Practice

- Fill in the missing plots:

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

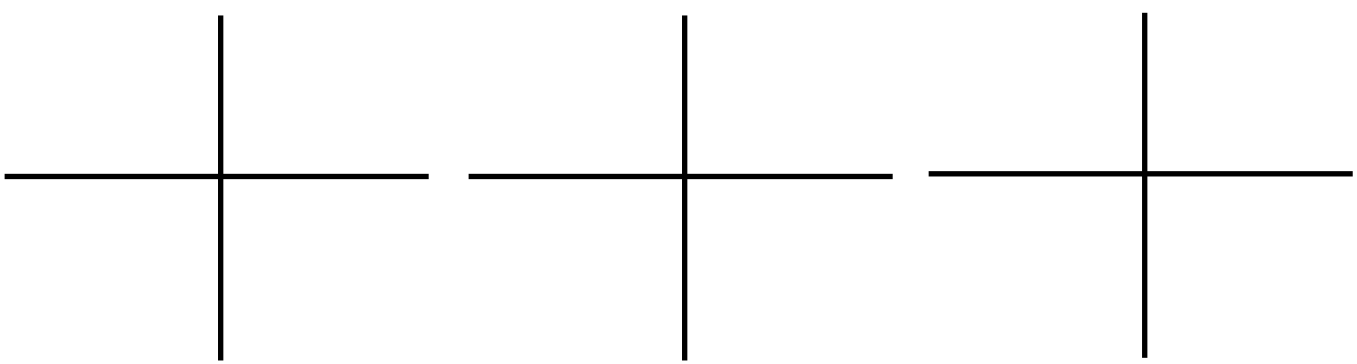
$$\mathbf{V}\mathbf{S}\mathbf{V}^T = \mathrm{eig}(\Sigma) \qquad \mathbf{J} = I - \mathbf{1}\mathbf{1}^T/n$$

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

$\mathbf{X}$ $\mathbf{Z}$

$\mu_X - \mu_Z$

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



Other dimensionality reduction

Machine Learning – CSE546
Kevin Jamieson
University of Washington

November 13, 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, $\mathbf{U}^T\mathbf{U} = I$, $\mathbf{V}^T\mathbf{V} = I$.

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

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

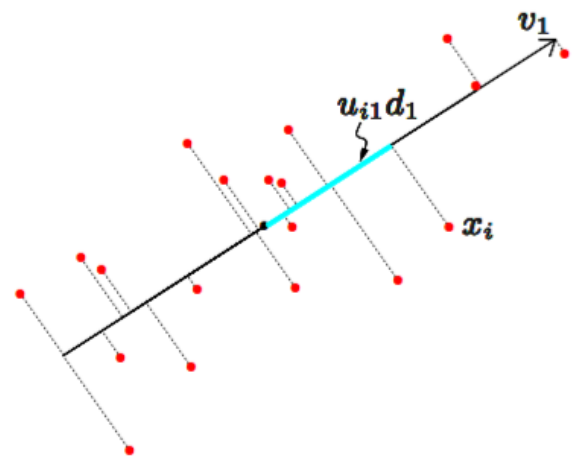
$$\mathbf{A}\mathbf{A}^T u_i = \mathbf{S}_{i,i}^2 u_i$$

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

Linear projections

Given $x_i \in \mathbb{R}^d$ and some $q < d$ consider

$$\min_{\mathbf{V}_q} \sum_{i=1}^{N} ||(x_i - \bar{x}) - \mathbf{V}_q \mathbf{V}_q^T (x_i - \bar{x})||^2.$$



where $\mathbf{V}_q = [v_1, v_2, \ldots, v_q]$ is orthonormal:

$$\mathbf{V}_q^T \mathbf{V}_q = I_q$$

$\mathbf{V}_q$ are the first q eigenvectors of Σ

$\mathbf{V}_q$ are the first q *principal components*

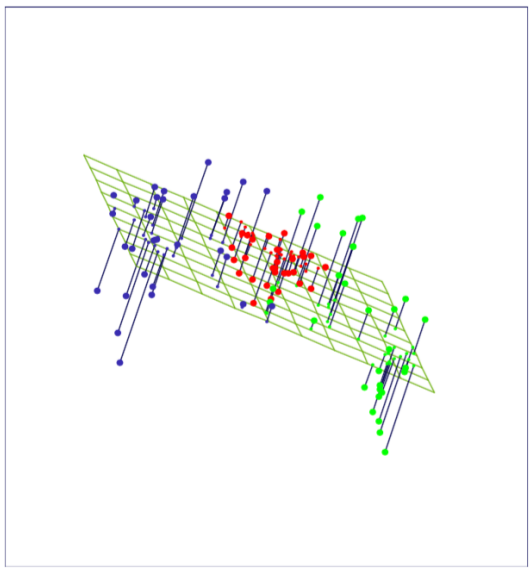
$$\Sigma := \sum_{i=1}^{N} (x_i - \bar{x})(x_i - \bar{x})^T$$

Principal Component Analysis (PCA) projects $(\mathbf{X} - \mathbf{1}\bar{x}^T)$ down onto $\mathbf{V}_q$

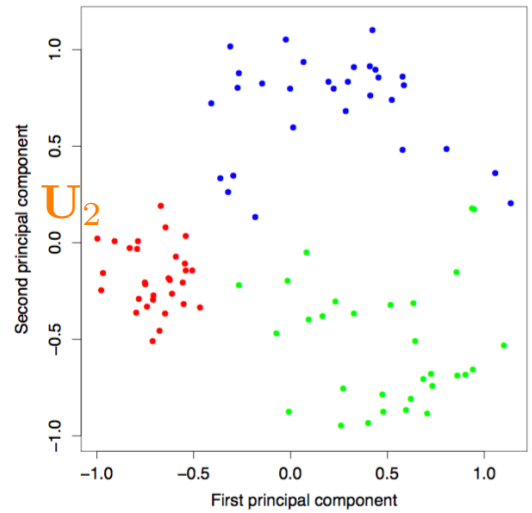
$$(\mathbf{X} - \mathbf{1}\bar{x}^T)\mathbf{V}_q = \mathbf{U}_q \mathrm{diag}(d_1, \ldots, d_q) \qquad \mathbf{U}_q^T \mathbf{U}_q = I_q$$

Dimensionality reduction

$\mathbf{V}_q$ are the first q eigenvectors of Σ and *SVD* $\mathbf{X} - \mathbf{1}\bar{x}^T = \mathbf{U}\mathbf{S}\mathbf{V}^T$



$\mathbf{X} - \mathbf{1}\bar{x}^T$



$\mathbf{U}_2$

$\mathbf{U}_1$

Kernel PCA

$\mathbf{V}_q$ are the first q eigenvectors of Σ and *SVD* $\mathbf{X} - \mathbf{1}\bar{x}^T = \mathbf{U}\mathbf{S}\mathbf{V}^T$

$$(\mathbf{X} - \mathbf{1}\bar{x}^T)\mathbf{V}_q = \mathbf{U_q}\mathbf{S_q} \in \mathbb{R}^{n \times q}$$

$$\mathbf{J}\mathbf{X} = \mathbf{X} - \mathbf{1}\bar{x}^T = \mathbf{U}\mathbf{S}\mathbf{V}^T \qquad \mathbf{J} = I - \mathbf{1}\mathbf{1}^T/n$$

$$(\mathbf{J}\mathbf{X})(\mathbf{J}\mathbf{X})^T = \mathbf{J}\mathbf{X}\mathbf{X}^T\mathbf{J} =: \mathbf{J}\mathbf{K}\mathbf{J} = \mathbf{U}\mathbf{S}^2\mathbf{U}^T \qquad \mathbf{K}_{i,j} = x_i^T x_j$$

Kernel PCA

$\mathbf{V}_q$ are the first q eigenvectors of Σ and *SVD* $\mathbf{X} - \mathbf{1}\bar{x}^T = \mathbf{U}\mathbf{S}\mathbf{V}^T$

$$(\mathbf{X} - \mathbf{1}\bar{x}^T)\mathbf{V}_q = \mathbf{U_q}\mathbf{S_q} \in \mathbb{R}^{n \times q}$$

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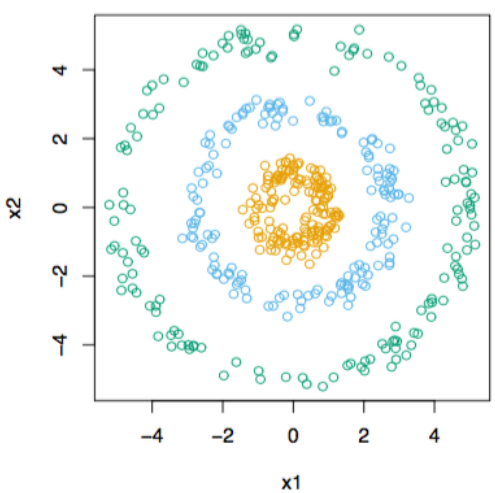
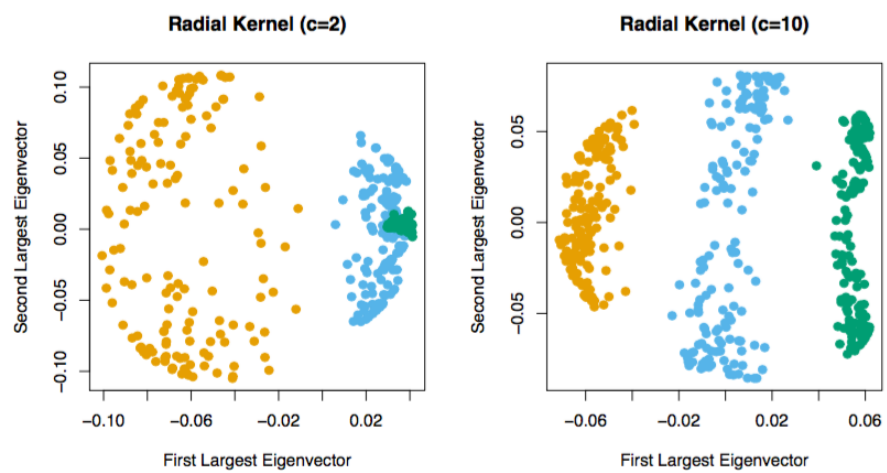
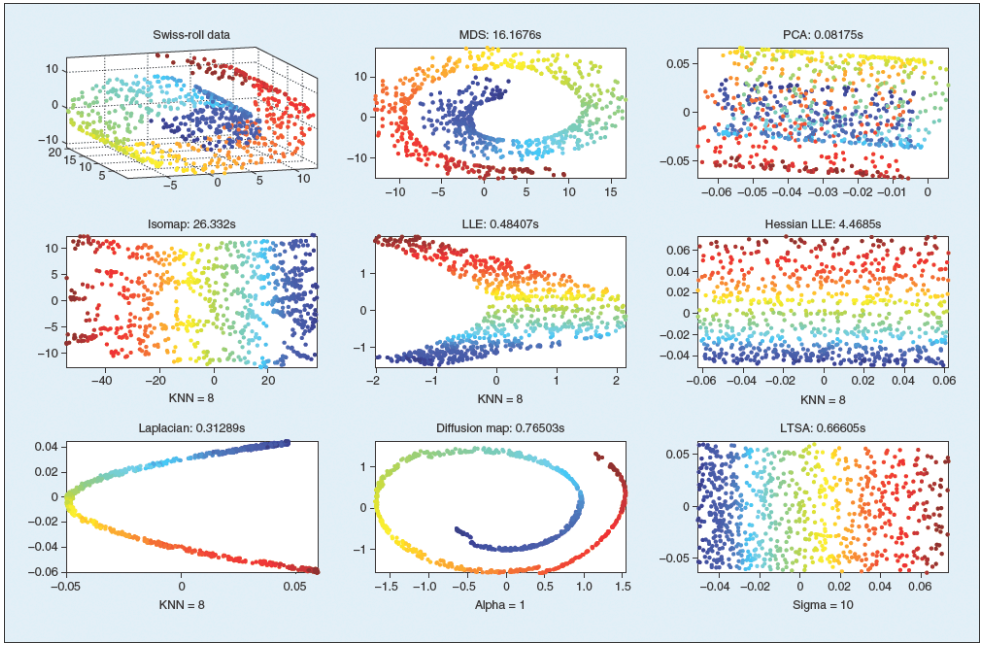




Nonlinear dimensionality reduction

Find a low dimensional representation that respects “local distances” in the higher dimensional space



Zhang et al 2010

Many methods:
- Kernel PCA
- ISOMAP
- Local linear embedding
- Maximum volume unfolding
- Non-metric multidimensional scaling
- Laplacian
- Neural network auto encoder
- …

Due to lack of agreed upon metrics, it is very hard to judge which is best. Also, results from 3 to 2 dims is probably not representative of 1000 to 2 dimensions.

Random projections

PCA finds a low-dimensional representation that reduces population variance

$$\min_{\mathbf{V}_q} \sum_{i=1}^{N} ||(x_i - \bar{x}) - \mathbf{V}_q \mathbf{V}_q^T (x_i - \bar{x})||^2.$$

$\mathbf{V}_q \mathbf{V}_q^T$ is a *projection matrix* that minimizes error in basis of size q

$\mathbf{V}_q$ are the first q eigenvectors of Σ

$$\Sigma := \sum_{i=1}^{N} (x_i - \bar{x})(x_i - \bar{x})^T$$

But what if I care about the reconstruction of the *individual* points?

$$\min_{\mathbf{W}_q} \max_{i=1,\ldots,n} ||(x_i - \bar{x}) - \mathbf{W}_q \mathbf{W}_q^T (x_i - \bar{x})||^2$$

Random projections

$$\min_{\mathbf{W}_q} \max_{i=1,\ldots,n} ||(x_i - \bar{x}) - \mathbf{W}_q \mathbf{W}_q^T (x_i - \bar{x})||^2$$

Johnson-Lindenstrauss (1983)

(q is independent of d)

Theorem Let $\epsilon \in \mathbb{R}^d$ and set $q = 20\epsilon^{-2}\log(n)$. Assume that the entries $A \in \mathbb{R}^{d\times q}$ are sampled iid from $\mathcal{N}(0, 1/q)$. Then for any $z \in \mathbb{R}^d$ we have with probability at least $1 - 2e^{(\epsilon^2-\epsilon^3)q/4}$ that

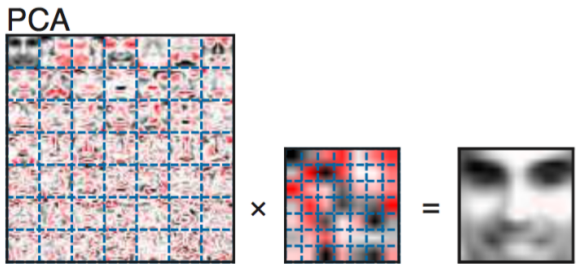
$$(1-\epsilon)\|z\|^2 \leq \|A^T z\|^2 \leq (1+\epsilon)\|z\|^2$$

Other matrix factorizations

$$\mathbf{X} = \mathbf{U}\,\mathbf{S}\,\mathbf{V}^{\mathbf{T}}$$

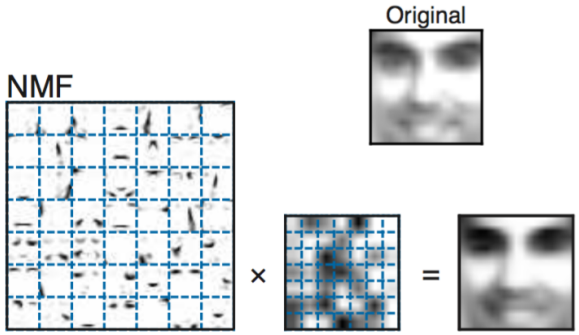
Singular value decomposition

Elements of $\mathbf{U}, \mathbf{S}, \mathbf{V}$ in $\mathbb{R}$



Nonnegative matrix factorization (NMF)

Elements of $\mathbf{U}, \mathbf{S}, \mathbf{V}$ in $\mathbb{R}_+$



Matrix Completion

Machine Learning – CSE546

Kevin Jamieson
University of Washington

November 13, 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, $\mathbf{U}^T\mathbf{U} = I$, $\mathbf{V}^T\mathbf{V} = I$.

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

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$\mathbf{V}$ are the first r eigenvectors of $\mathbf{A}^T\mathbf{A}$ with eigenvalues $\mathrm{diag}(\mathbf{S})$
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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, $\mathbf{U}^T\mathbf{U} = I$, $\mathbf{V}^T\mathbf{V} = I$.

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

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

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)

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

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

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

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

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

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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
⋮					

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

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

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 13, 2016

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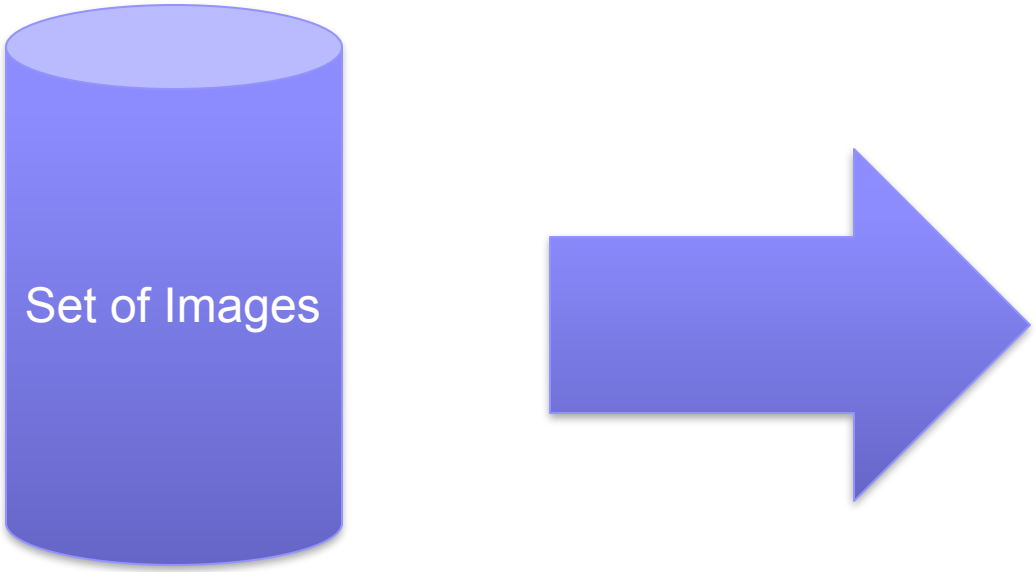
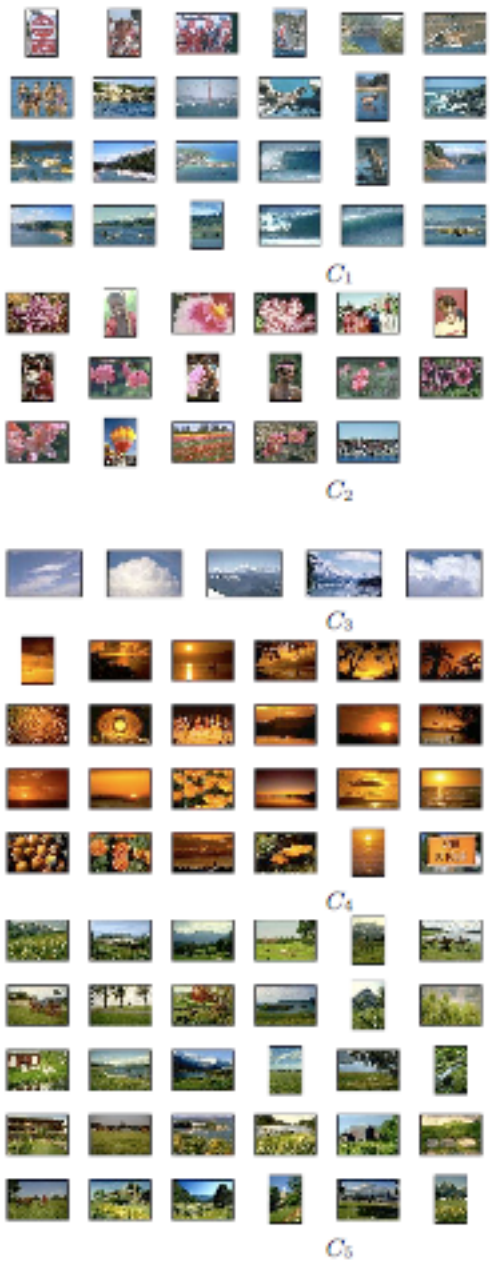
Clustering images





[Goldberger et al.]

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Clustering web search results

web news images wikipedia blogs jobs more »

race Search advanced preferences

clusters sources sites

remix

All Results (238)

- 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

1. 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) - [cache] - Live, Ask
2. 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
3. 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/backgrounder/usa/race - [cache] - Ask
4. 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
5. 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
6. **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
7. 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

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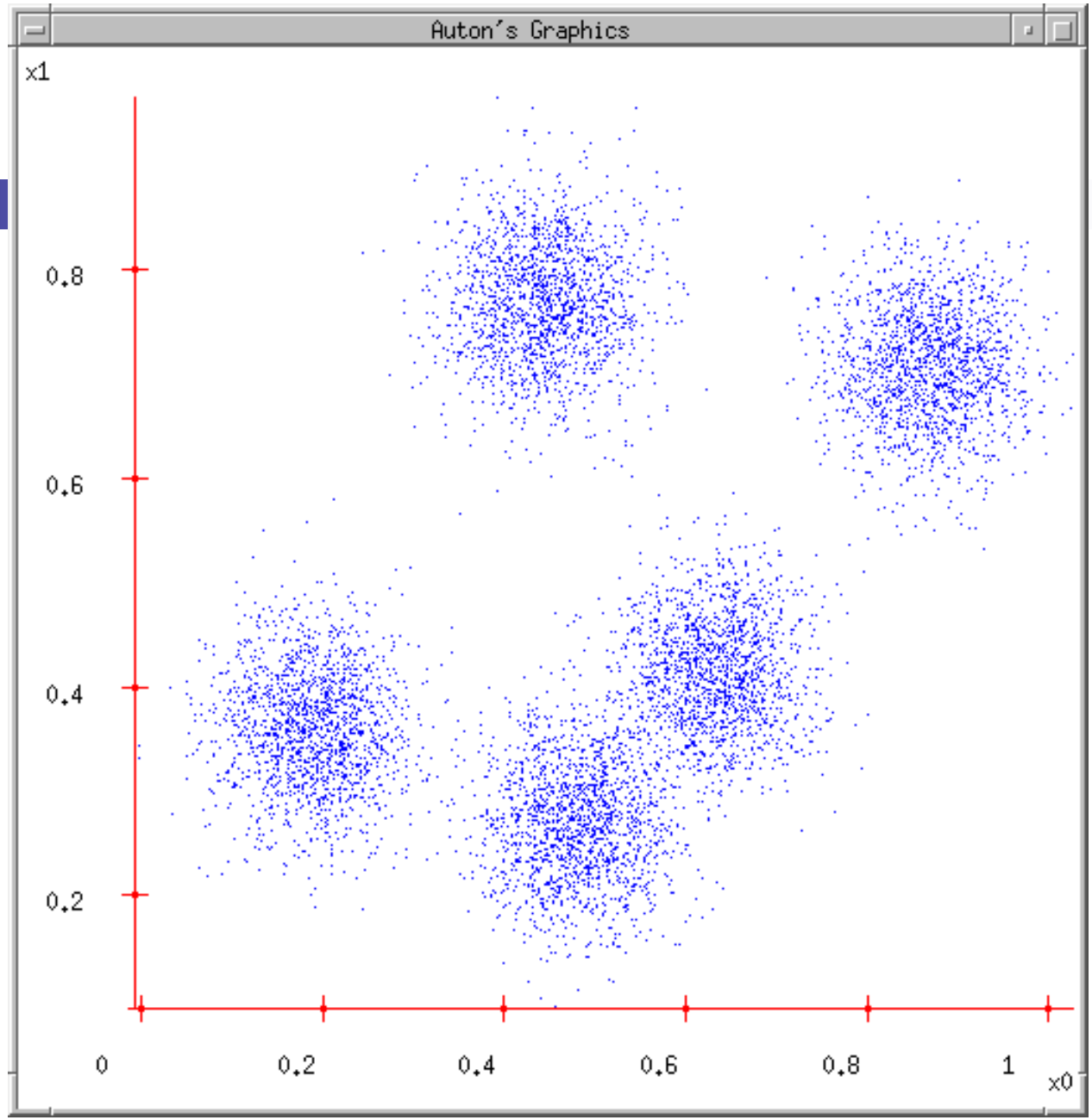
Some Data



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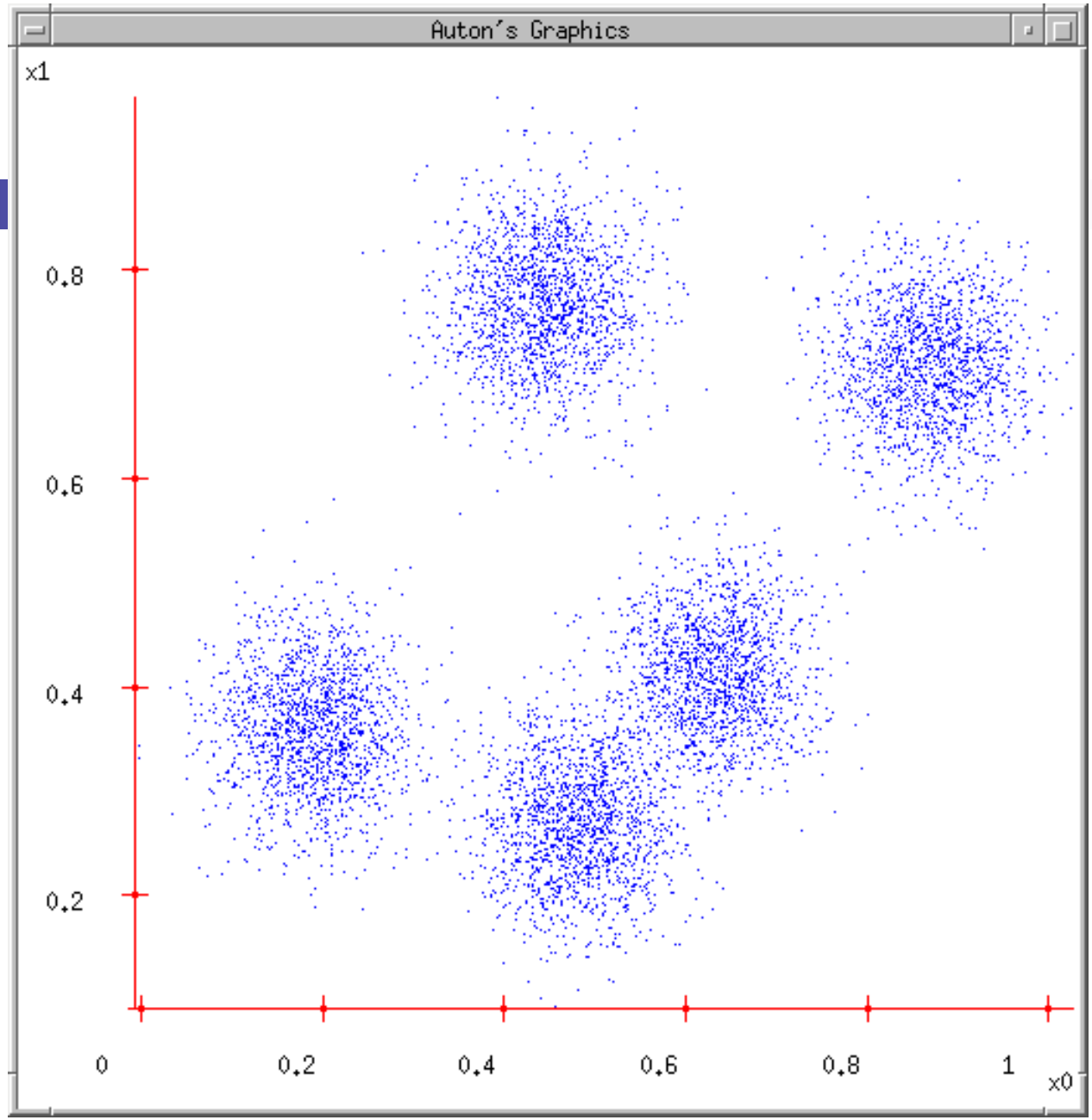
K-means

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



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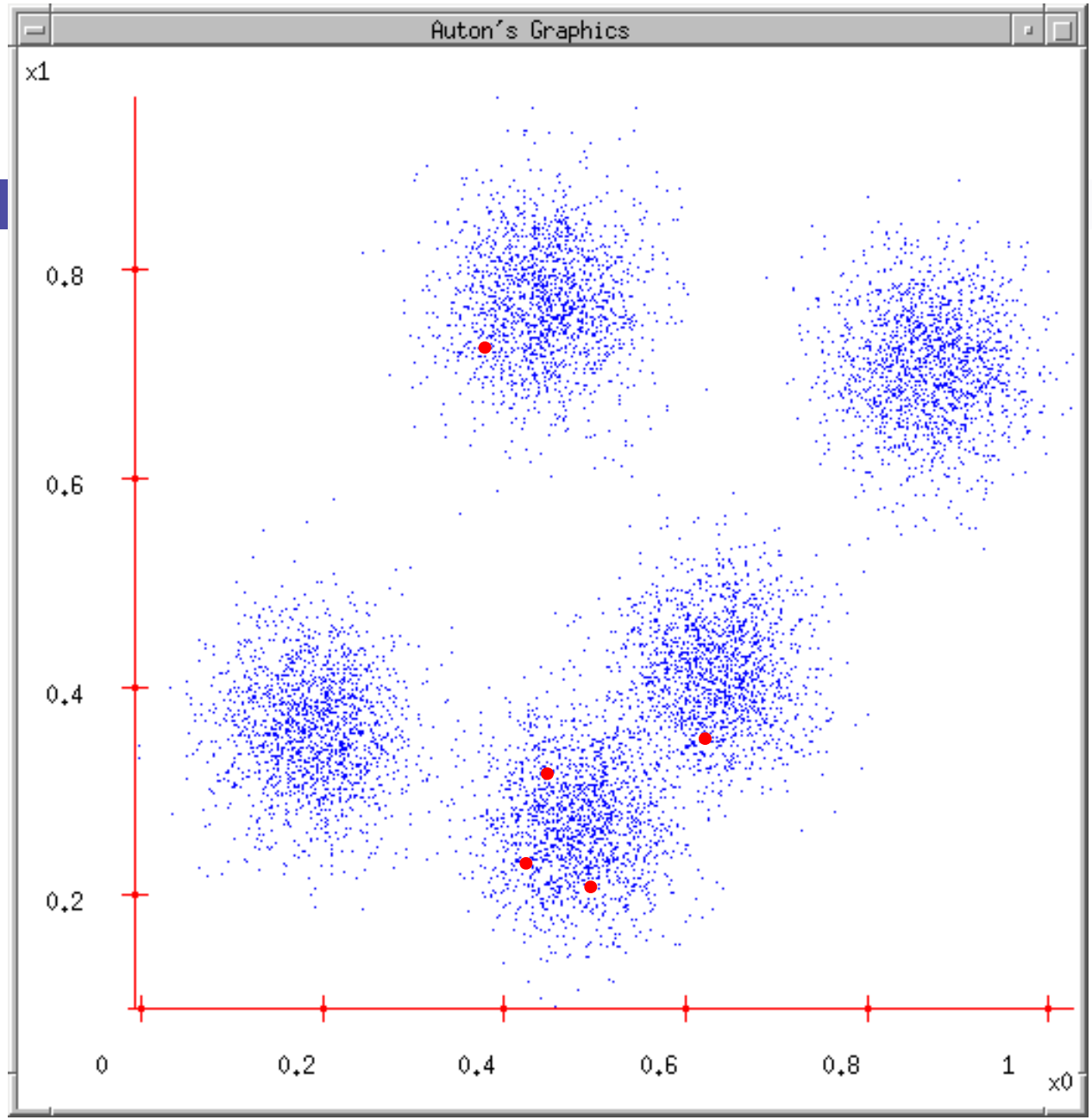
K-means

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



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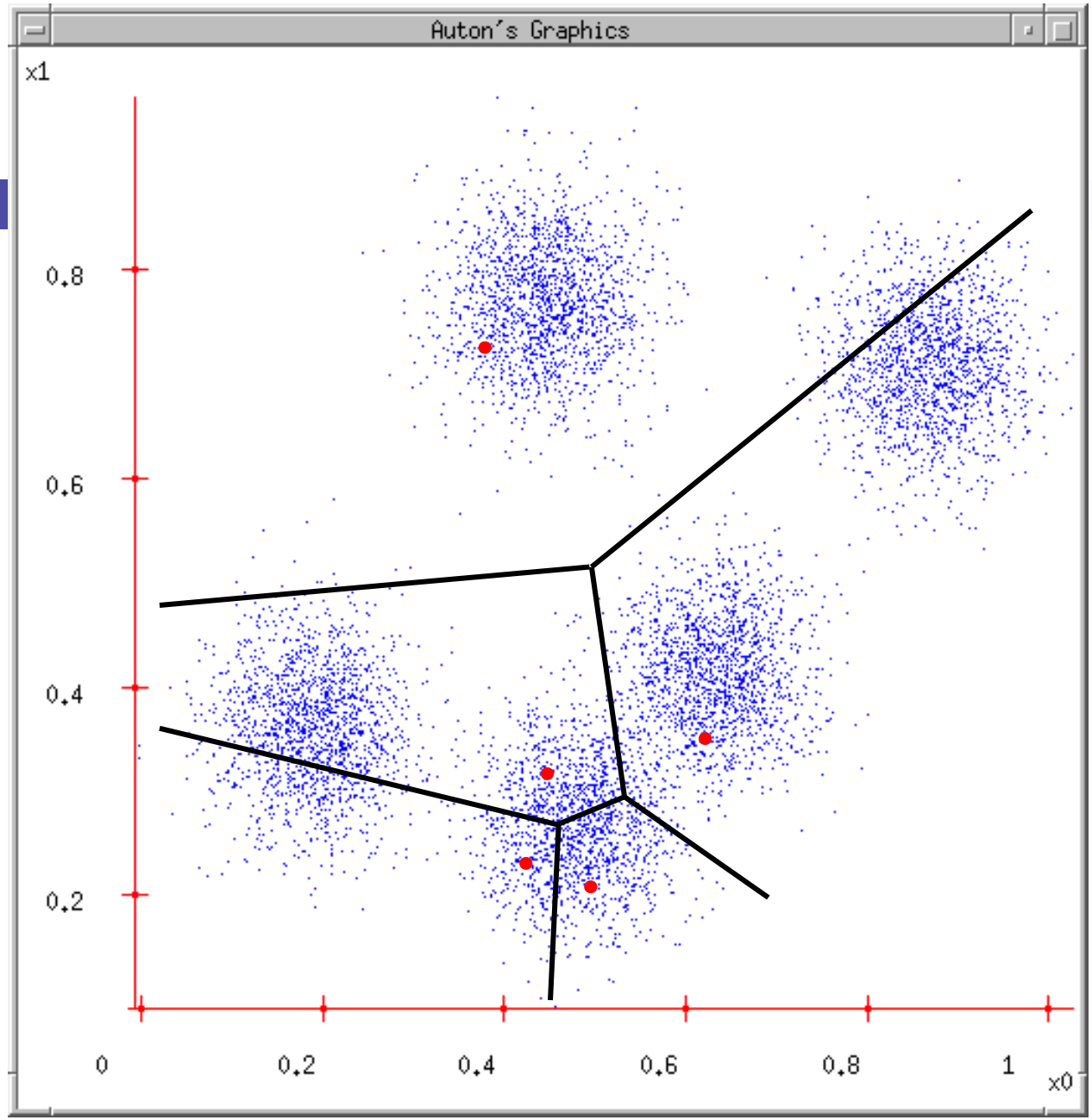
K-means

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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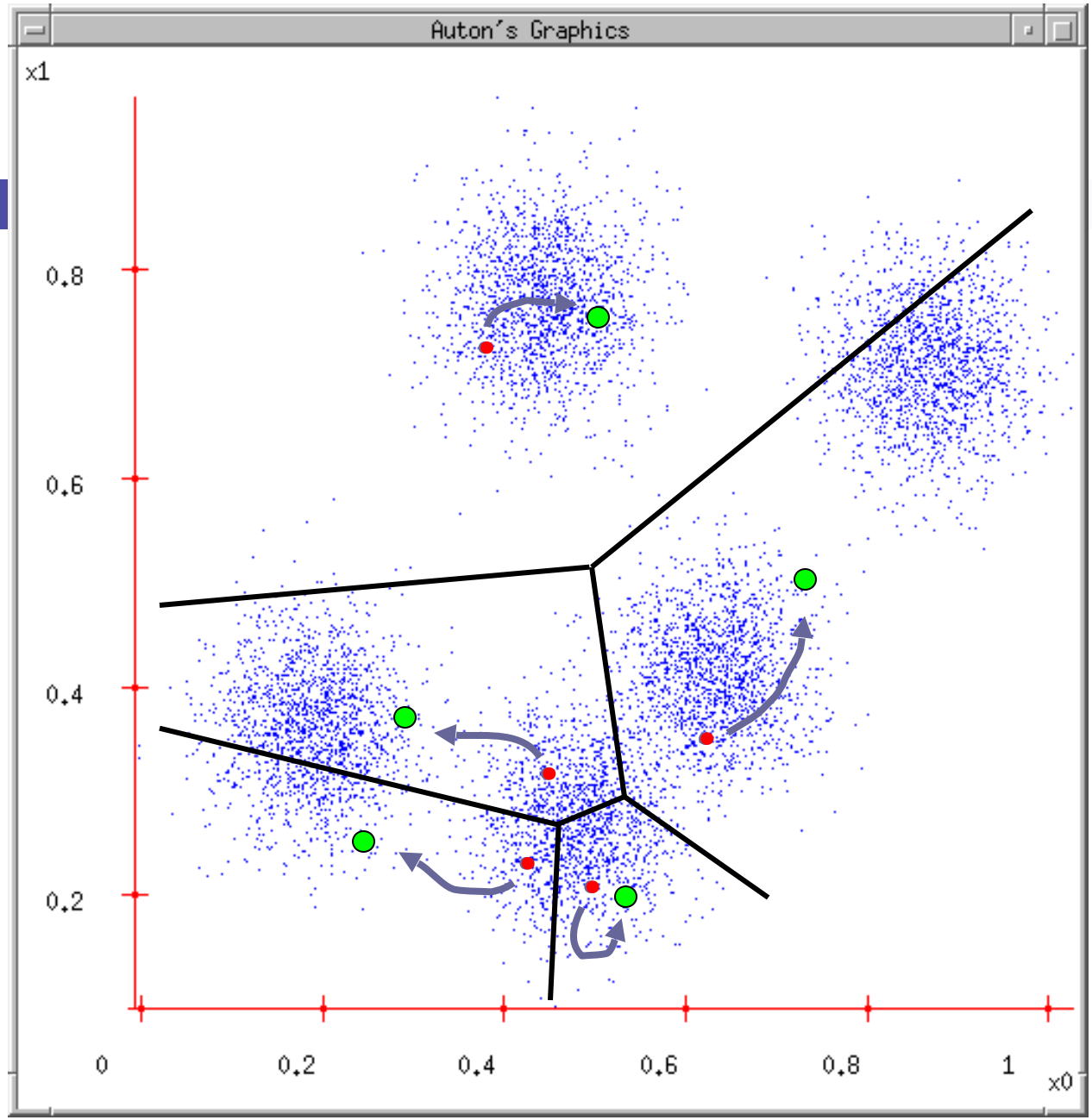
K-means

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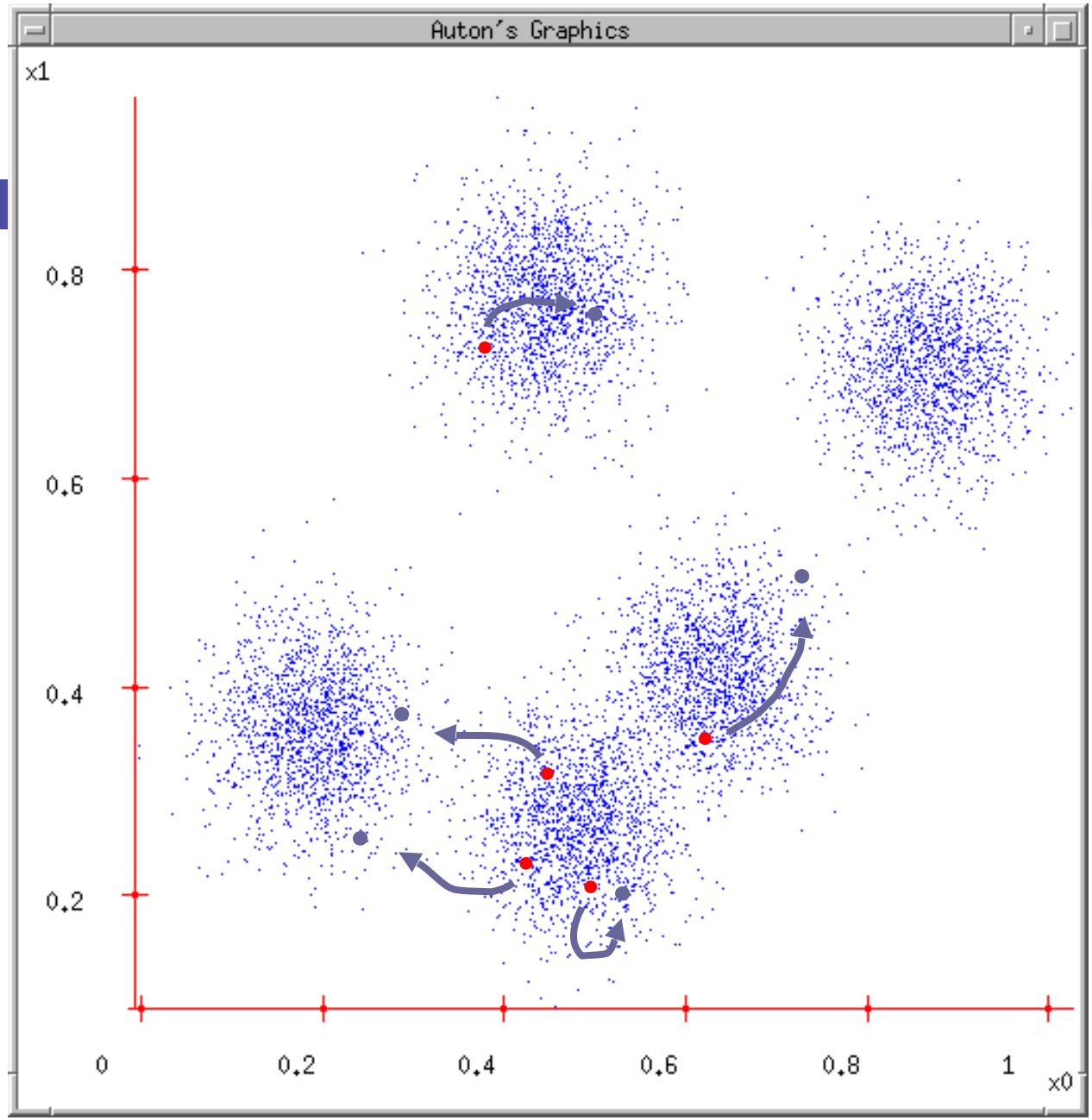
K-means

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!



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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.

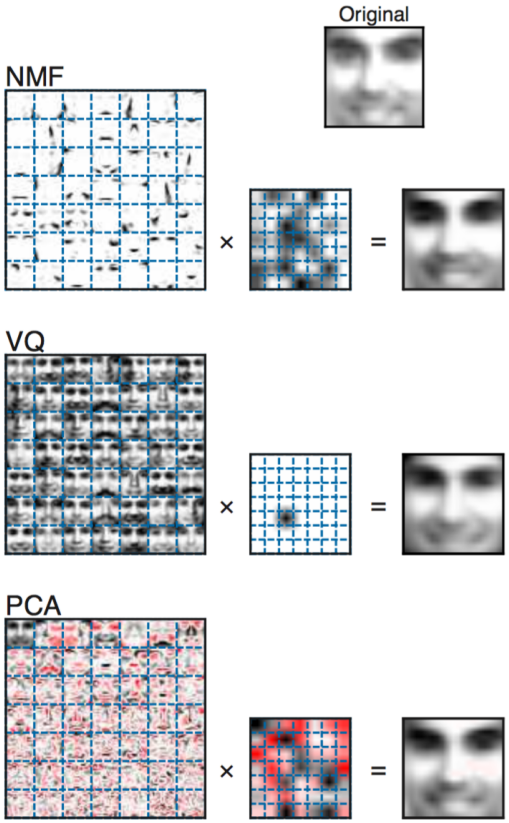
FIGURE 14.9. *Sir Ronald A. Fisher (1890 – 1962) was one of the founders of modern day statistics, to whom we owe maximum-likelihood, sufficiency, and many other fundamental concepts. The image on the left is a 1024×1024 grayscale image at 8 bits per pixel. The center image is the result of 2 × 2 block 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*

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*



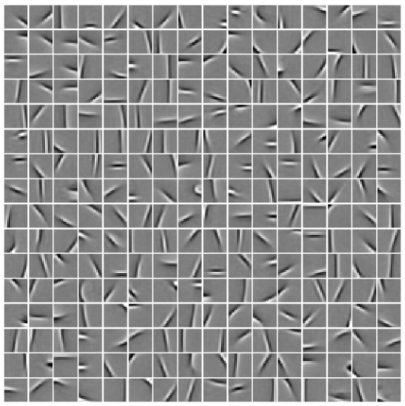
Vector Quantization, Fisher Vectors

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*

Typical output of k-means on patches

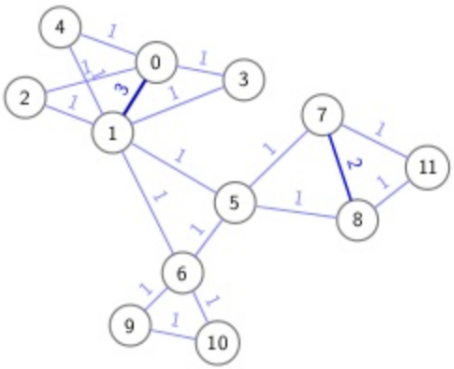


Similar reduced representation can be used as a feature vector

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:

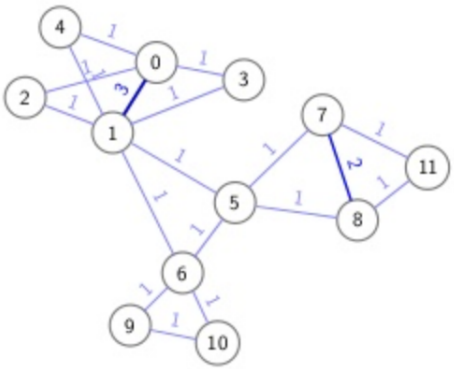
- k-nearest neighbor graph with weights in {0,1}
- weighted graph with arbitrary *similarities* $\mathbf{W}_{i,j} = e^{-\gamma||x_i - x_j||^2}$

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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Spectral Clustering

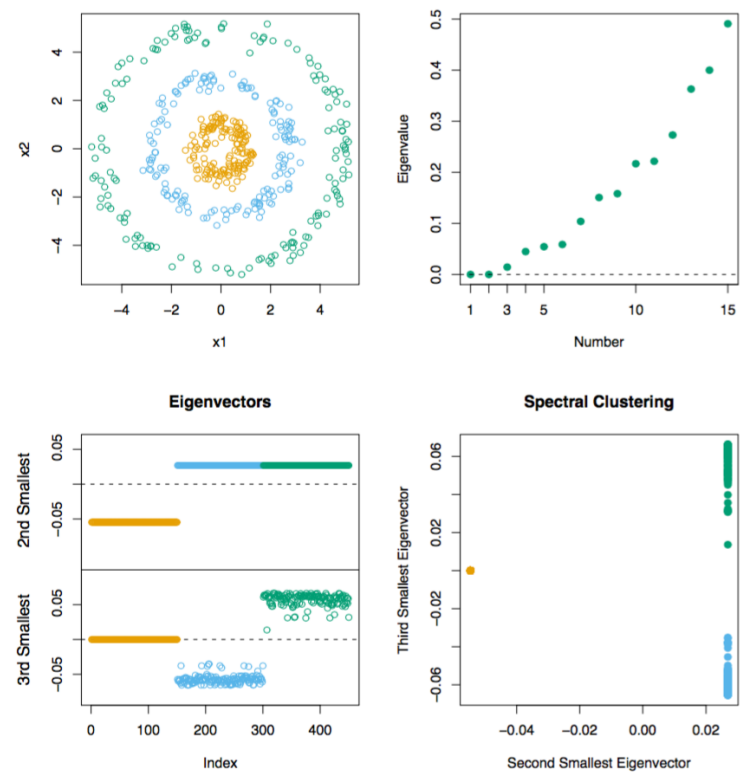
Adjacency matrix: $\mathbf{W}$

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

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

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 13, 2016

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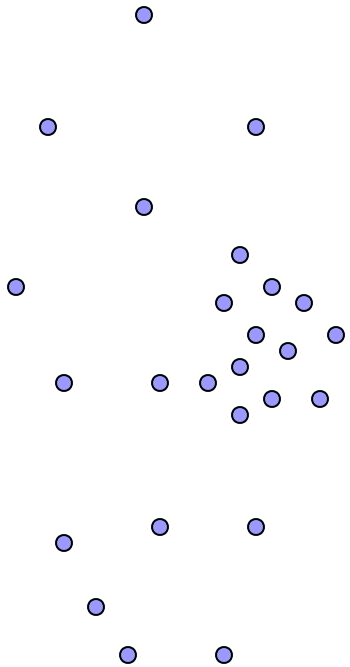
(One) bad case for k-means



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

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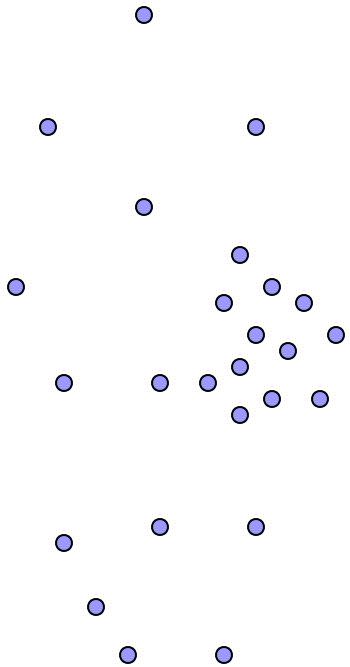
(One) bad case for k-means



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

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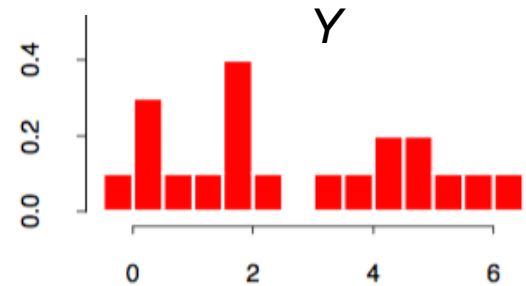
Mixture models

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

$\Delta \in \{0,1\}$ 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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Y &= (1-\Delta)\cdot Y_1 + \Delta \cdot Y_2,
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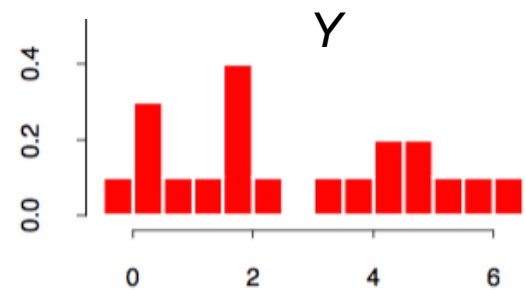
$$

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

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

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

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

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

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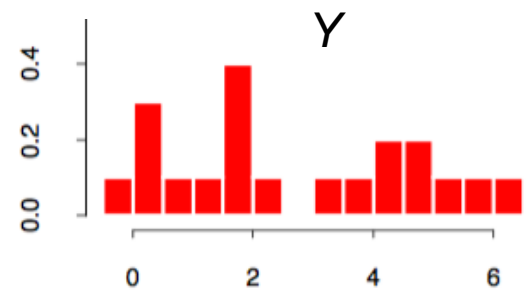
$\theta = (\pi, \theta_1, \theta_2) = (\pi, \mu_1, \sigma_1^2, \mu_2, \sigma_2^2)$



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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 Δ, how would we choose θ?

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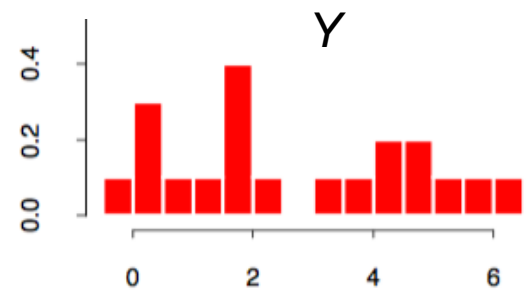
Mixture models

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

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

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



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

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Mixture models

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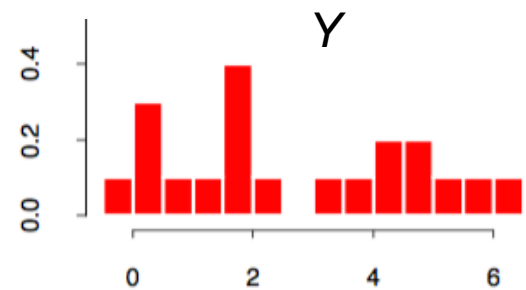
Y_2 &\sim N(\mu_2, \sigma_2^2), \\
Y &= (1-\Delta)\cdot Y_1 + \Delta \cdot Y_2,
\end{aligned}
$$

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

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

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

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

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

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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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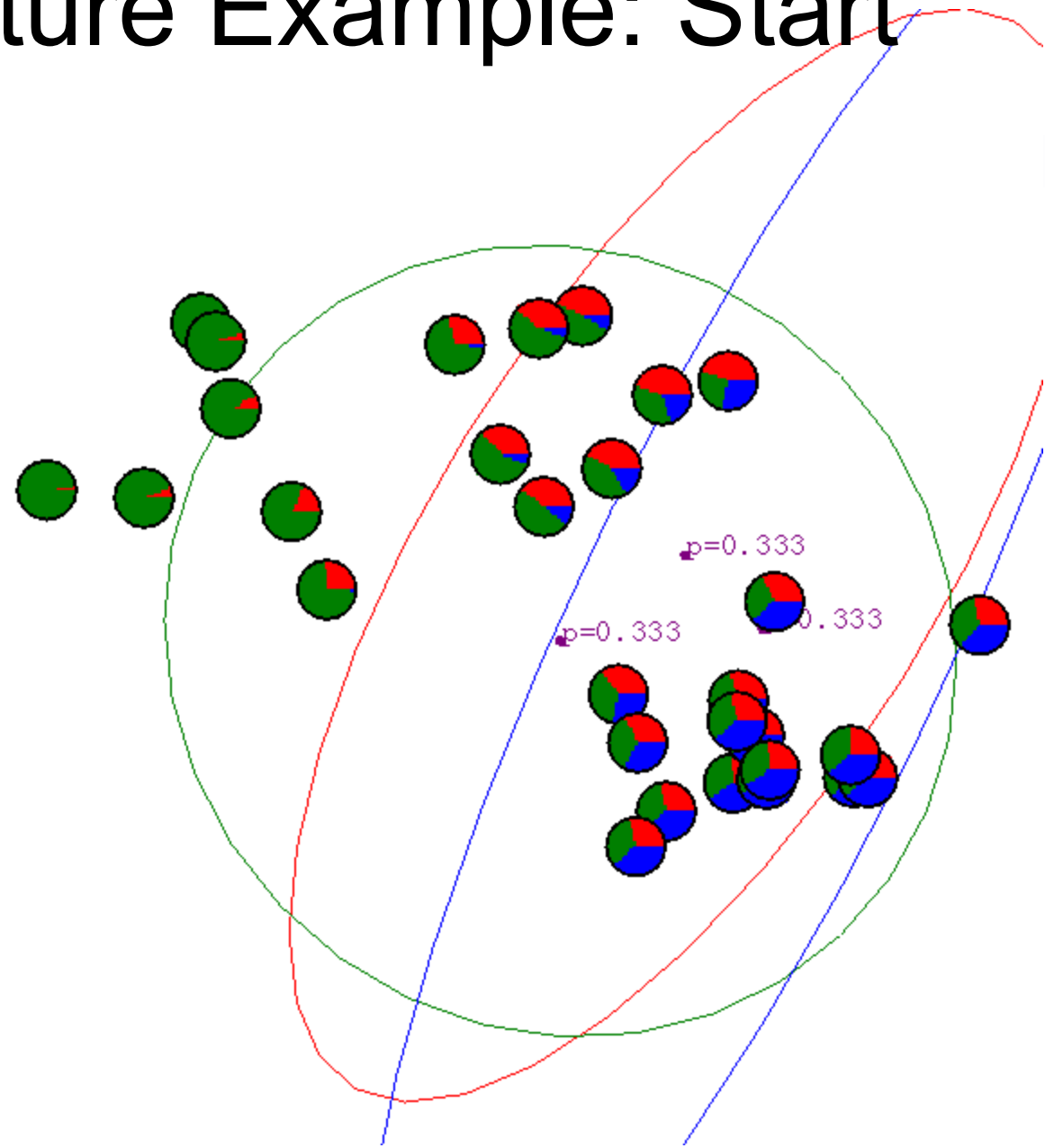
Gaussian Mixture Example: Start



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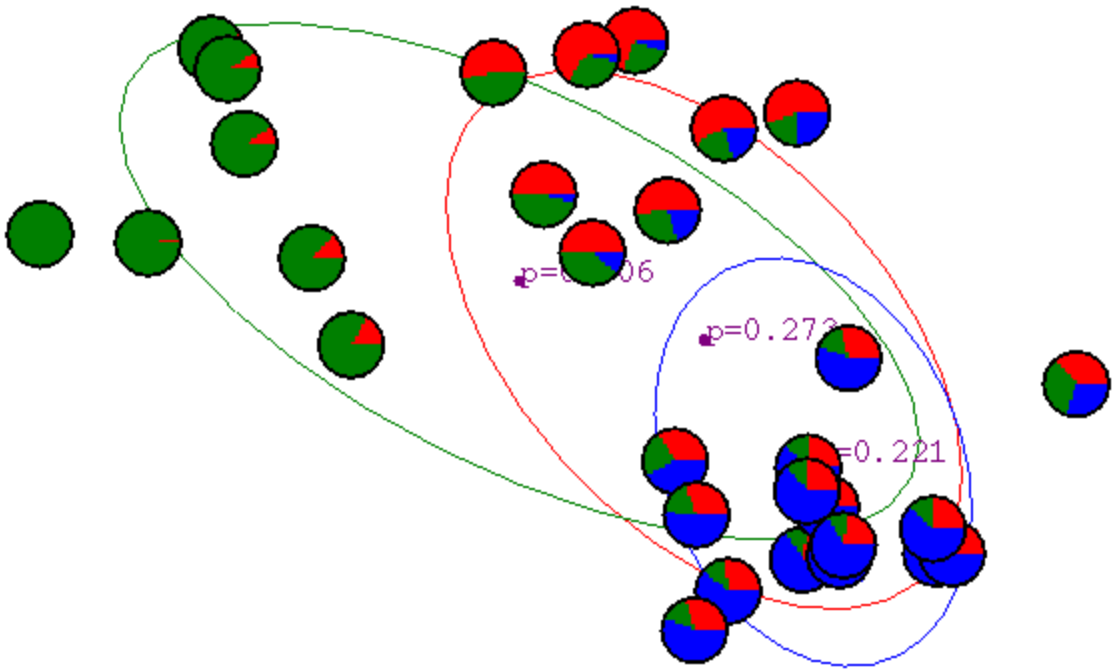
After first iteration



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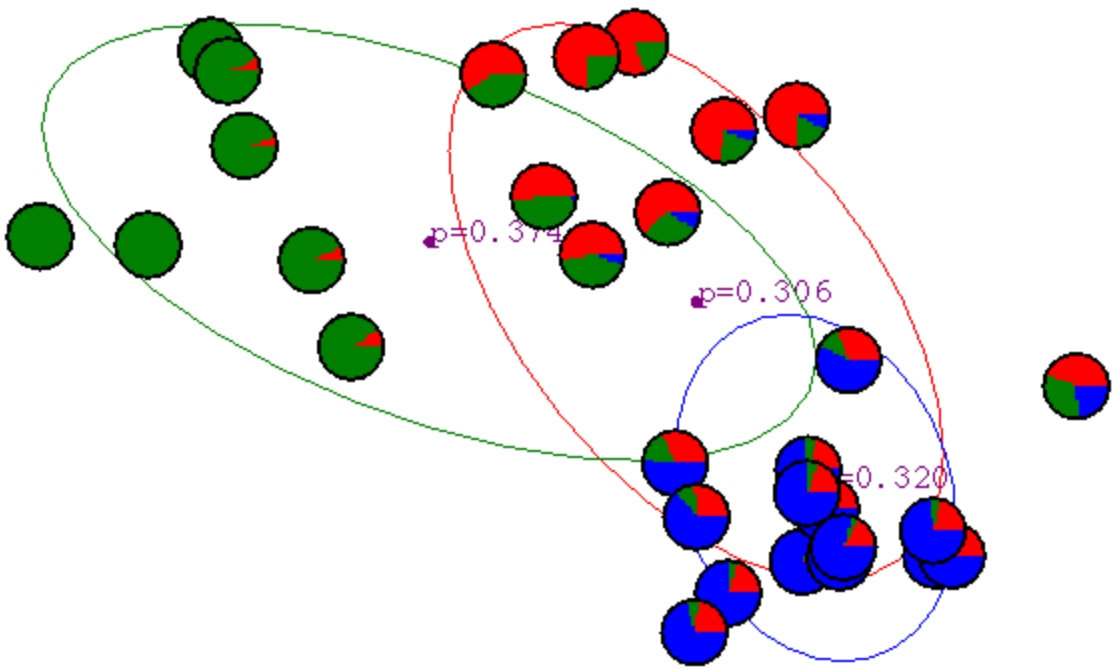
After 2nd iteration



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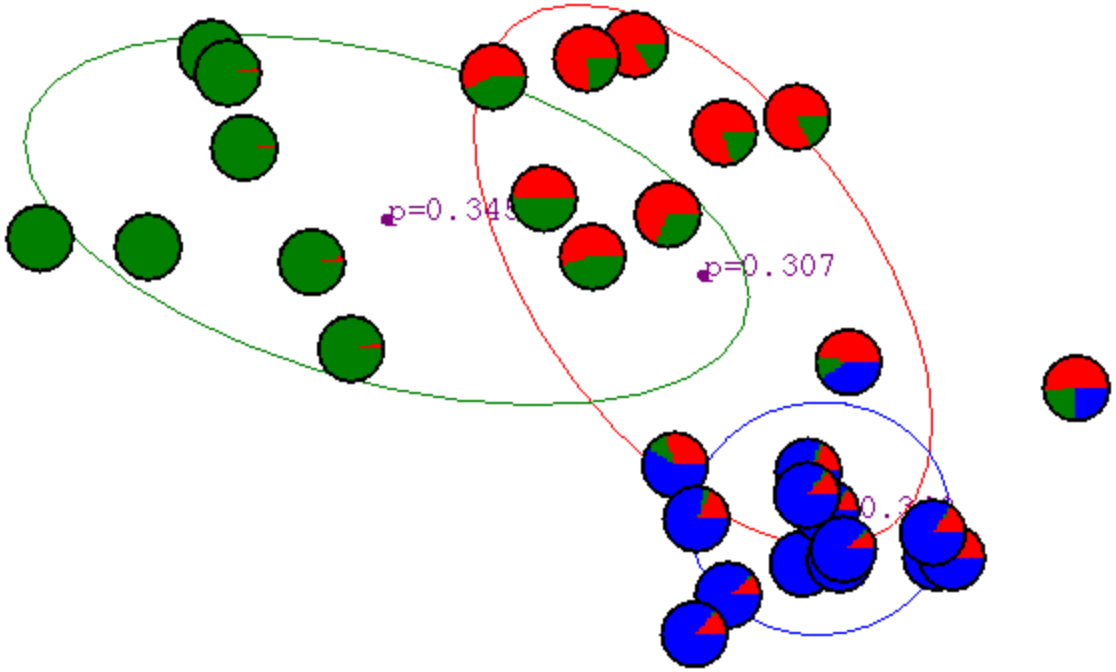
After 3rd iteration



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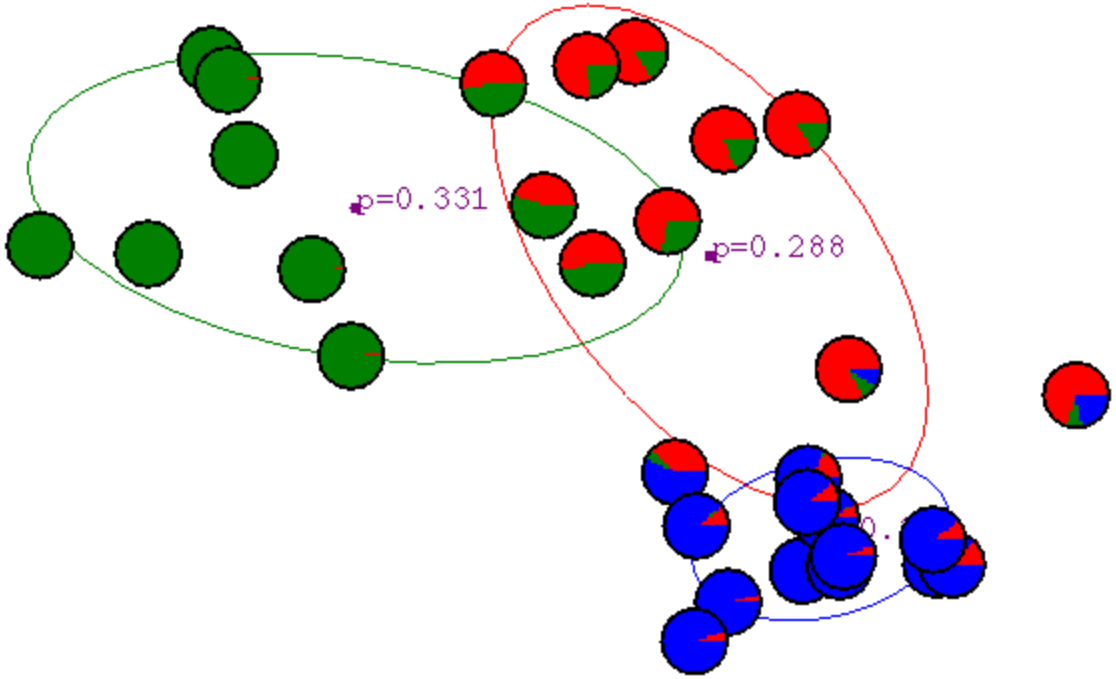
After 4th iteration



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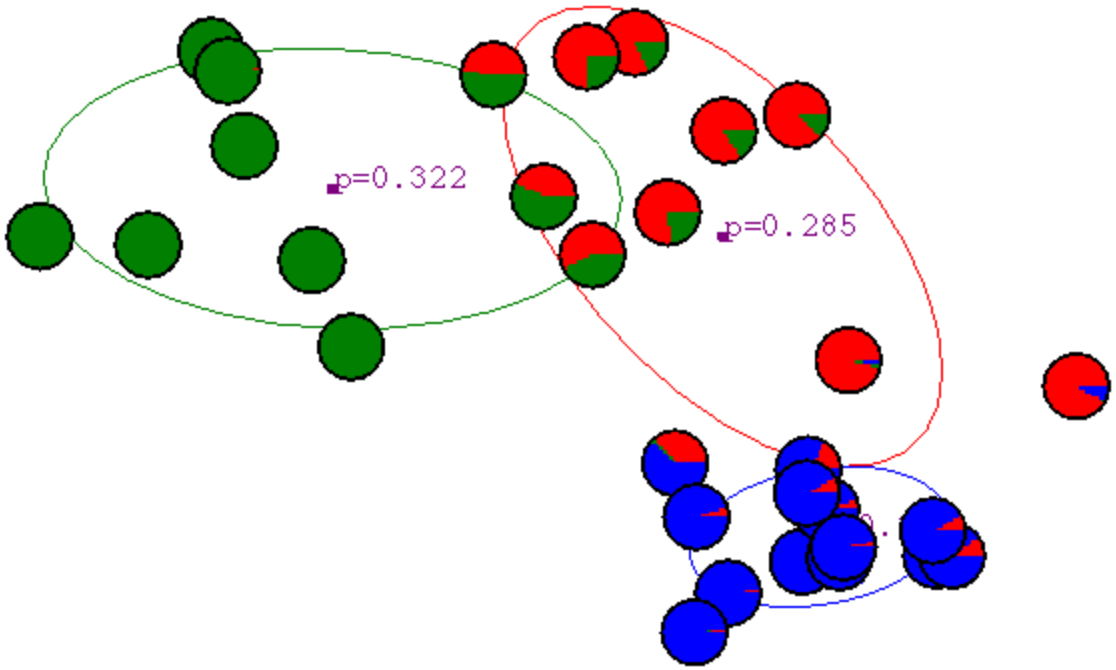
After 5th iteration



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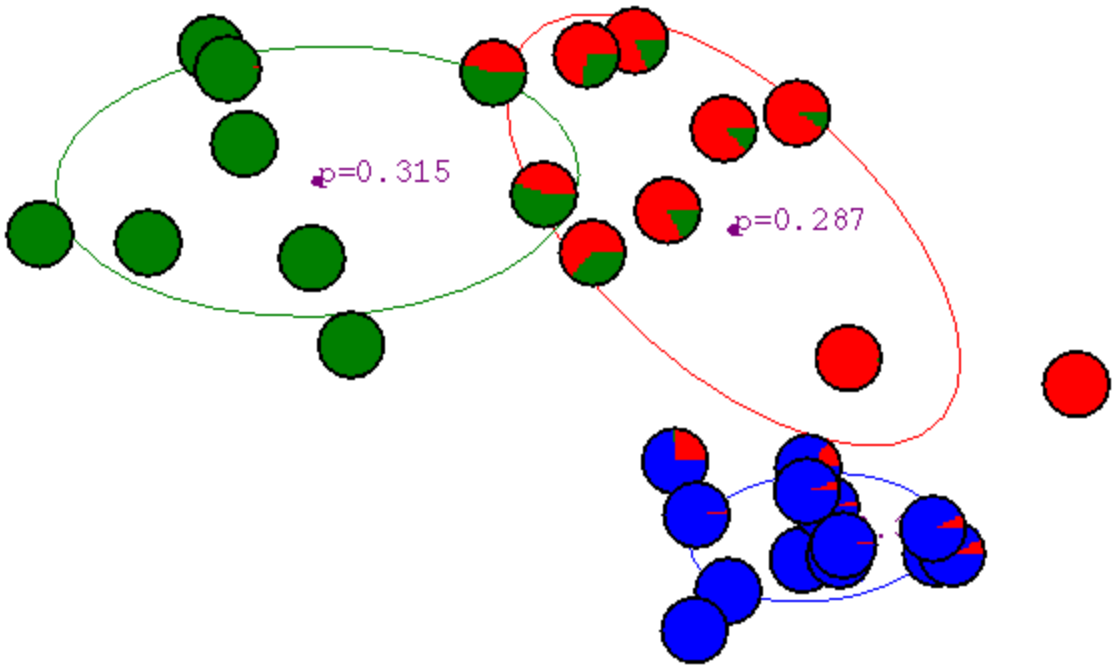
After 6th iteration



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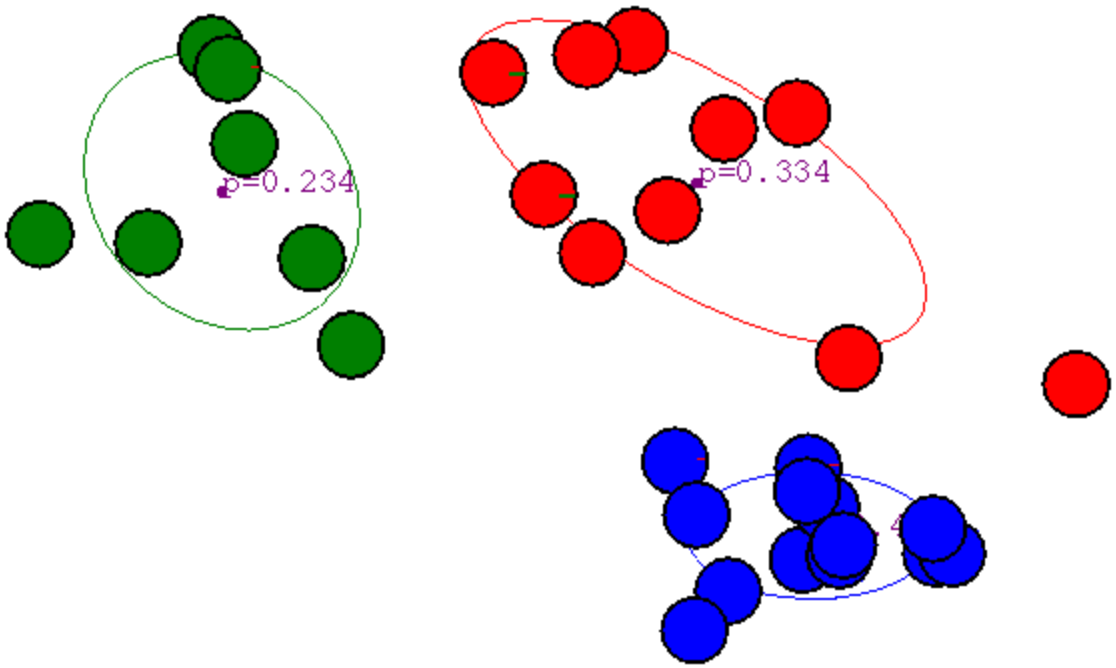
After 20th iteration



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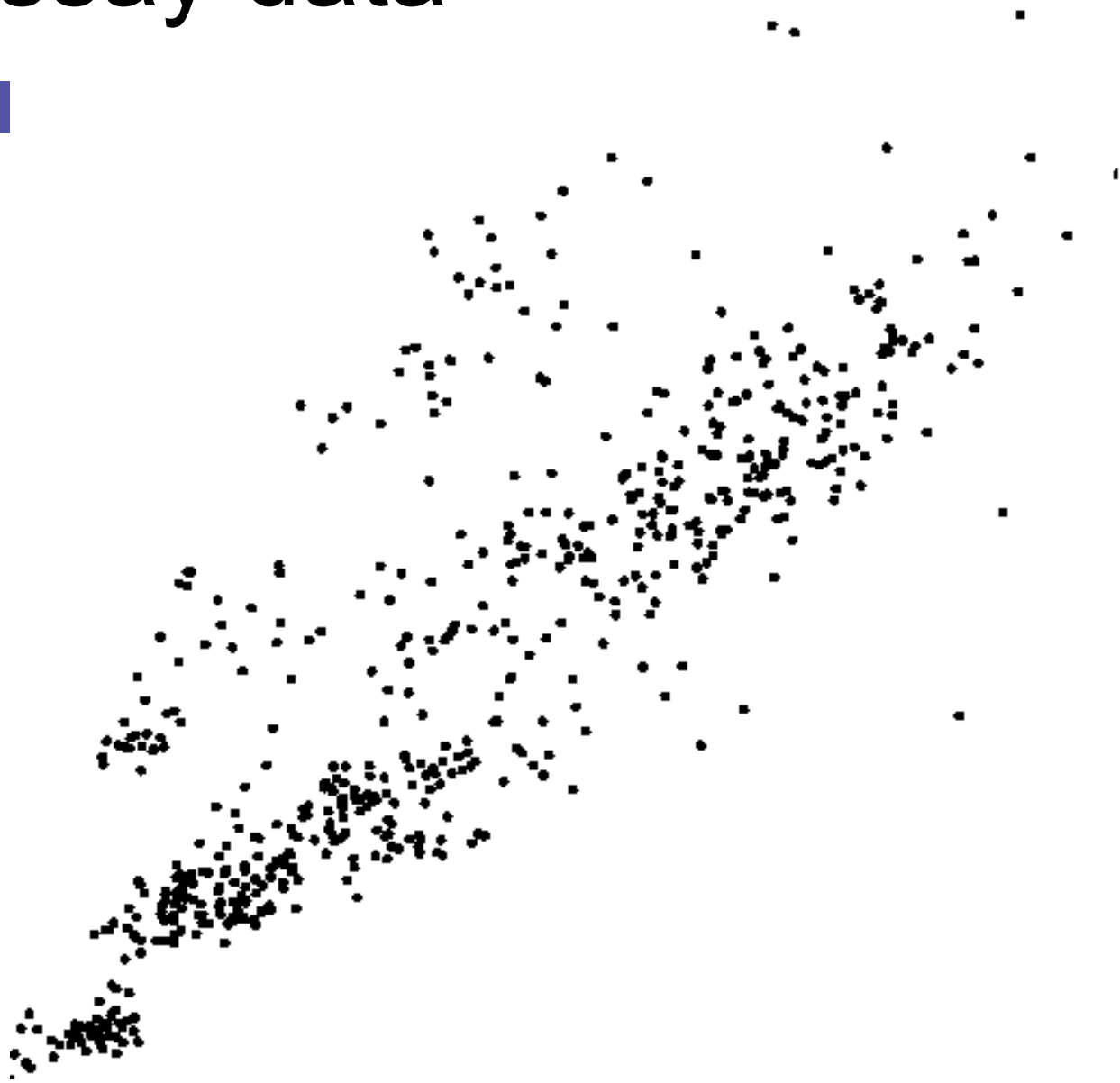
Some Bio Assay data



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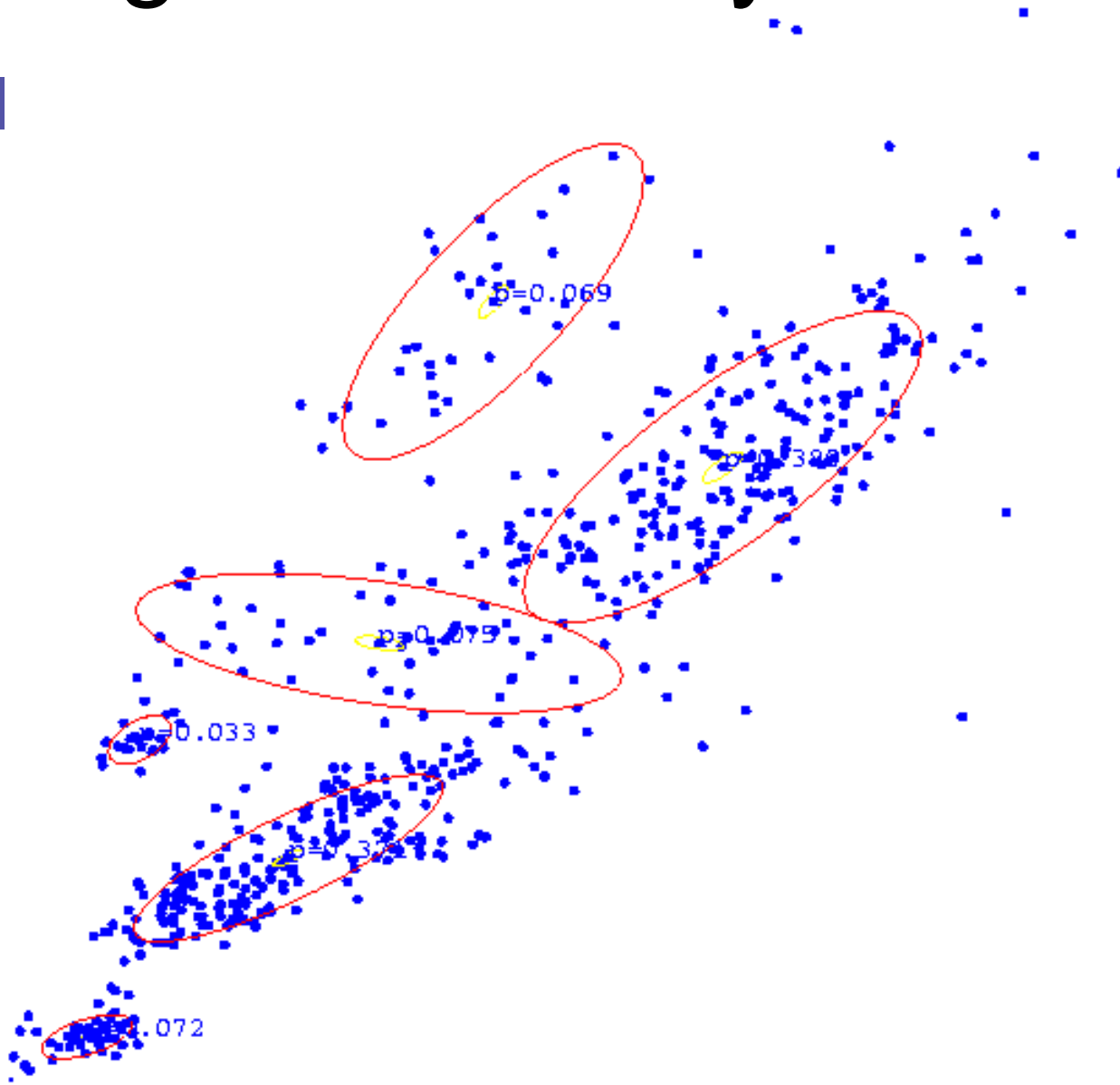
GMM clustering of the assay data



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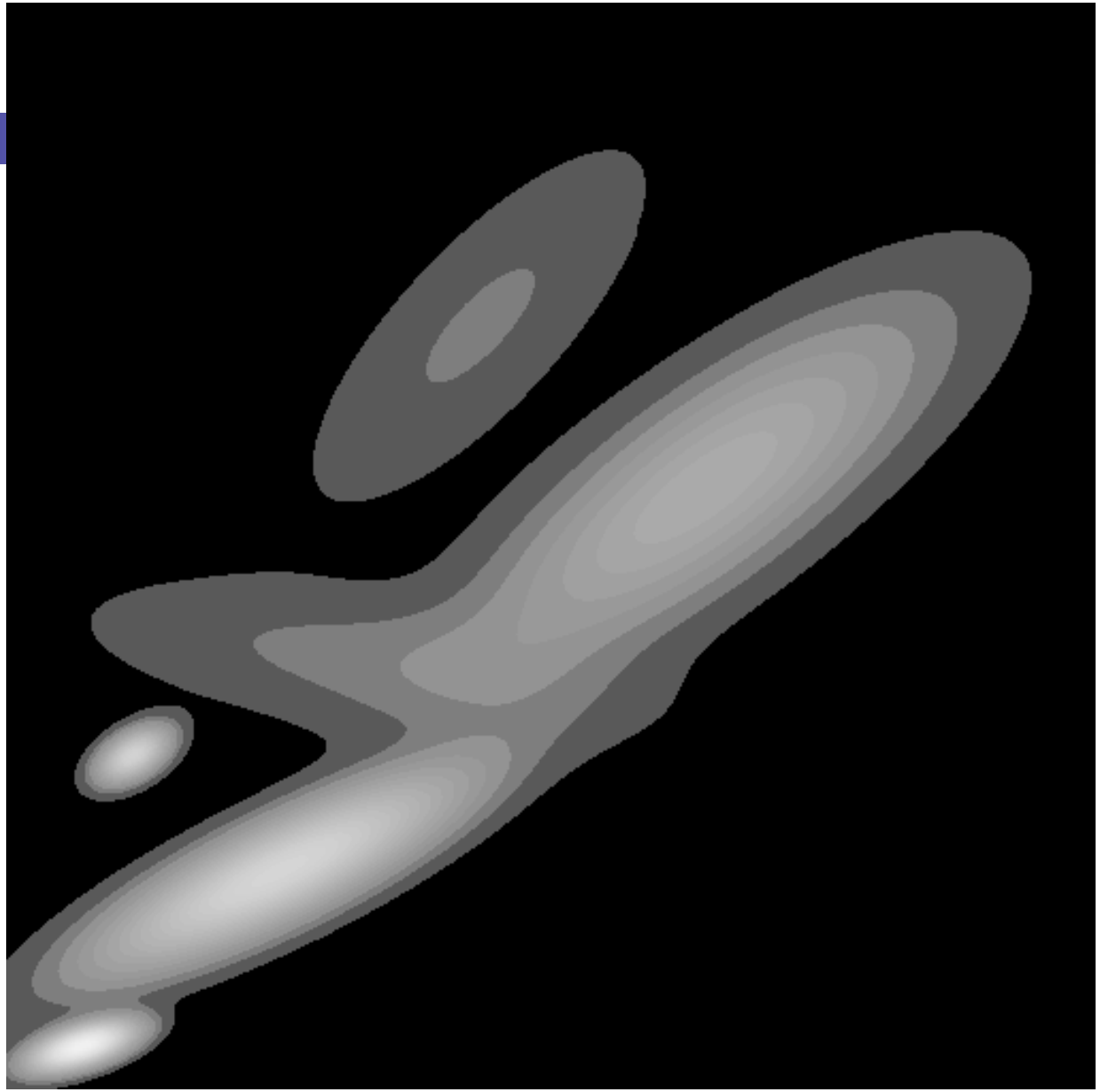
Resulting Density Estimator



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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 jth step, compute

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

   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

$\mathbf{\Delta}$ is unobserved data

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

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Density Estimation

Machine Learning – CSE546

Kevin Jamieson
University of Washington

November 13, 2016

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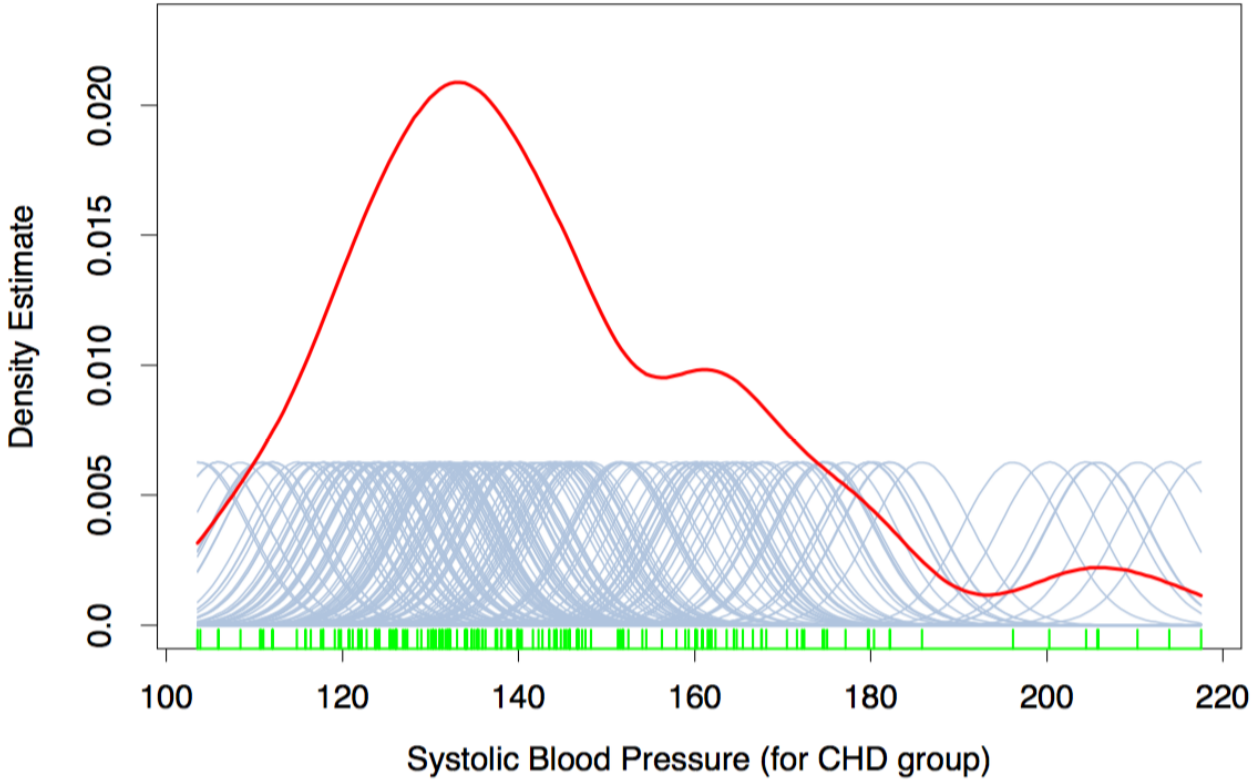
Kernel Density Estimation



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

A very “lazy” GMM

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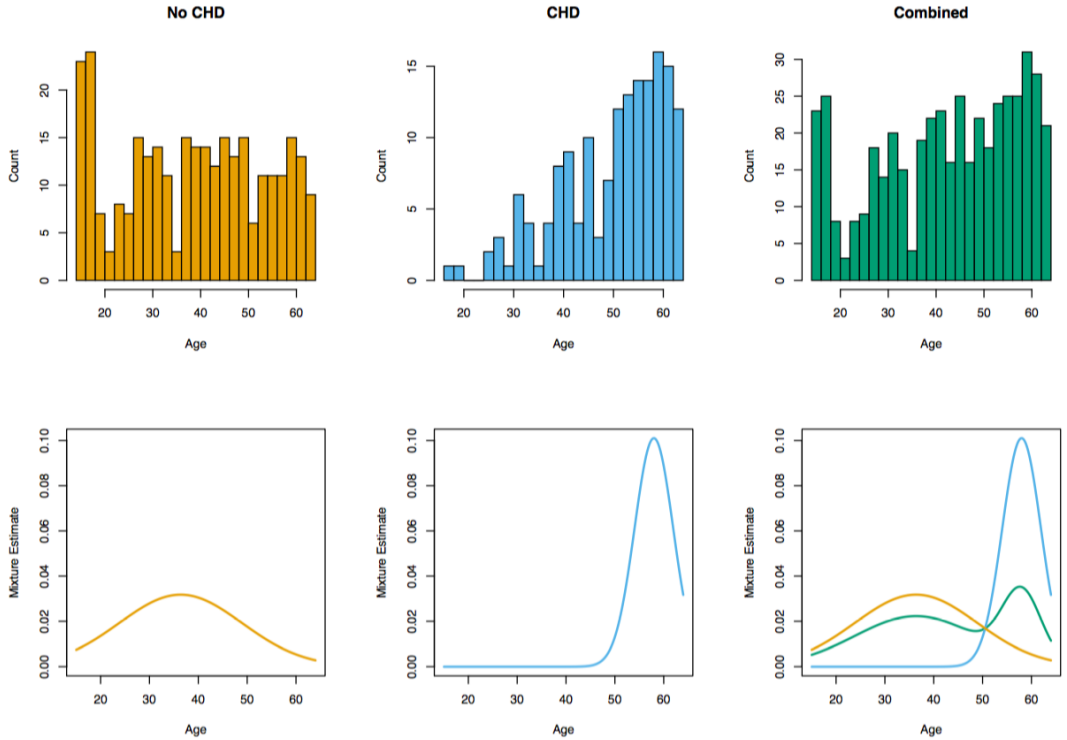
Kernel Density Estimation



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

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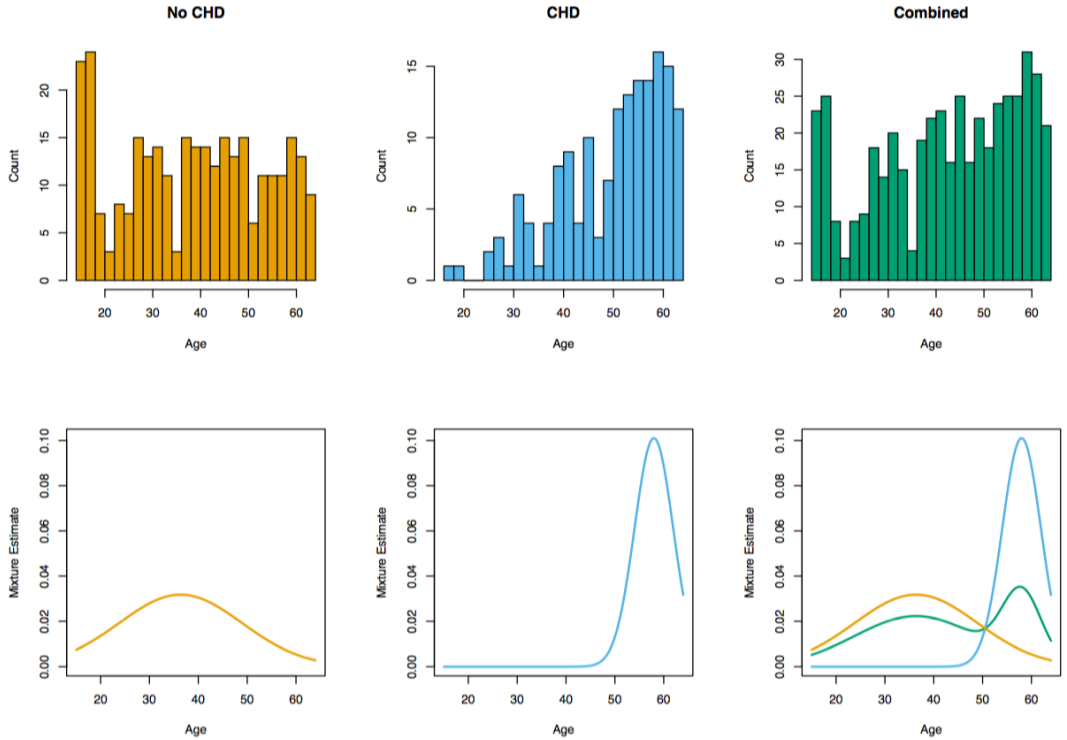
Kernel Density Estimation



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 $\arg\max_m \widehat{r}_{im}$

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Generative vs Discriminative

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