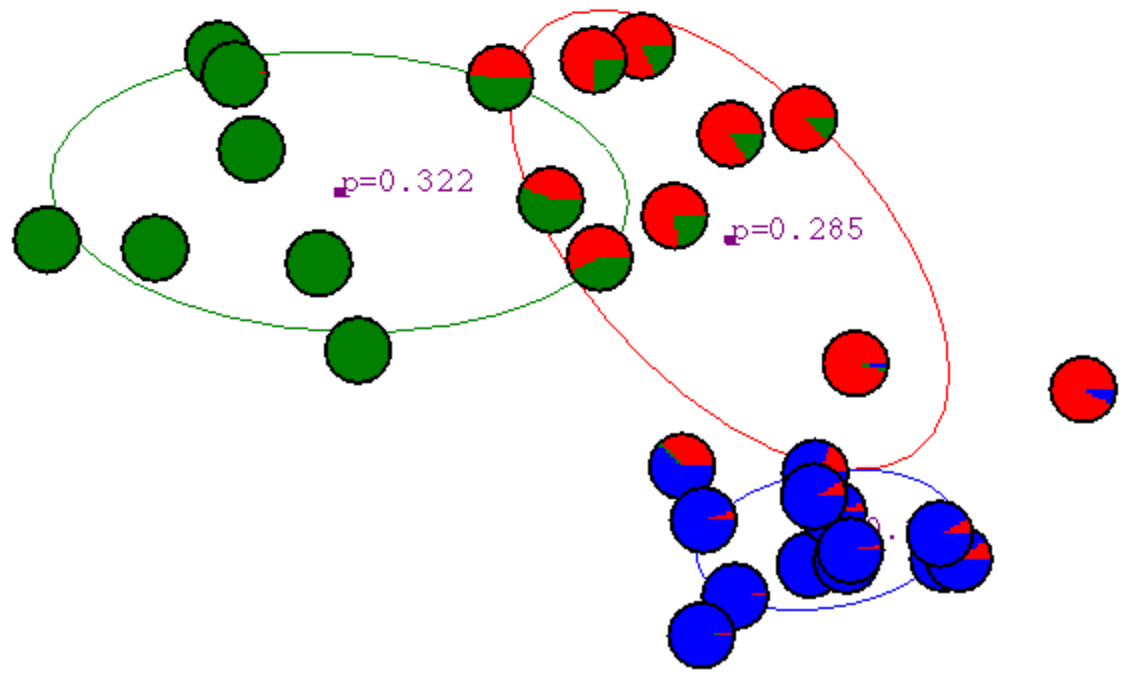
After 5th iteration



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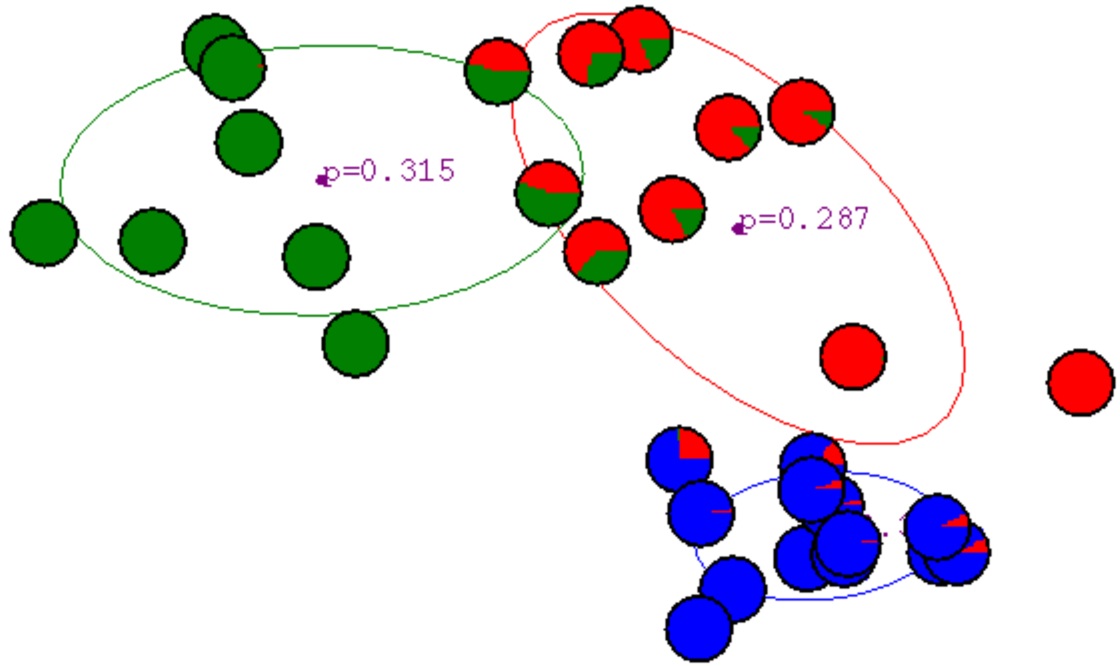
After 6th iteration



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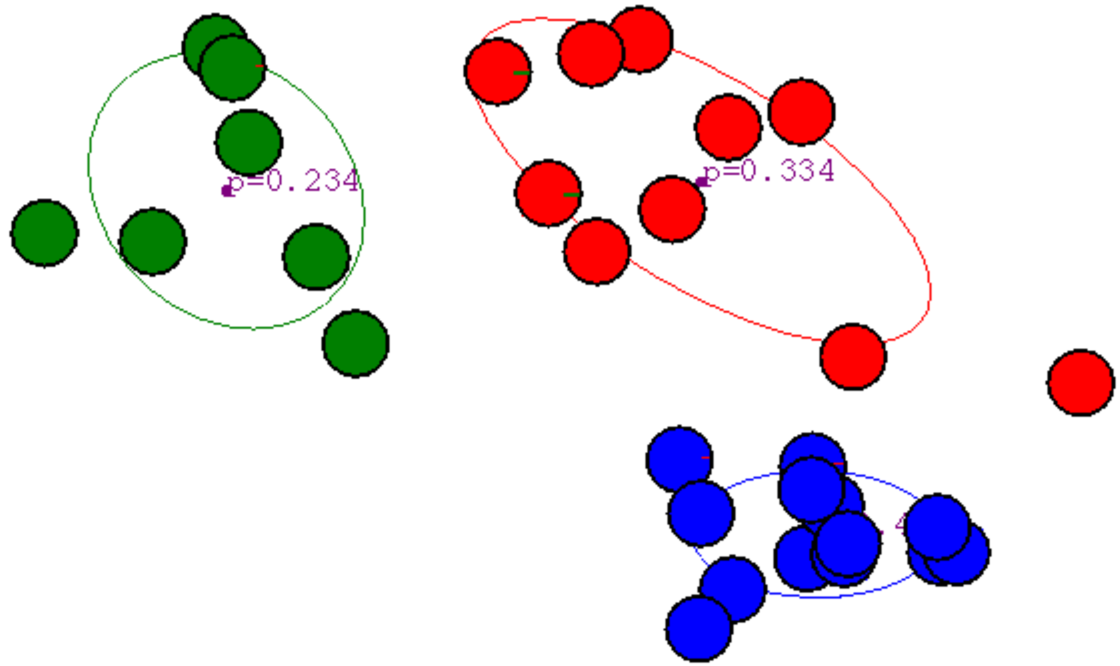
After 20th iteration



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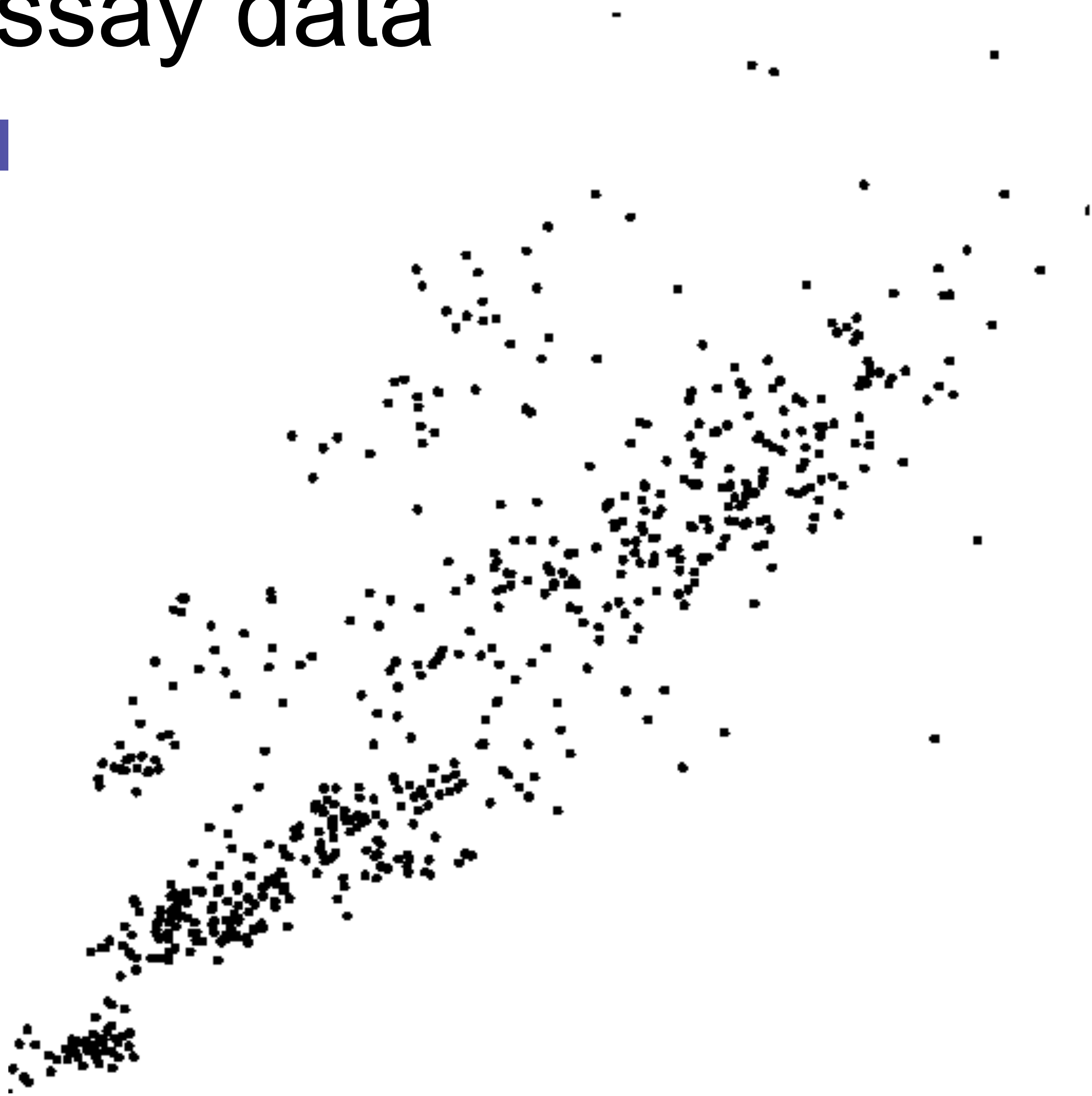
Some Bio Assay data



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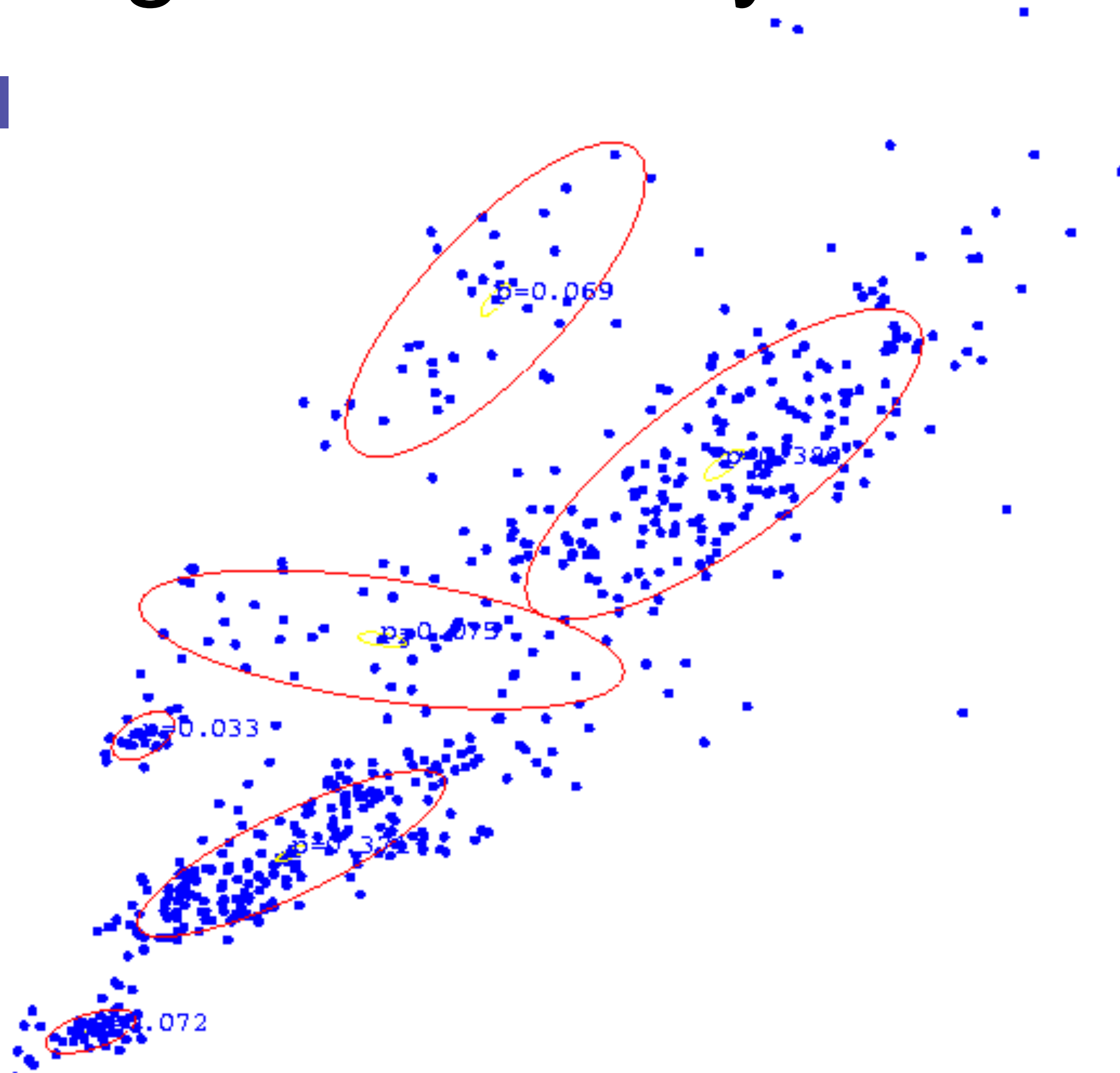
GMM clustering of the assay data



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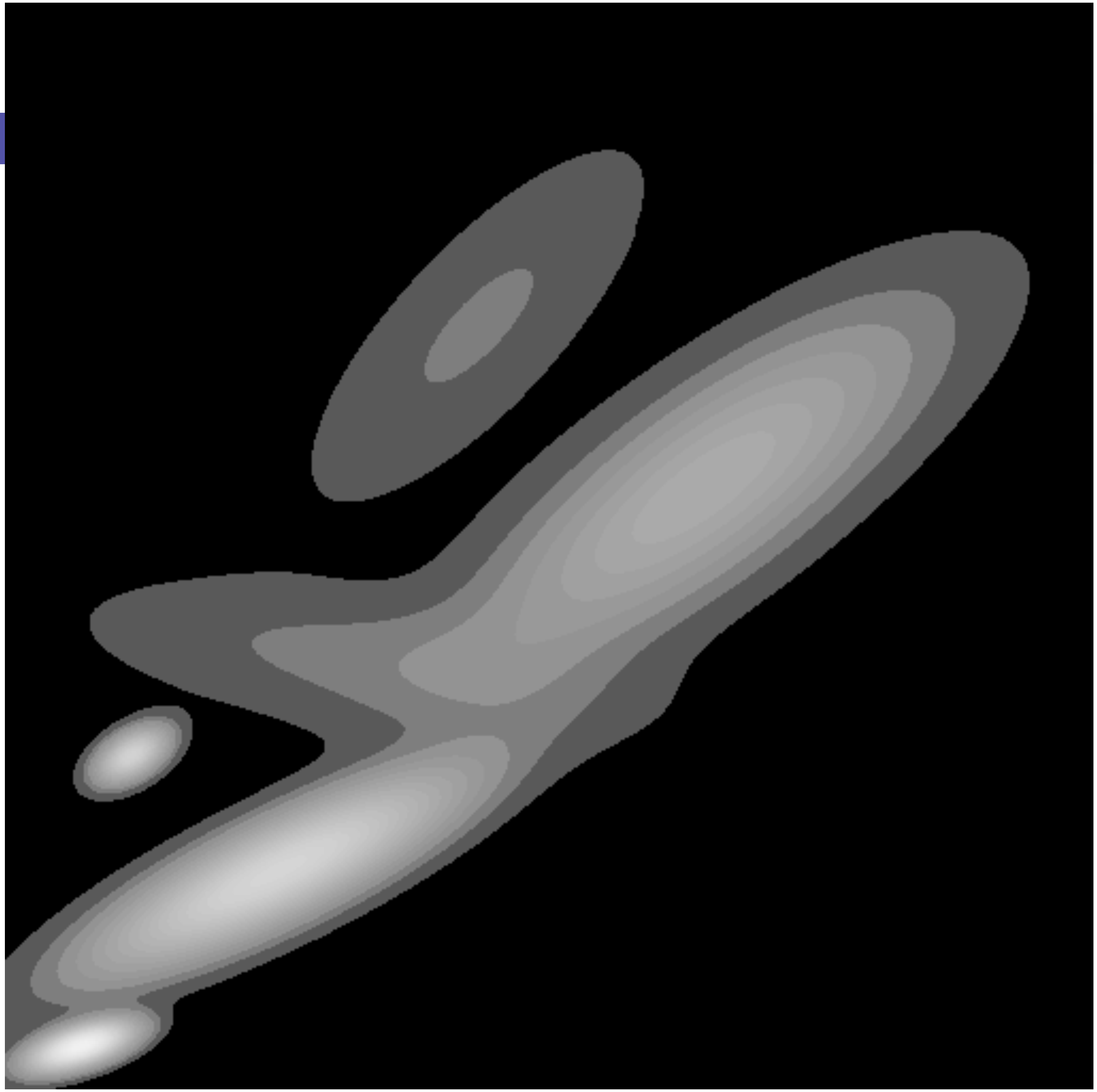
Resulting Density Estimator



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