Unsupervised Learning
Clustering

Jun Zhu
dcszj@mail.tsinghua.edu.cn
http://bigml.cs.tsinghua.edu.cn/~jun
State Key Lab of Intelligent Technology & Systems
Tsinghua University

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Unsupervised Learning

- Task: learn an explanatory function $f(x), \; x \in \mathcal{X}$
- Aka "Learning without a teacher"

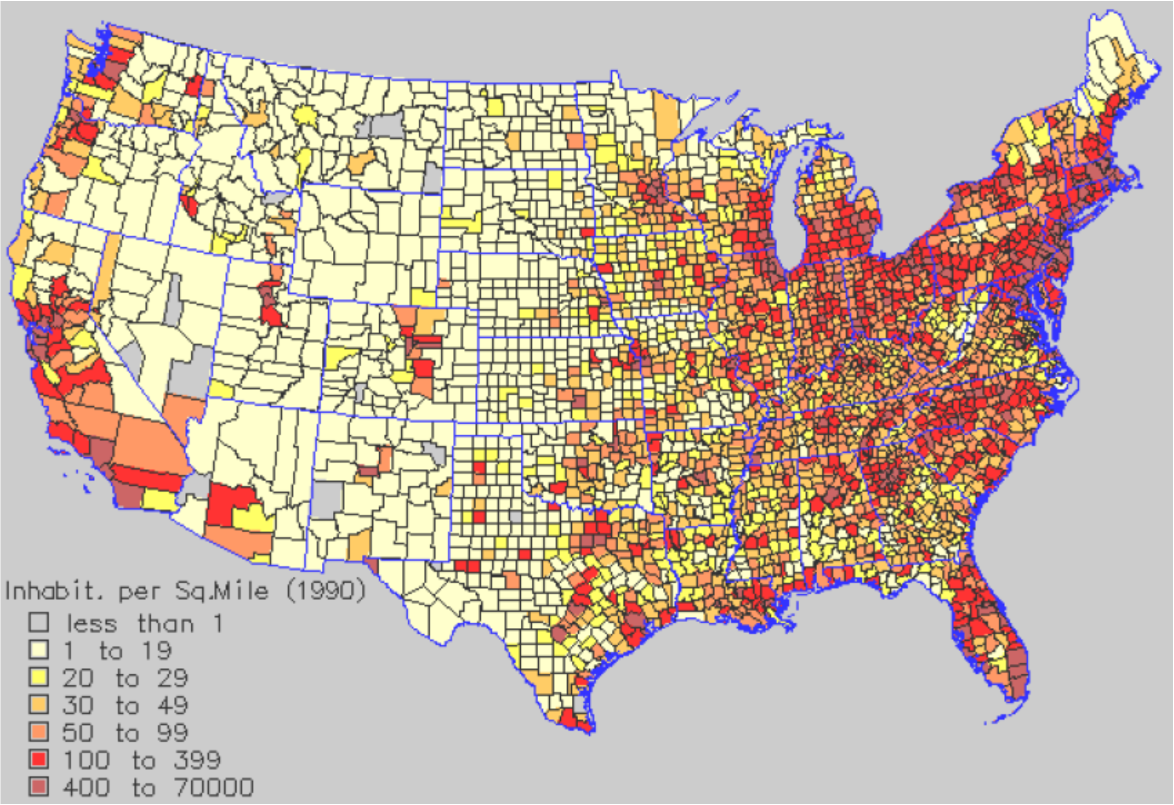
Feature space $\mathcal{X}$

Words in documents

Word distribution
(probability of a word)

- No training/test split

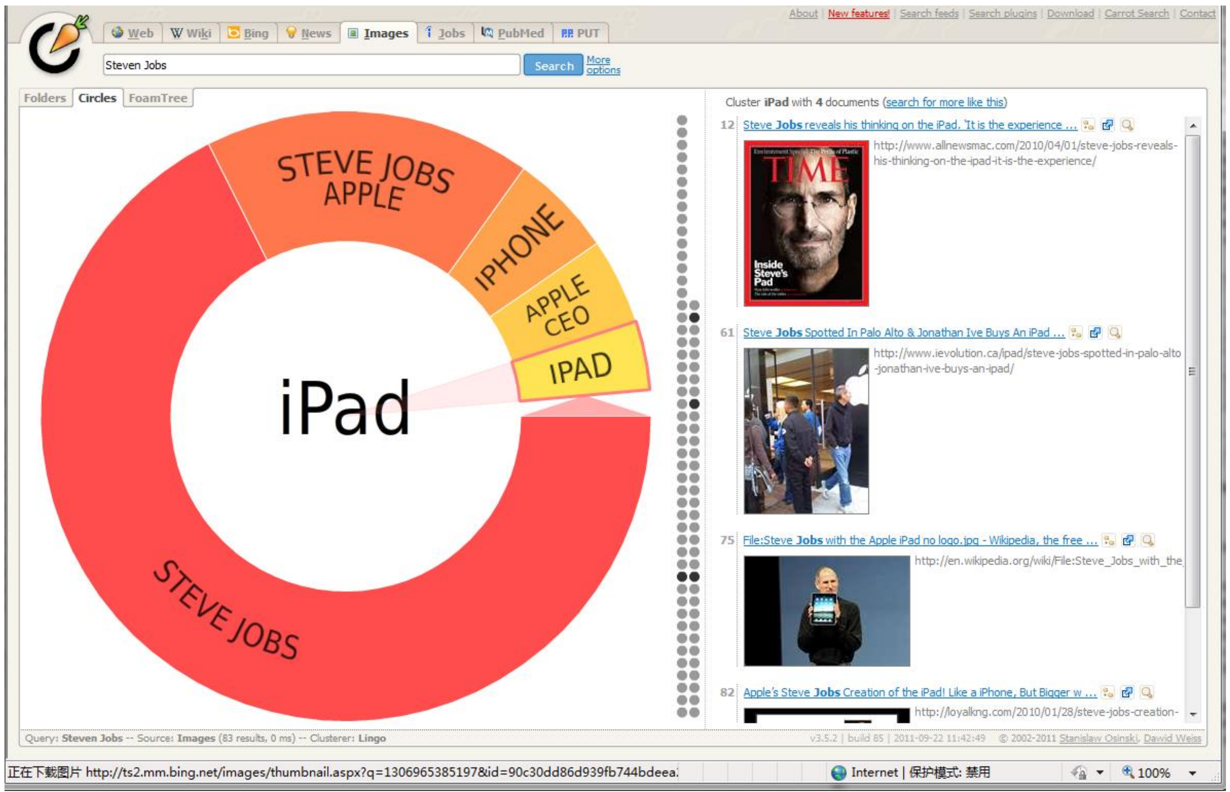
Unsupervised Learning – density estimation



Feature space $\mathcal{X}$
geographical information of a location

Density function
$f(x), \;\; x \in \mathcal{X}$

Unsupervised Learning – clustering



http://search.carrot2.org/stable/search

Feature space $\mathcal{X}$

Attributes (e.g., pixels & text) of images

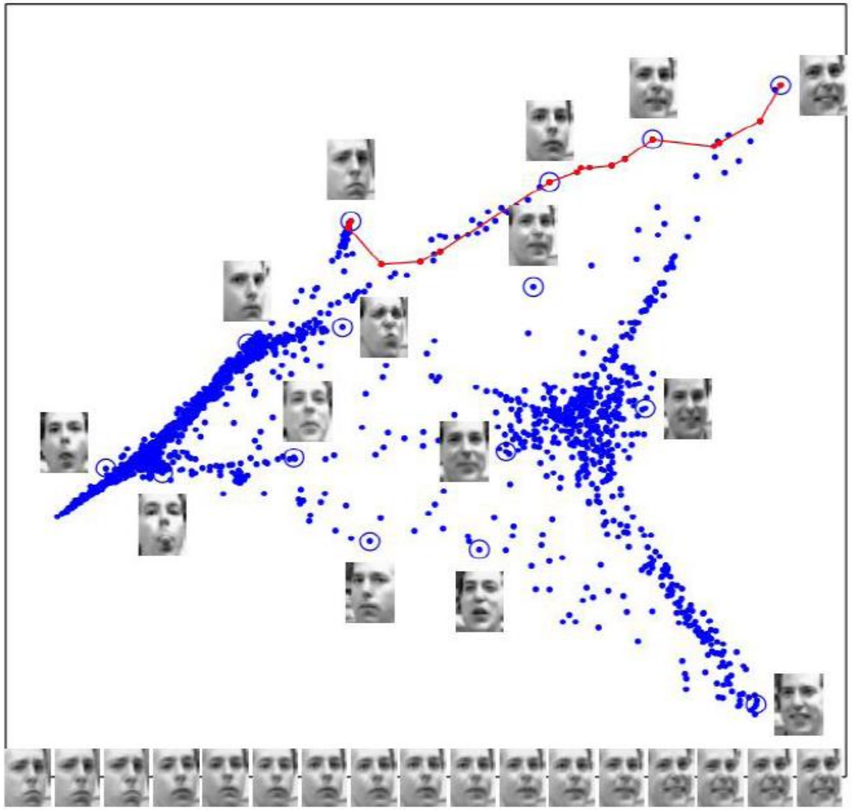
Cluster assignment function

$f(x), \ x \in \mathcal{X}$

Unsupervised Learning – dimensionality reduction

Images have thousands or millions of pixels

Can we give each image a coordinate, such that similar images are near each other ?



Feature space $\mathcal{X}$
pixels of images

Coordinate function in 2D space

$$f(x), \ x \in \mathcal{X}$$

Clustering
(K-*Means*, Gaussian *Mixtures*)

What is clustering?

- Clustering: the process of grouping a set of objects into classes of similar objects
  - High intra-class similarity
  - Low inter-class similarity

- A common and important task that finds many applications in science, engineering, information science, etc
  - Group genes that perform the same function
  - Group individuals that has similar political view
  - Categorize documents of similar topics
  - Identify similar objects from pictures
  - …

The clustering problem

- **Input**: training data $D = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$, where $\mathbf{x} \in \mathbb{R}^d$, integer K clusters
- **Output**: a set of clusters $C_1, \ldots, C_K$

Machine learning

From Wikipedia, the free encyclopedia

For the journal, see Machine Learning (journal).

See also: Pattern recognition

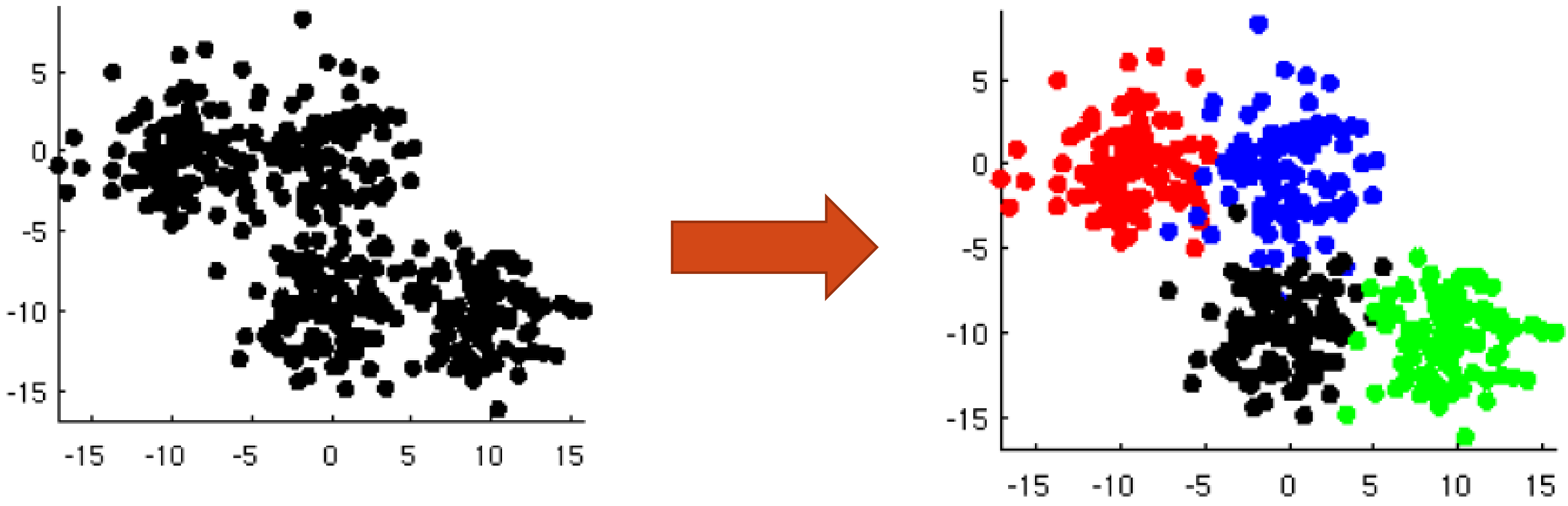
Machine learning is a scientific discipline that explores the construction and study of algorithms that can learn from data.[1] Such algorithms operate by building a model from example inputs and using that to make predictions or decisions,[2]:2 rather than following strictly static program instructions. Machine learning is closely related to and often overlaps with computational statistics; a discipline which also specializes in prediction-making.

$$\left\{\begin{array}{c} 4 \\ 4 \\ \vdots \\ 0 \\ \vdots \\ 1 \end{array}\right\} \qquad \left\{\begin{array}{c} \text{machine} \\ \text{learning} \\ \vdots \\ \text{JMLR} \\ \vdots \\ \text{prediction} \end{array}\right\}$$

Word Vector Space **Vocabulary**

The clustering problem

- **Input**: training data $D = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$, where $\mathbf{x} \in \mathbb{R}^d$, integer K clusters
- **Output**: a set of clusters $C_1, \ldots, C_K$

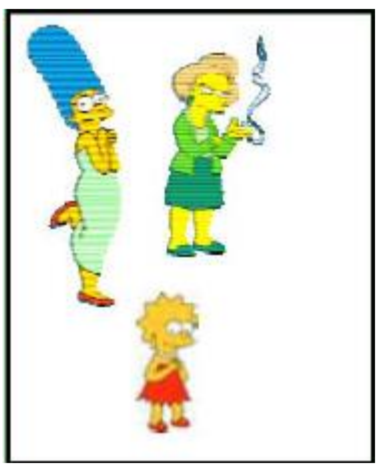


Issues for clustering

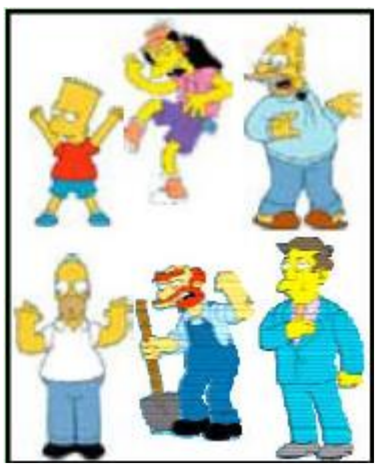
- What is a natural grouping among these objects?
  - Definition of "groupness"
- What makes objects "related"?
  - Definition of "similarity/distance"
- Representation for objects
  - Vector space? Normalization?
- How many clusters?
  - Fixed a priori?
  - Completely data driven?
- Clustering algorithms
  - Partitional algorithms
  - Hierarchical algorithms
- Formal foundation and convergence

What is a natural grouping among objects?

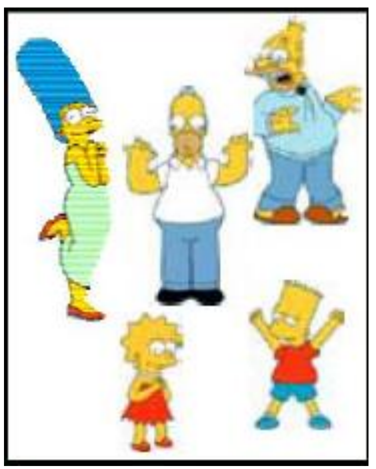
Clustering is subjective



Females



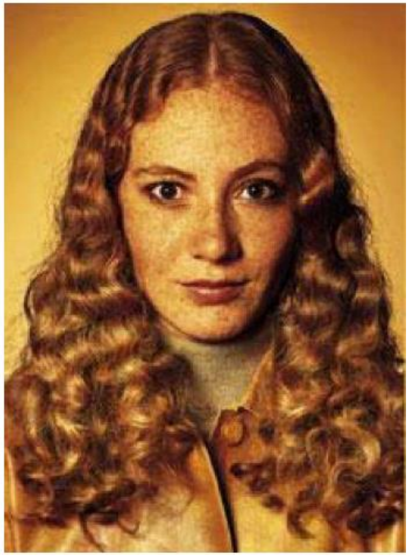
Males



Simpson's Family

School Employees

What is similarity?



- The real meaning of similarity is a philosophical question.
- Depends on representation and algorithm. For many rep./alg., easier to think in terms of distance between vectors

Desirable distance measure properties

- $d(A,B) = d(B,A)$ Symmetry
  - Otherwise you could claim "Alex looks like Bob, but Bob looks nothing like Alex"
- $d(A,A) = 0$ Constancy of Self-Similarity
  - Otherwise you could claim "Alex looks more like Bob, than Bob does"
- $d(A,B) = 0$ iff $A=B$ Positivity Separation
  - Otherwise there are objects that are different, but you can't tell apart
- $d(A,B) \leq d(A,C)+d(B,C)$ Triangular Inequality
  - Otherwise you could claim "Alex is very like Bob, and Alex is very like Carl, but Bob is very unlike Carl"

Minkowski Distance

$$dist(\mathbf{x},\mathbf{y}) = \sqrt[r]{\sum_{i=1}^{d} |x_i - y_i|^r}$$

- Common Minkowski distances
  - Euclidean distance (r=2):

$$dist(\mathbf{x},\mathbf{y}) = \sqrt{\sum_{k=1}^{d} (x_k - y_k)^2} = \|\mathbf{x}-\mathbf{y}\|_2$$

  - Manhattan distance (r=1):

$$dist(\mathbf{x},\mathbf{y}) = \sum_{k=1}^{d} |x_k - y_k| = \|\mathbf{x}-\mathbf{y}\|_1$$

  - "Sup" distance ($r = \infty$):

$$dist(\mathbf{x},\mathbf{y}) = \sup_{k=1}^{d} |x_k - y_k| = \|\mathbf{x}-\mathbf{y}\|_\infty$$

Hamming distance

- Manhattan distance is called Hamming distance when all features are binary

  - E.g., gene expression levels under 17 conditions (1-high; 0-low)

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
GeneA	0	1	1	0	0	1	0	0	1	0	0	1	1	1	0	0	1
GeneB	0	1	1	1	0	0	0	0	1	1	1	1	1	1	0	1	1

  - Hamming distance: $\#(0\ 1) + \#(1\ 0) = 4 + 1 = 5$

Correlation coefficient

- Pearson correlation coefficient

$$s(\mathbf{x}, \mathbf{y}) = \frac{(\mathbf{x} - \bar{x}\mathbf{1})^\top (\mathbf{y} - \bar{y}\mathbf{1})}{\|\mathbf{x} - \bar{x}\mathbf{1}\|_2 \|\mathbf{y} - \bar{y}\mathbf{1}\|_2}$$

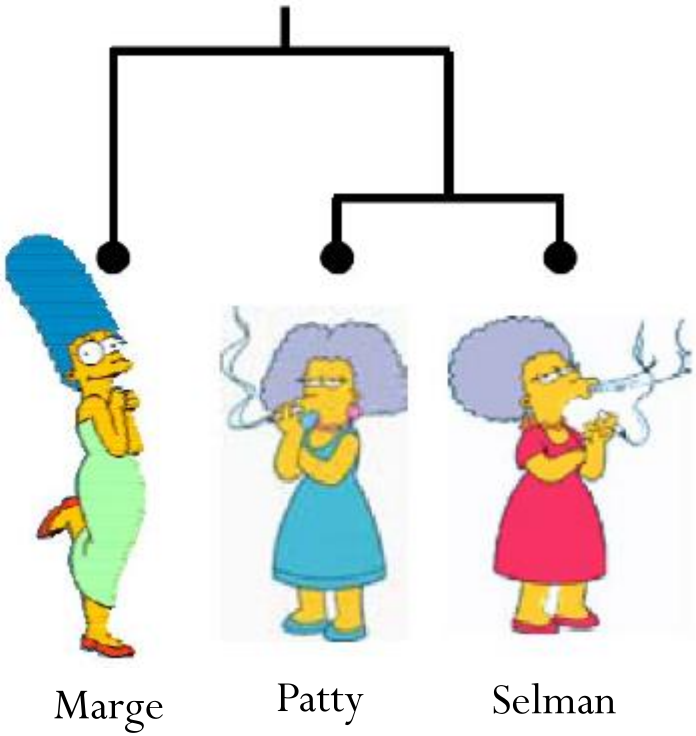
$$\text{where } \bar{x} = \frac{1}{d}\sum_i x_i, \;\; \bar{y} = \frac{1}{d}\sum_i y_i$$

  - Cosine Similarity:

$$\cos(\mathbf{x}, \mathbf{y}) = \frac{\mathbf{x}^\top \mathbf{y}}{\|\mathbf{x}\|_2 \|\mathbf{y}\|_2}$$

Edit Distance

- To measure the similarity between two objects, transform one into the other, and measure how much effort it took. The measure of effort becomes the distance measure



The distance between Patty and Selma.

Change dress color, 1 point
Change earring shape, 1 point
Change hair part, 1 point

D(Patty,Selma) = 3

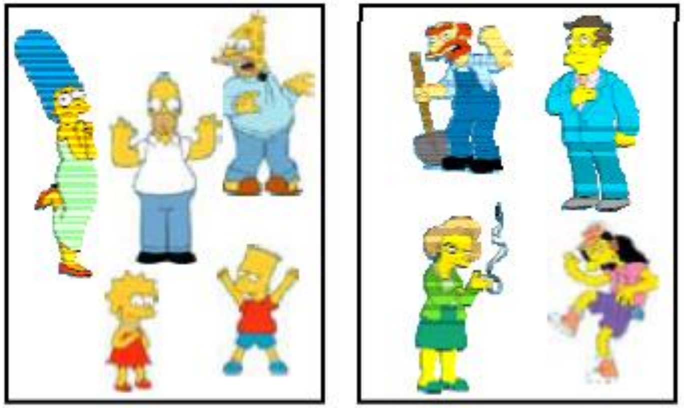
The distance between Marge and Selma

Change dress color, 1 point
Add earrings, 1 point
Decrease height, 1 point
Take up smoking, 1 point
Loss weight, 1 point

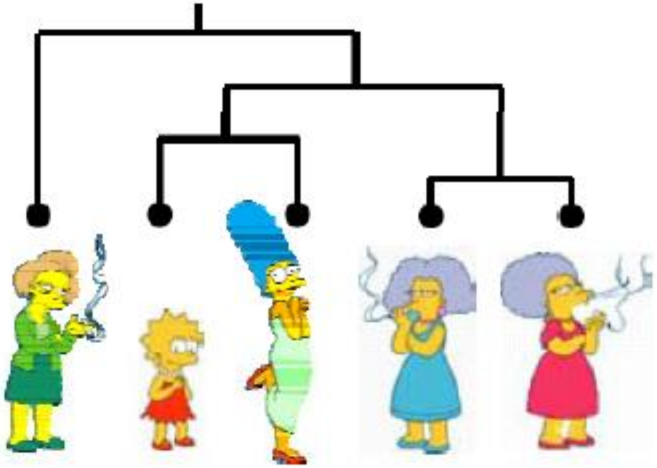
D(Marge, Selma) = 5

Clustering algorithms

- Partitional algorithms
  - Usually start with a random (partial) partitioning
  - Refine it iteratively
    - K-means
    - Mixture-Model based clustering

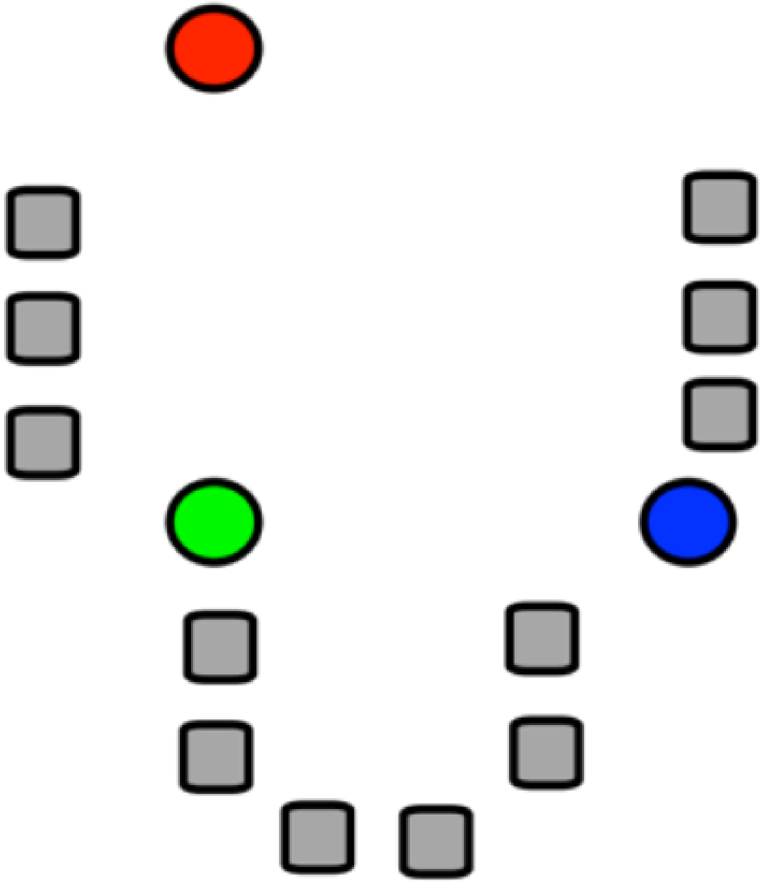


- Hierarchical algorithms
  - Bottom-up, agglomerative
  - Top-down, divisive



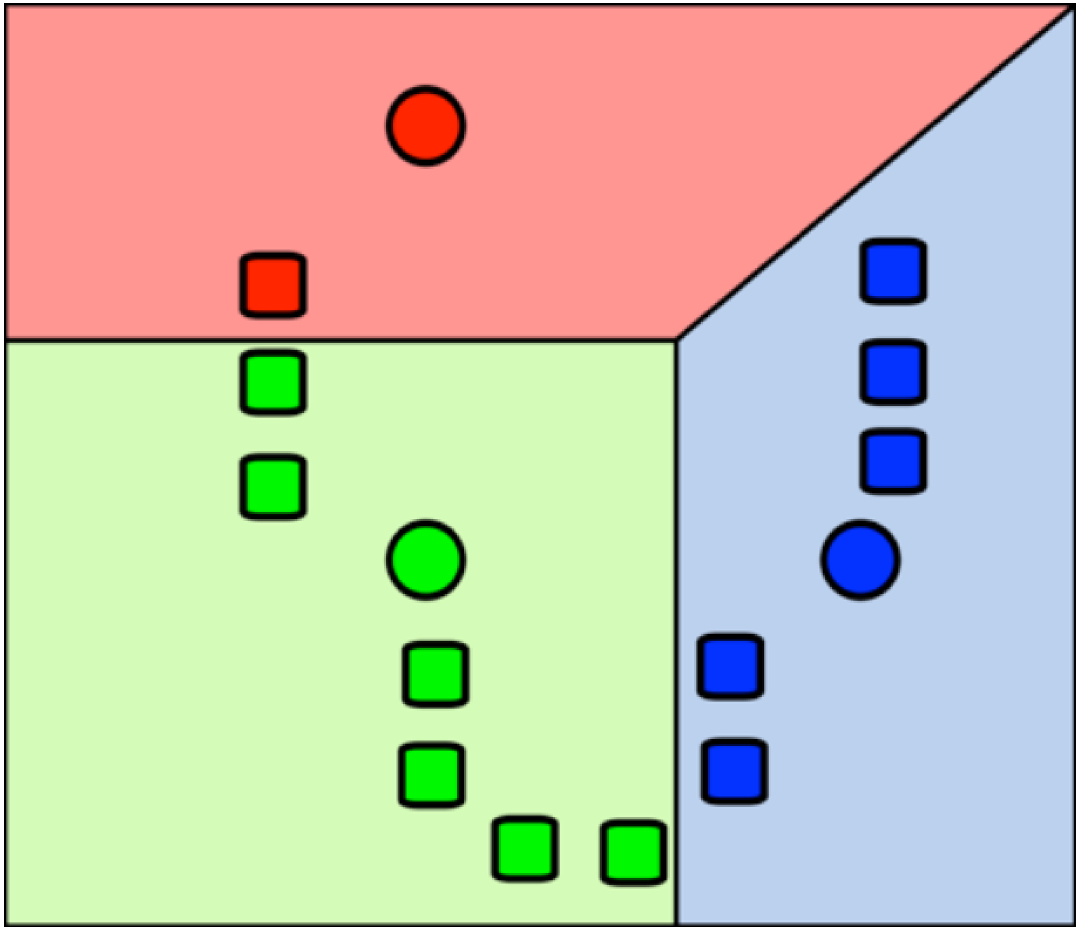
K-means Algorithm

- 1. Initialize the centroids $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K$



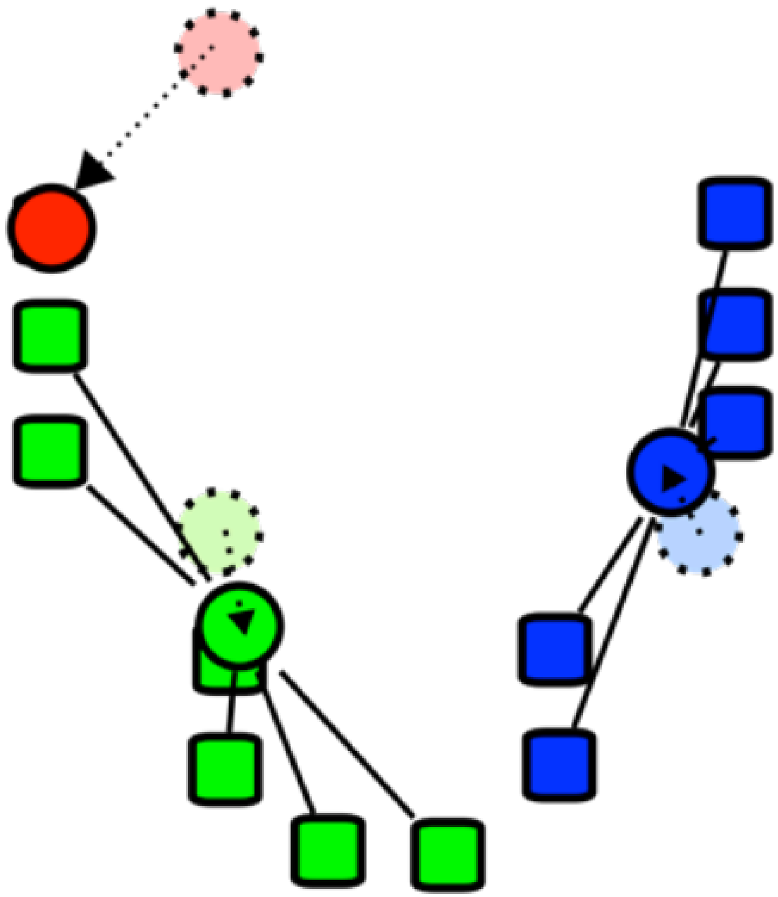
K-means Algorithm

- 2. for each k, $C_k = \{i, \text{ s.t. } \mathbf{x}_i \text{ is closest to } \boldsymbol{\mu}_k\}$



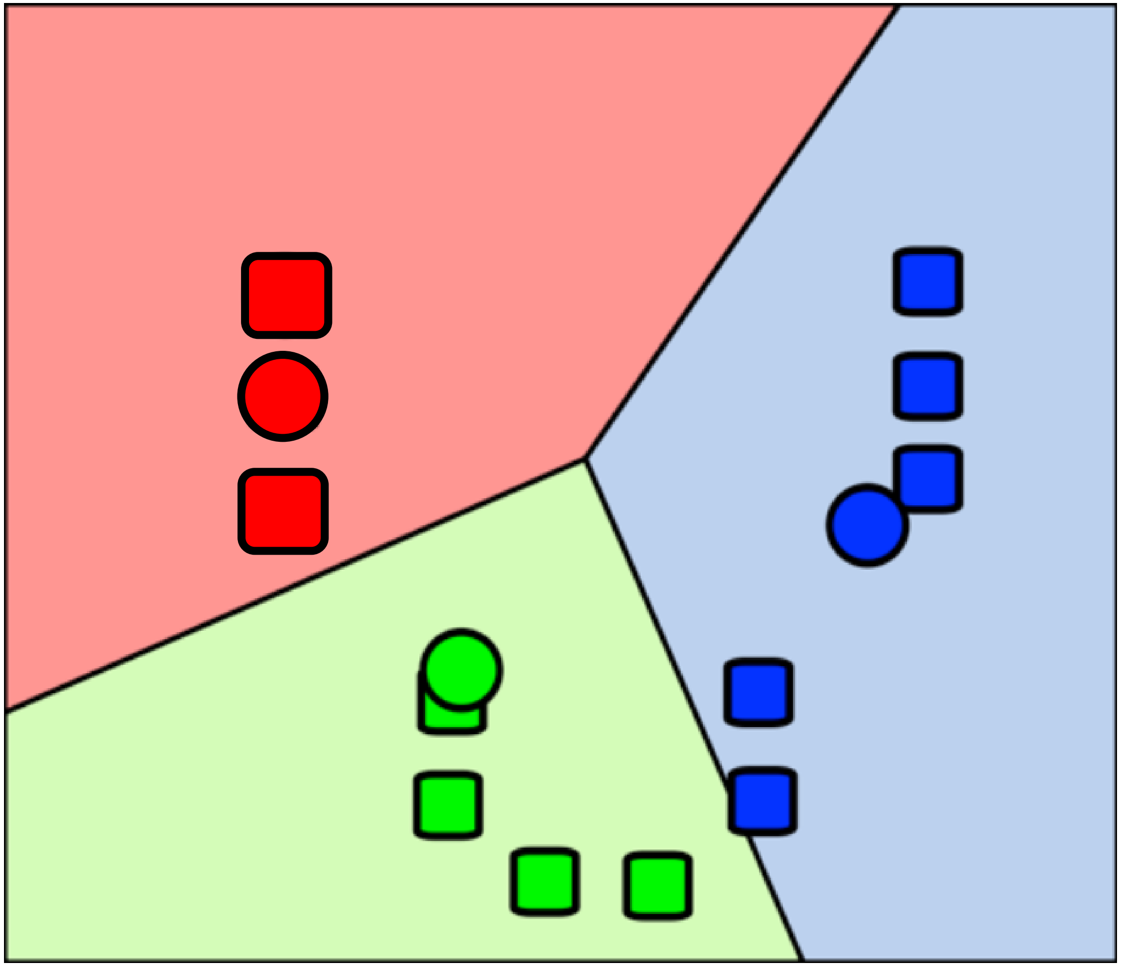
K-means Algorithm

- 3. for each k, $\boldsymbol{\mu}_k \leftarrow \frac{1}{|C_k|} \sum_{j \in C_k} \mathbf{x}_j$ (sample mean)



K-means Algorithm

- Repeat until no further change in cluster assignment



Summary of K-means Algorithm

- 1. Initialize centroids $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K$
- 2. Repeat until no change of cluster assignment
  - (1) for each *k*:

$$C_k = \{i, \text{ s.t. } \mathbf{x}_i \text{ is closest to } \boldsymbol{\mu}_k\}$$

  - (2) for each *k*:

$$\boldsymbol{\mu}_k \leftarrow \frac{1}{|C_k|} \sum_{j \in C_k} \mathbf{x}_j$$

- **Note**: each iteration requires $O(NK)$ operations

K-means Questions

- What is it trying to optimize?
- Are we sure it will terminate?
- Are we sure it will find an optimal clustering?
- How should we start it?
- How could we automatically choose the number of centers?

Theory: K-Means as an Opt. Problem

- The opt. problem

$$\min_{\{C_k\}_{k=1}^{K}} \quad \sum_{k=1}^{K} \sum_{\mathbf{x} \in C_k} \|\mathbf{x} - \boldsymbol{\mu}_k\|_2^2$$

$$\text{s.t}: \quad \boldsymbol{\mu}_k = \frac{1}{|C_k|} \sum_{\mathbf{x} \in C_k} \mathbf{x}$$

- **Theorem**: *K-means iteratively leads to a non-increasing of the objective, until local minimum is achieved*
  - *Proof ideas:*
    - *Each operation leads to non-increasing of the objective*
    - *The objective is bounded and the number of clusters is finite*

K-means as gradient descent

- Find K prototypes to minimize the ***quantization error*** (i.e., the average distance between a data to its closest prototype):

$$\min_{\{\boldsymbol{\mu}_c\}_{c=1}^{K}} \quad \sum_{i=1}^{N} \min_k \|\mathbf{x}_i - \boldsymbol{\mu}_k\|_2^2$$

  - First-order gradient descent applies
  - Newton method leads to the same update rule:

$$\boldsymbol{\mu}_k = \frac{1}{|C_k|} \sum_{\mathbf{x} \in C_k} \mathbf{x}$$

- *See [Bottou & Bengio, NIPS'95] for more details*

Trying to find a good optimum

- **Idea 1**: Be careful about where you start
- **Idea 2**: Do many runs of k-means, each from a different random start configuration
- Many other ideas floating around.

- **Note**: *K*-means is often used to initialize other clustering methods

Mixture of Gaussians and EM algorithm

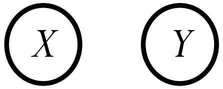
Basics of Probability & MLE

Basics of Probabilities

Independence

- Independent random variables:

$$P(X,Y) = P(X)P(Y)$$



$$P(X|Y) = P(X)$$

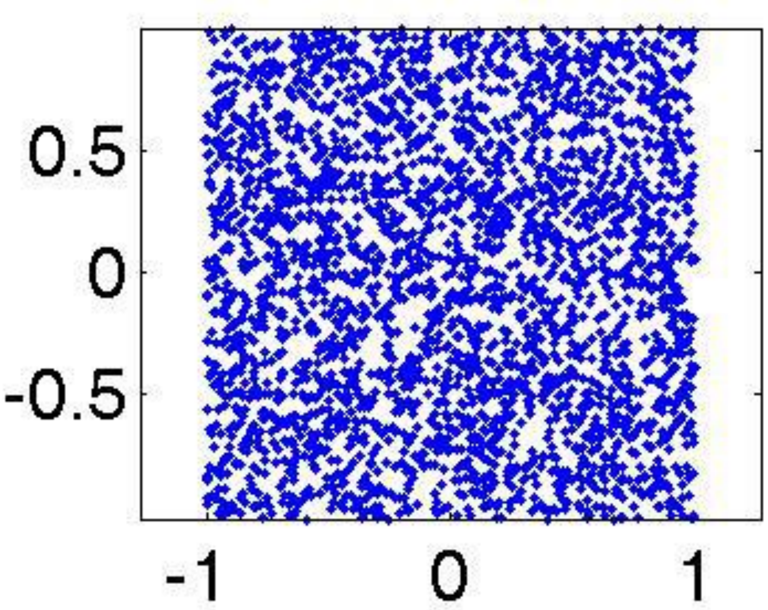
  - Y and X don't contain information about each other

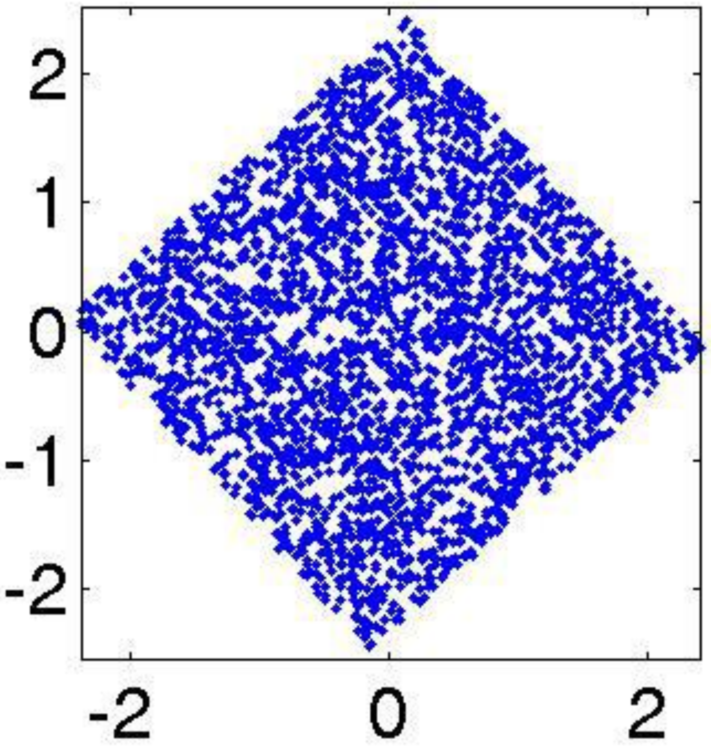
    Observing Y doesn't help predicting X

    Observing X doesn't help predicting Y

- Examples:
  - Independent:
    - winning on roulette this week and next week
  - Dependent:
    - Russian roulette

Dependent / Independent?



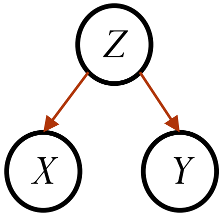


Conditional Independence

- Conditionally independent:

$$P(X, Y|Z) = P(X|Z)P(Y|Z)$$

  - knowing Z makes X and Y independent



- Examples:

London taxi drivers: A survey has pointed out a positive and significant correlation between the number of accidents and wearing coats. They concluded that coats could hinder movements of drivers and be the cause of accidents. A new law was prepared to prohibit drivers from wearing coats when driving.

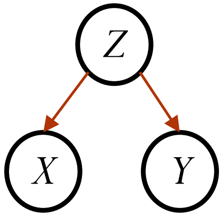
Finally another study pointed out that people wear coats when it rains…

Conditional Independence

- Conditionally independent:

$$P(X,Y|Z) = P(X|Z)P(Y|Z)$$

  - knowing Z makes X and Y independent



- Equivalent to:

$$\forall(x,y,z)\colon\ P(X=x|Y=y,Z=z) = P(X=x\ |Z=z)$$

  - E.g.:

$$P(Thunder\ |\ Rain, Lighting) = \mathrm{P}(Thunder\ |\ Lighting)$$

Maximum Likelihood Estimation (MLE)

Flipping a Coin

- What's the probability that a coin will fall with a head up (if flipped)?
- Let us flip it a few times to estimate the probability

The estimated probability is: 3/5 "frequency of heads"

Questions:

The estimated probability is: 3/5 "frequency of heads"

- Why frequency of heads?
- How good is this estimation?
- Why is this a machine learning problem?

Question (1)

- Why frequency of heads?
  - Frequency of heads is exactly the Maximum Likelihood Estimator for this problem

  - MLE has nice properties

    (interpretation, statistical guarantees, simple)

MLE for Bernoulli Distribution

Data, D =

$$D = \{X_i\}_{i=1}^{n}, \; X_i \in \{\text{H}, \text{T}\}$$

$$P(Head) = \theta \qquad P(Tail) = 1 - \theta$$

- Flips are i.i.d:
  - **Independent** events that are **identically distributed** according to Bernoulli distribution
- **MLE**: choose θ that maximizes the probability of observed data

Maximum Likelihood Estimation (MLE)

- MLE: choose θ that maximizes the probability of observed data

$$\hat{\theta}_{MLE} = \arg\max_{\theta} P(D|\theta)$$

$$= \arg\max_{\theta} \prod_{i=1}^{n} P(X_i|\theta)$$ Independent draws

$$= \arg\max_{\theta} \prod_{i:X_i=H} \theta \prod_{i:X_i=T} (1-\theta)$$ Identically distributed

$$= \arg\max_{\theta} \theta^{N_H} (1-\theta)^{N_T}$$

Maximum Likelihood Estimation (MLE)

- MLE: choose θ that maximizes the probability of observed data

$$\hat{\theta}_{MLE} = \arg\max_{\theta} P(D|\theta)$$
$$= \arg\max_{\theta} \theta^{N_H}(1-\theta)^{N_T}$$

- Solution?

$$\hat{\theta}_{MLE} = \frac{N_H}{N_H + N_T}$$

  - Exactly the "**Frequency of heads**"

Question (2)

- How good is the MLE estimation?

$$\hat{\theta}_{MLE} = \frac{N_H}{N_H + N_T}$$

  - Is it biased?

How many flips do I need?

- I flipped the coins 5 times: 3 heads, 2 tails

$$\hat{\theta}_{MLE} = \frac{3}{5}$$

- What if I flipped 30 heads and 20 tails?

$$\hat{\theta}_{MLE} = \frac{30}{50}$$

- Which estimator should we trust more?

A Simple Bound

- Let $\theta^\star$ be the true parameter. For n data points, and

$$\hat{\theta}_{MLE} = \frac{N_H}{N_H + N_T}$$

- Then, for any ε>0 , we have the Hoeffding's Inequality:

$$P(|\hat{\theta} - \theta^\star| \geq \epsilon) \leq 2e^{-2n\epsilon^2}$$

Probably Approximately Correct (PAC) Learning

- I want to know the coin parameter θ, within ε=0.1 error with probability at least 1-δ (e.g., 0.95)
- How many flips do I need?

$$P(|\hat{\theta} - \theta^{\star}| \geq \epsilon) \leq 2e^{-2n\epsilon^2} \leq \delta$$

- Sample complexity:

$$n \geq \frac{\ln(2/\delta)}{2\epsilon^2}$$

Question (3)

- Why is this a machine learning problem?
  - Improve their performance (accuracy of the estimated prob.)
  - At some task (estimating the probability of heads)
  - With experience (the more coin flips the better we are)

How about continuous features?

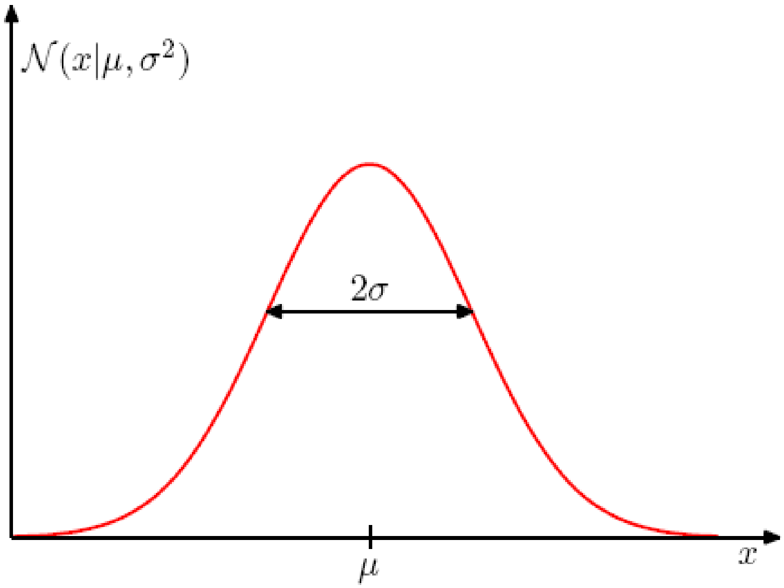
Gaussian Distributions

Carl F. Gauss (1777 – 1855)

- Univariate Gaussian distribution

$$p(x|\mu,\sigma^2) = \frac{1}{\sqrt{2\pi}\sigma}\exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

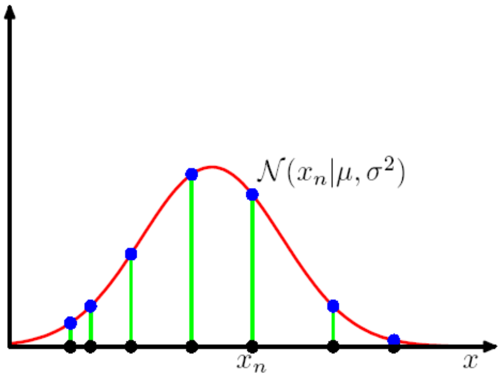
- Given parameters, we can draw samples and plot distributions



Maximum Likelihood Estimation

- Given a data set $\mathcal{D} = \{x_1, \ldots, x_N\}$, the likelihood is

$$p(\mathcal{D}|\mu, \sigma^2) = \prod_{n=1}^{N} p(x_n|\mu, \sigma^2)$$



- MLE estimates the parameters as

$$(\mu_{\mathrm{ML}}, \sigma^2_{\mathrm{ML}}) = \operatorname*{argmax}_{\mu, \sigma^2} \log p(\mathcal{D}|\mu, \sigma^2)$$

$$\mu_{\mathrm{ML}} = \frac{1}{N} \sum_{n=1}^{N} x_n$$ sample mean

$$\sigma^2_{\mathrm{ML}} = \frac{1}{N} \sum_{n=1}^{N} (x_n - \mu_{\mathrm{ML}})^2$$ sample variance

Note: MLE for the variance of a Gaussian is biased

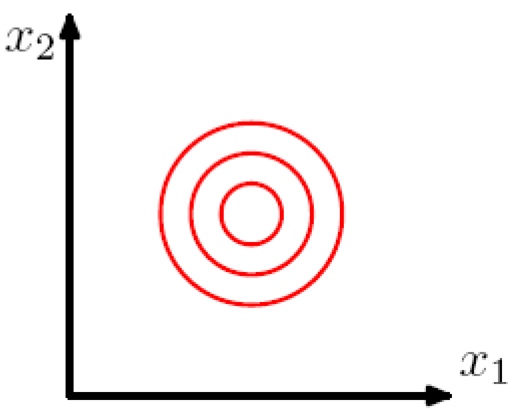
Gaussian Distributions

Carl F. Gauss (1777 – 1855)

- *d*-dimensional multivariate Gaussian

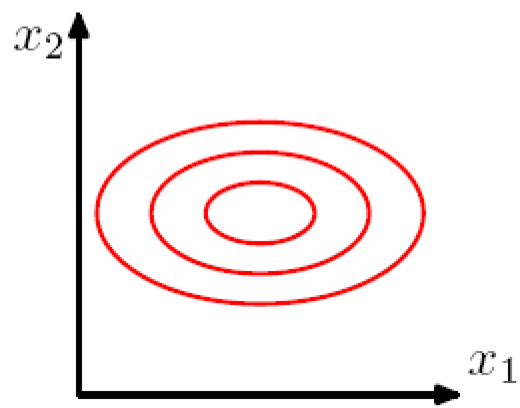
$$p(\mathbf{x}|\mu,\Sigma) = \frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \exp\Big(-\frac{1}{2}(\mathbf{x}-\mu)\Sigma^{-1}(\mathbf{x}-\boldsymbol{\mu})\Big)$$

- Given parameters, we can draw samples and plot distributions



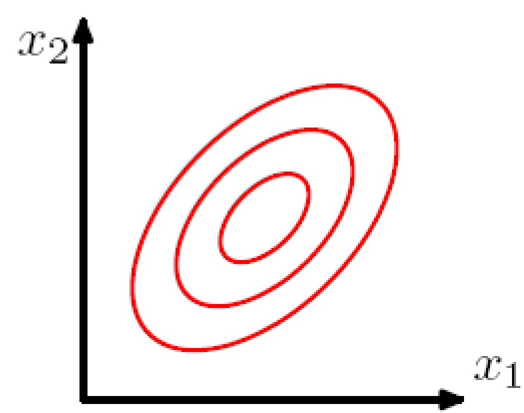
Isotropic

$$\Sigma = \sigma^2 \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$



Diagonal

$$\Sigma = \begin{bmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{bmatrix}$$



General

$$\Sigma = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}$$

Maximum Likelihood Estimation

- Given a data set $\mathcal{D} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$, the likelihood is

$$p(\mathcal{D}|\mu, \Sigma) = \prod_{n=1}^{N} p(\mathbf{x}_n|\mu, \Sigma)$$

- MLE estimates the parameters as

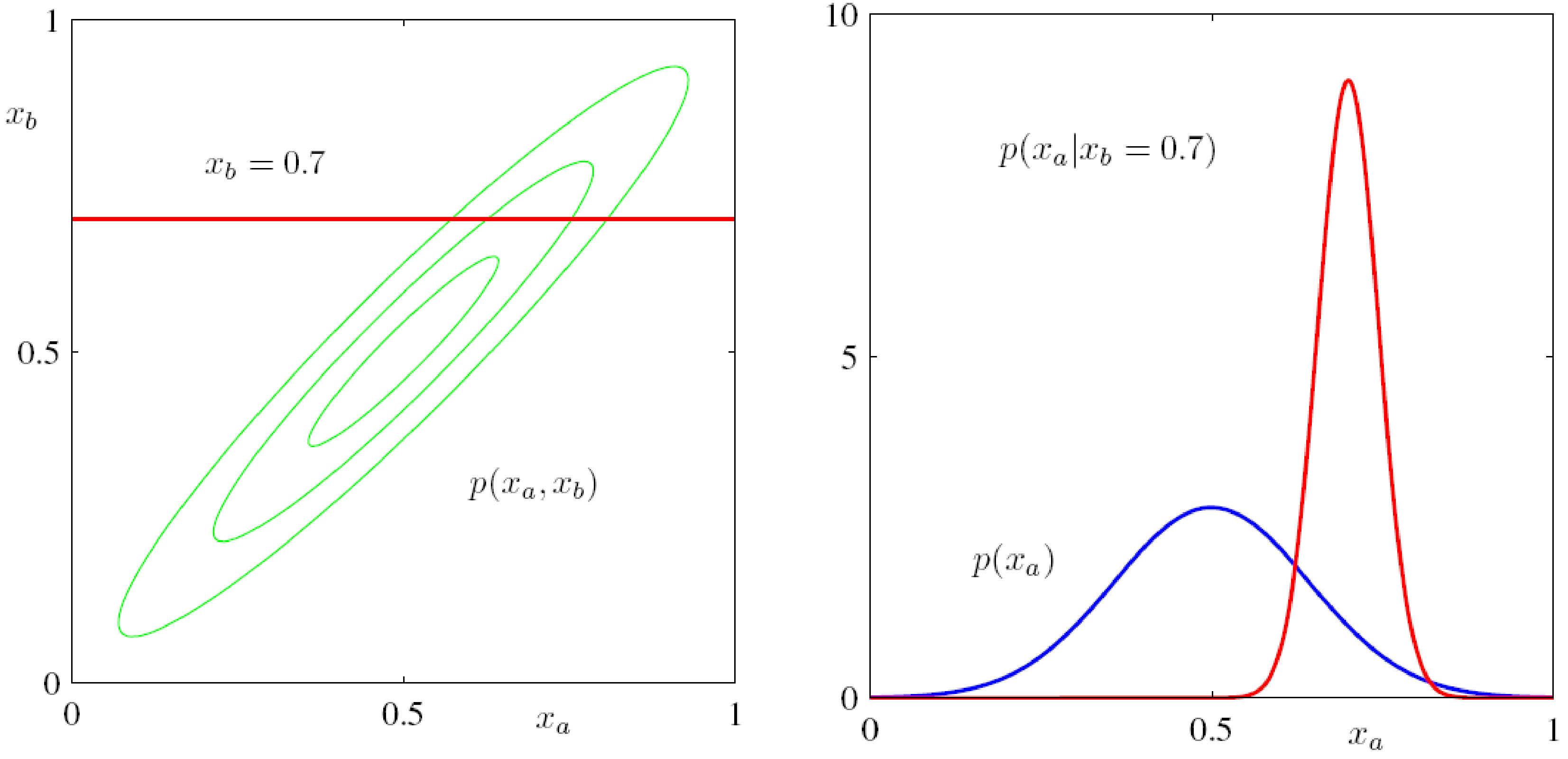
$$(\mu_{\mathrm{ML}}, \Sigma_{\mathrm{ML}}) = \underset{\mu, \Sigma}{\operatorname{argmax}} \log p(\mathcal{D}|\mu, \Sigma)$$

$$\mu_{\mathrm{ML}} = \frac{1}{N} \sum_{n=1}^{N} \mathbf{x}_n$$ sample mean

$$\Sigma_{\mathrm{ML}}^2 = \frac{1}{N} \sum_{n=1}^{N} (x_n - \mu_{\mathrm{ML}})(x_n - \mu_{\mathrm{ML}})^\top$$ sample covariance

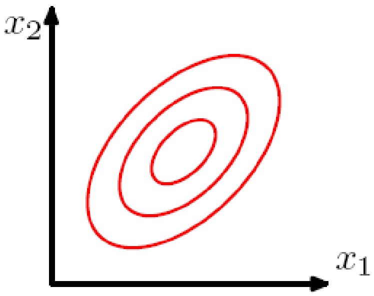
Other Nice Analytic Properties

- Marginal is Gaussian
- Conditional is Gaussian

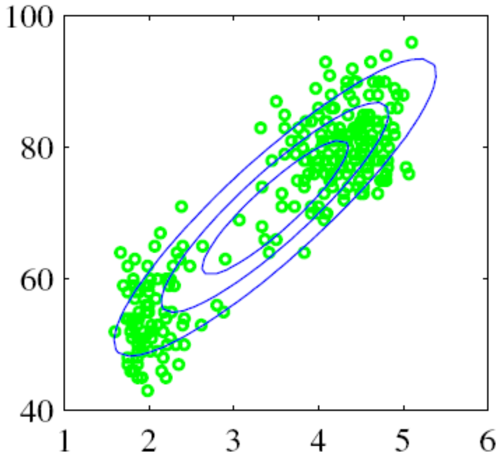


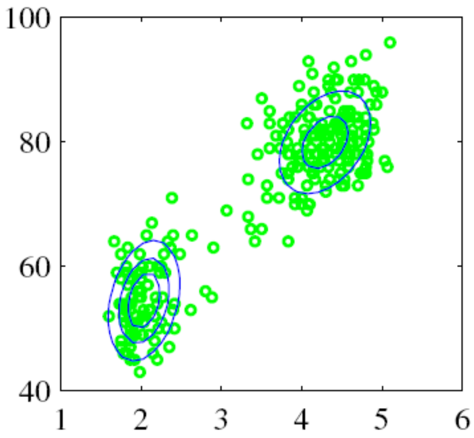
Limitations of Single Gaussians

- Single Gaussian is unimodal



- … can't fit well multimodal data, which is more realistic!

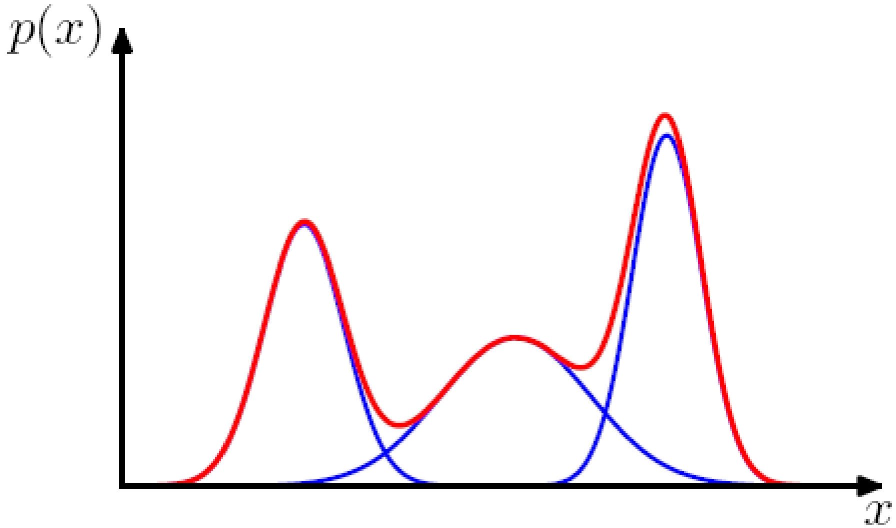




Mixture of Gaussians

- A simple family of multi-modal distributions
  - treat unimodal Gaussians as basis (or component) distributions
  - superpose multiple Gaussians via linear combination

$$p(x) = \sum_{k=1}^{K} \pi_k \mathcal{N}(x|\mu_k, \sigma_k^2)$$

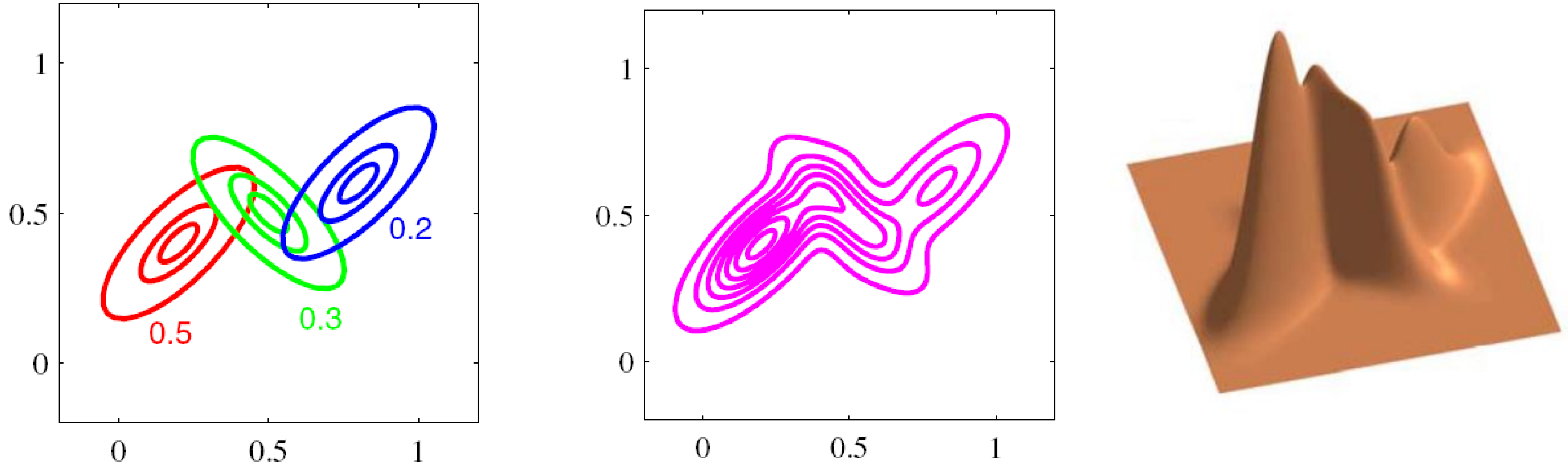


Mixture of Gaussians

- A simple family of multi-modal distributions
  - treat unimodal Gaussians as basis (or component) distributions
  - superpose multiple Gaussians via linear combination

$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\mu_k, \Sigma_k)$$

What conditions should the mixing coefficients satisfy ?



MLE for Mixture of Gaussians

- Log-likelihood

$$\log p(\mathcal{D}|\pi, \mu, \Sigma) = \sum_{n=1}^{N} \log \left(\sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\mu_k, \Sigma_k) \right)$$

  - this is complicated … ☹
  - … but, we know the MLE for single Gaussians are easy

- A heuristic procedure (can we iterate?)
  - allocate data into different components
  - estimate each component Gaussian analytically

Optimal Conditions

- Some math

$$\mathcal{L}(\boldsymbol{\mu}, \Sigma) = \log p(\mathcal{D}|\boldsymbol{\mu}, \Sigma) = \sum_{n=1}^{N} \log \left(\sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \Sigma_k) \right)$$

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{\mu}_k} = 0 \quad \Rightarrow \quad \sum_{n=1}^{N} \underbrace{\frac{\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \Sigma_k)}{\sum_j \pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j, \Sigma_j)}}_{\gamma(z_{nk})} \Sigma_k^{-1}(\mathbf{x}_n - \boldsymbol{\mu}_k) = 0$$

$$\Rightarrow \quad \boldsymbol{\mu}_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) \mathbf{x}_n \qquad N_k = \sum_{n=1}^{N} \gamma(z_{nk})$$

A weighted sample mean!

Optimal Conditions

- Some math

$$\mathcal{L}(\boldsymbol{\mu}, \Sigma) = \log p(\mathcal{D}|\boldsymbol{\mu}, \Sigma) = \sum_{n=1}^{N} \log \left(\sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \Sigma_k) \right)$$

$$\frac{\partial \mathcal{L}}{\partial \Sigma_k} = 0 \quad \Rightarrow \quad \Sigma_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk})(\mathbf{x}_n - \boldsymbol{\mu}_k)(\mathbf{x}_n - \boldsymbol{\mu}_k)^\top$$

A weighted sample variance!

Optimal Conditions

- Some math

$$\mathcal{L}(\boldsymbol{\mu}, \Sigma) = \log p(\mathcal{D}|\boldsymbol{\mu}, \Sigma) = \sum_{n=1}^{N} \log \left(\sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \Sigma_k) \right)$$

Note: constraints exist for mixing coefficients!

$$L = \mathcal{L}(\boldsymbol{\mu}, \Sigma) + \lambda \left(\sum_{k=1}^{K} \pi_k - 1 \right)$$

$$\frac{\partial L}{\partial \pi_k} = 0 \quad \Rightarrow \quad \sum_{n=1}^{N} \frac{\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \Sigma_k)}{\sum_j \pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j, \Sigma_j)} + \lambda = 0$$

$$\Rightarrow \quad \pi_k = \frac{N_k}{N}$$

The ratio of data assigned to component k!

Optimal Conditions – summary

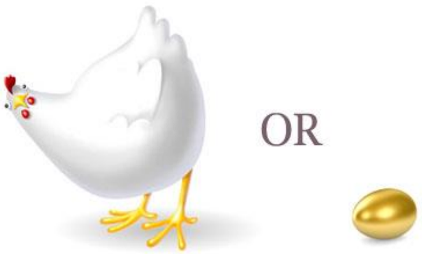
- The set of couple conditions

$$\boldsymbol{\mu}_k = \frac{1}{N_k}\sum_{n=1}^{N}\gamma(z_{nk})\mathbf{x}_n$$

$$\Sigma_k = \frac{1}{N_k}\sum_{n=1}^{N}\gamma(z_{nk})(\mathbf{x}_n - \boldsymbol{\mu}_k)(\mathbf{x}_n - \boldsymbol{\mu}_k)^{\top}$$

$$\pi_k = \frac{N_k}{N}$$

- The key factor to get them coupled



$$\gamma(z_{nk}) = \frac{\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \Sigma_k)}{\sum_j \pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j, \Sigma_j)}$$

- If we know $\gamma(z_{nk})$, each component Gaussian is easy to estimate!

The EM Algorithm

- **E-step**: estimate the responsibilities

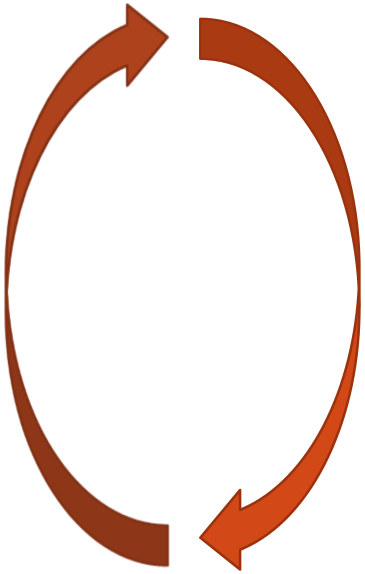
$$\gamma(z_{nk}) = \frac{\pi_k \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \Sigma_k)}{\sum_j \pi_j \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_j, \Sigma_j)}$$

- **M-step**: re-estimate the parameters

$$\boldsymbol{\mu}_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) \mathbf{x}_n$$

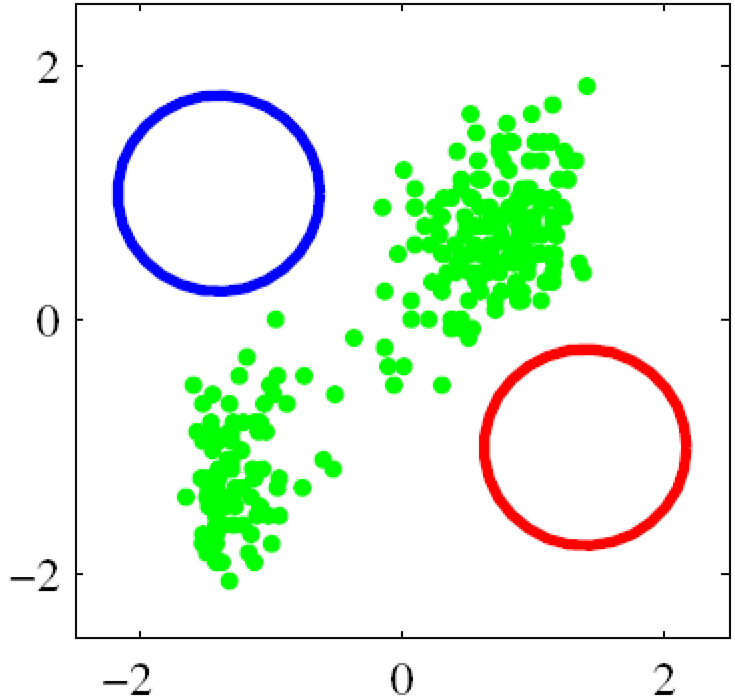
$$\Sigma_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) (\mathbf{x}_n - \boldsymbol{\mu}_k)(\mathbf{x}_n - \boldsymbol{\mu}_k)^\top$$

$$\pi_k = \frac{N_k}{N}$$



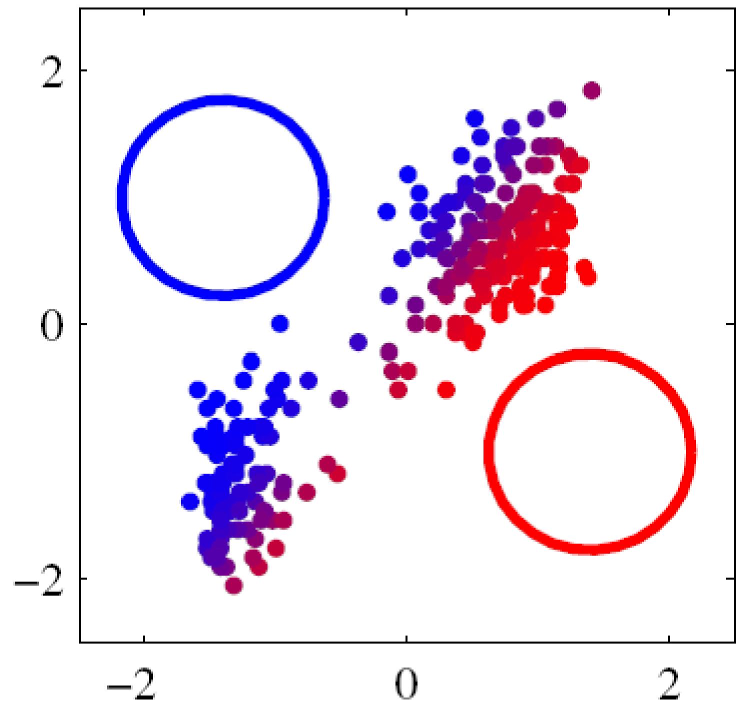
Initialization plays a key role to succeed!

A Running Example



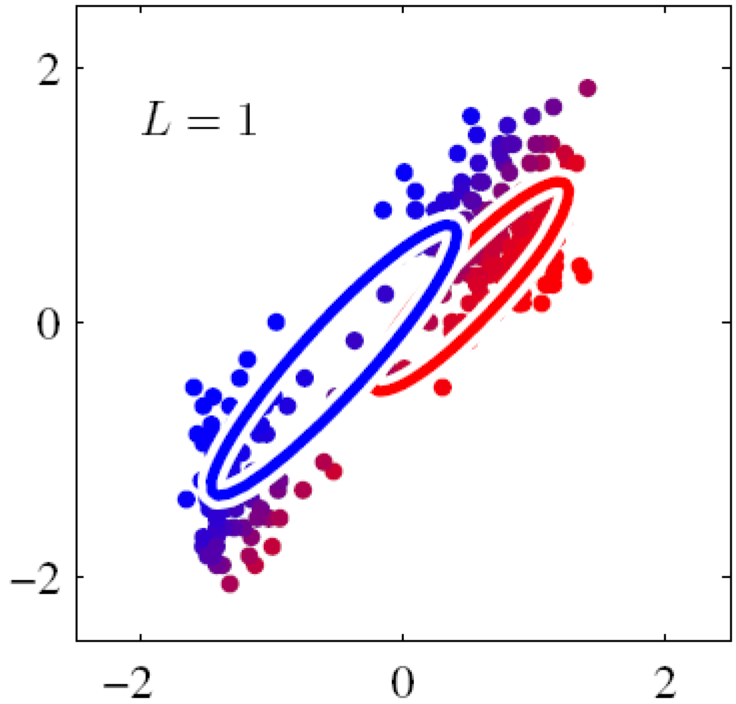
◈ The data and a mixture of two isotropic Gaussians

A Running Example



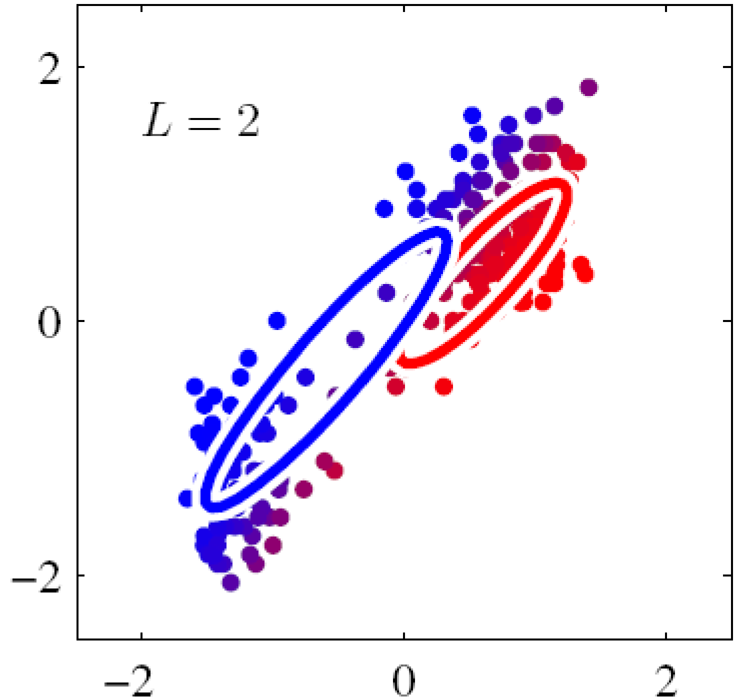
- Initial E-step

A Running Example



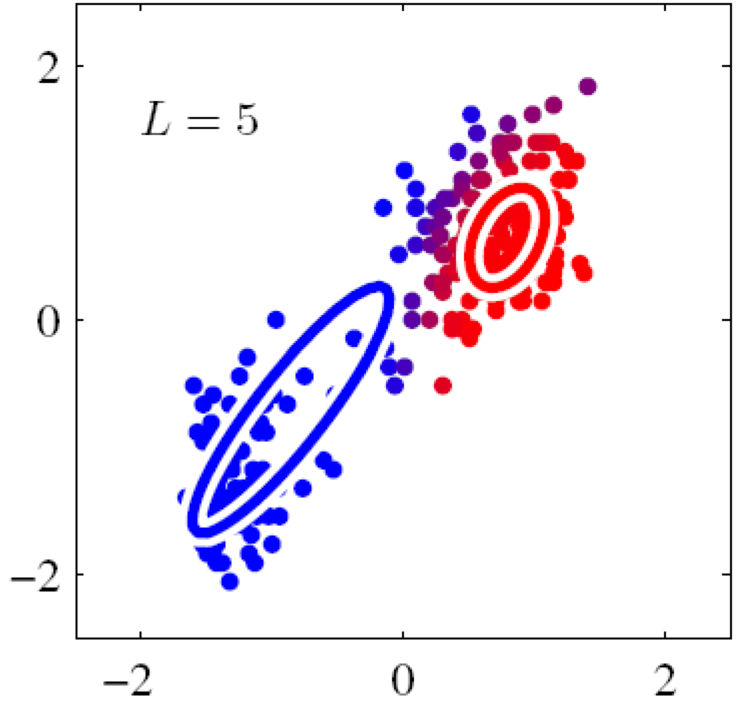
- Initial M-step

A Running Example



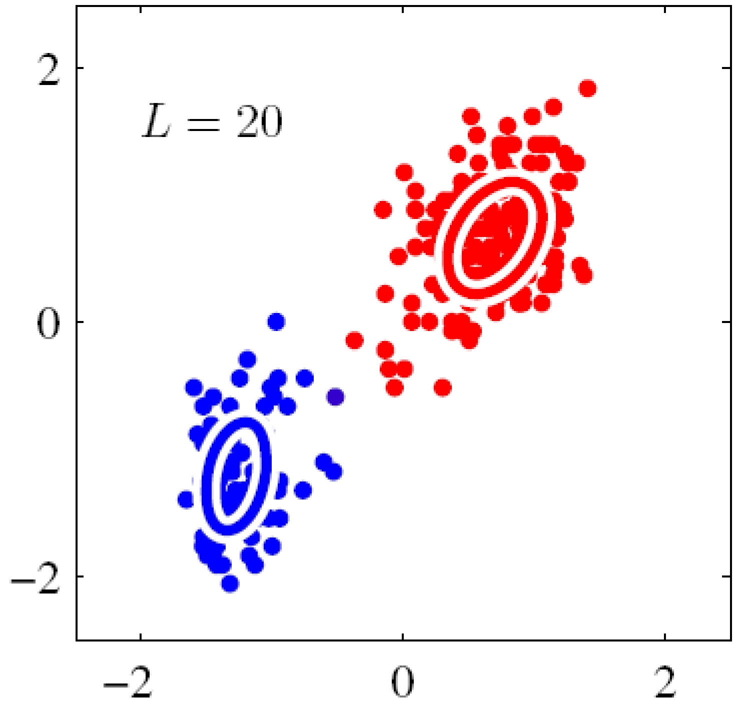
- The 2nd M-step

A Running Example



- The 5[th] M-step

A Running Example

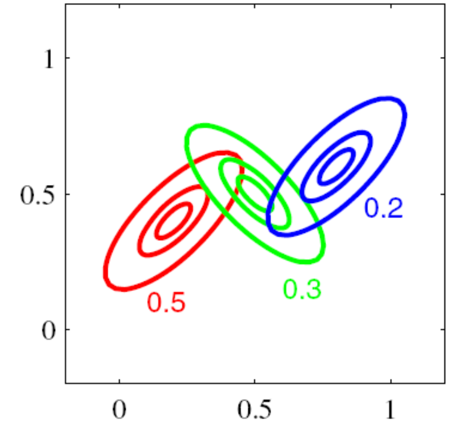


- The 20th M-step

Theory

- Let's take the latent variable view of mixture of Gaussians

$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\mu_k, \Sigma_k)$$

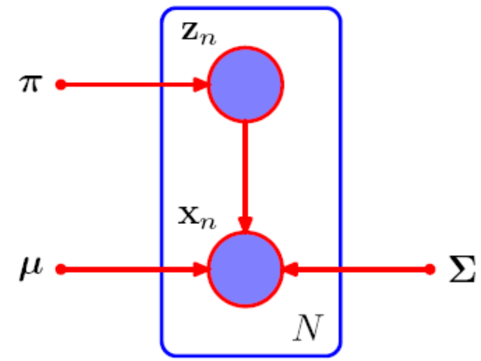


- Indicator (selecting) variable

$$\mathbf{z} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

$$\Rightarrow \quad p(\mathbf{x}, \mathbf{z}) = \prod_{k=1}^{K} \pi_k^{z_k} \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \Sigma_k)^{z_k}$$

$$\Rightarrow \quad p(\mathbf{x}) \stackrel{?}{=} \sum_{\mathbf{z}} p(\mathbf{x}, \mathbf{z})$$



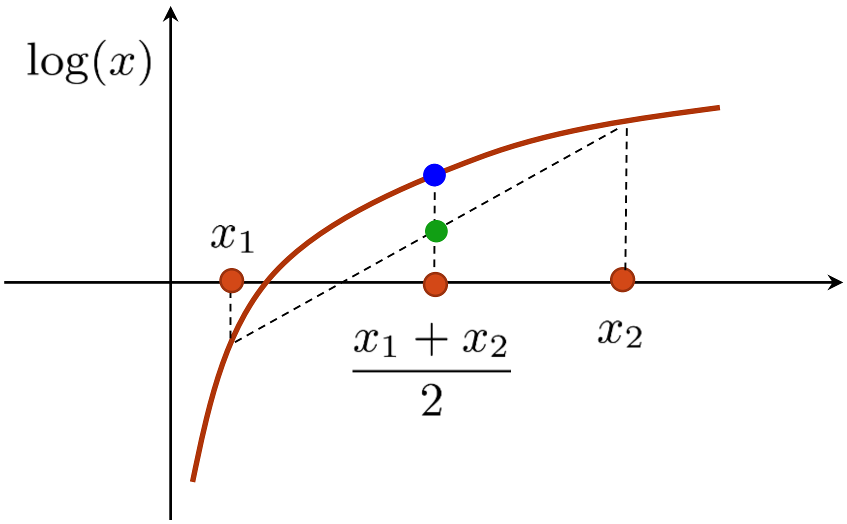
Note: the idea of data augmentation is influential in statistics and machine learning!

Theory

- Re-visit the log-likelihood

$$\log p(\mathcal{D}|\Theta) = \sum_{n=1}^{N} \log \left(\sum_{\mathbf{z}_n} p(\mathbf{x}_n, \mathbf{z}_n) \right)$$

- Jensen's inequality



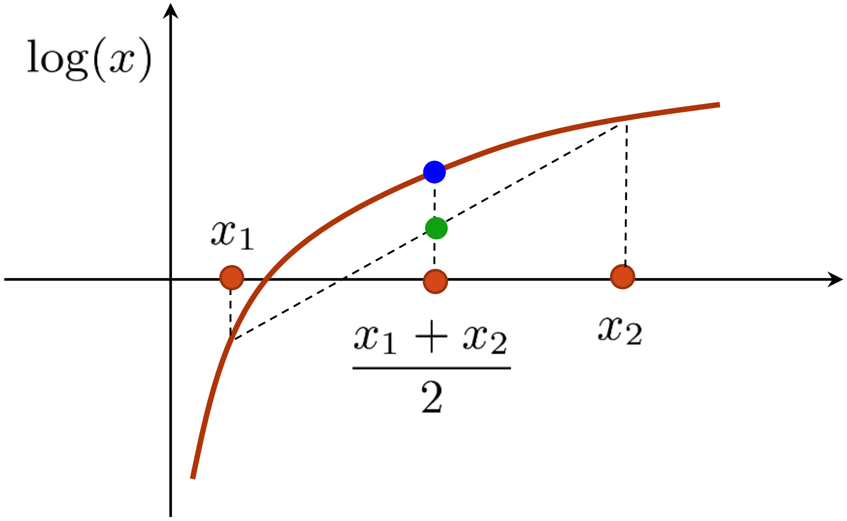
$$\boxed{\log \frac{x_1 + x_2}{2} \geq \frac{\log x_1 + \log x_2}{2}}$$

Theory

- Re-visit the log-likelihood

$$\log p(\mathcal{D}|\Theta) = \sum_{n=1}^{N} \log\left(\sum_{\mathbf{z}_n} p(\mathbf{x}_n, \mathbf{z}_n)\right)$$

- Jensen's inequality



$$\boxed{\log \mathbb{E}_{p(x)}[x] \geq \mathbb{E}_{p(x)}[\log x]}$$

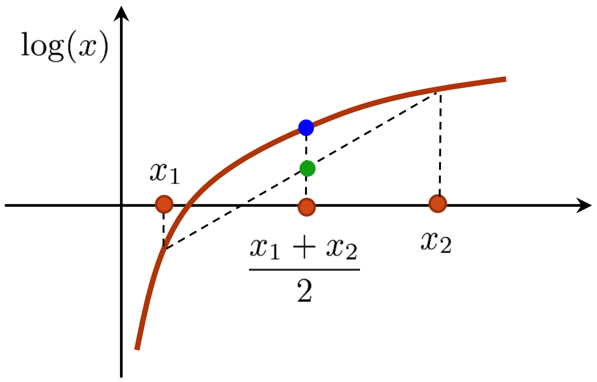
Theory

- Re-visit the log-likelihood

$$\log p(\mathcal{D}|\Theta) = \sum_{n=1}^{N} \log \left(\sum_{\mathbf{z}_n} p(\mathbf{x}_n, \mathbf{z}_n) \right)$$

- Jensen's inequality

$$\boxed{\log \mathbb{E}_{p(x)}[x] \geq \mathbb{E}_{p(x)}[\log x]}$$



- How to apply?

$$\log p(\mathcal{D}|\Theta) = \sum_{n=1}^{N} \log \left(\sum_{\mathbf{z}_n} q(\mathbf{z}_n) \frac{p(\mathbf{x}_n, \mathbf{z}_n)}{q(\mathbf{z}_n)} \right)$$

$$\geq \sum_{n=1}^{N} \sum_{\mathbf{z}_n} q(\mathbf{z}_n) \log \left(\frac{p(\mathbf{x}_n, \mathbf{z}_n)}{q(\mathbf{z}_n)} \right)$$

Theory

- What we have is a lower bound

$$\log p(\mathcal{D}|\Theta) \geq \sum_{n=1}^{N} \sum_{\mathbf{z}_n} q(\mathbf{z}_n) \log \left(\frac{p(\mathbf{x}_n, \mathbf{z}_n)}{q(\mathbf{z}_n)} \right) \triangleq \mathcal{L}(\Theta, q(\mathbf{Z}))$$

- What's the GAP?

$$\begin{aligned}
\mathcal{L}(\Theta, q(\mathbf{Z})) &= \sum_{n=1}^{N} \Big\{ \sum_{\mathbf{z}_n} q(\mathbf{z}_n) \log p(\mathbf{x}_n, \mathbf{z}_n) - \sum_{\mathbf{z}_n} q(\mathbf{z}_n) \log q(\mathbf{z}_n) \Big\} \\
&= \sum_{n=1}^{N} \Big\{ \sum_{\mathbf{z}_n} q(\mathbf{z}_n) \log \left(\frac{p(\mathbf{x}_n, \mathbf{z}_n)}{p(\mathbf{x}_n)} \right) + \log p(\mathbf{x}_n) - \sum_{\mathbf{z}_n} q(\mathbf{z}_n) \log q(\mathbf{z}_n) \Big\} \\
&= \log p(\mathcal{D}|\Theta) + \sum_{n=1}^{N} \Big\{ \sum_{\mathbf{z}_n} q(\mathbf{z}_n) \log p(\mathbf{z}_n|\mathbf{x}_n) - \sum_{\mathbf{z}_n} q(\mathbf{z}_n) \log q(\mathbf{z}_n) \Big\} \\
&= \log p(\mathcal{D}|\Theta) - \mathrm{KL}(q(\mathbf{Z}) \| p(\mathbf{Z}|\mathcal{D}))
\end{aligned}$$

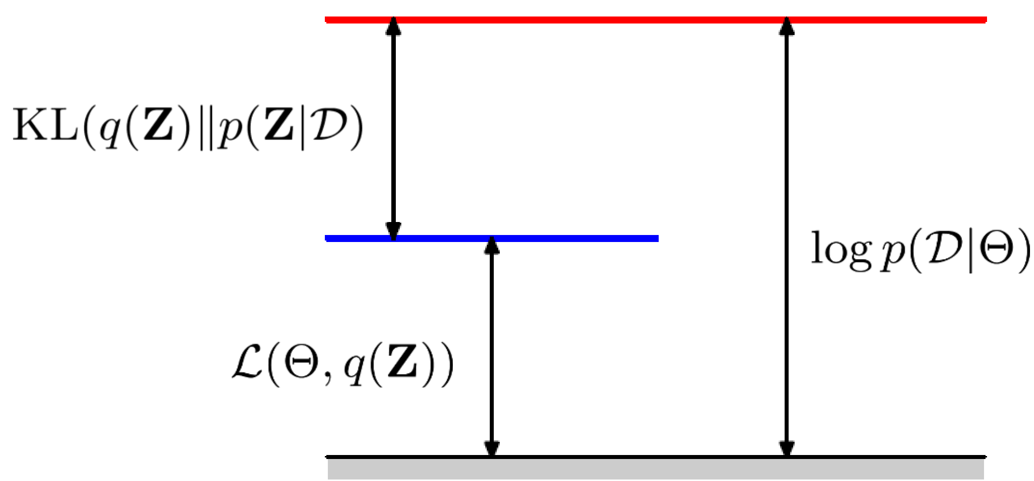
Theory

- What we have is a lower bound

$$\log p(\mathcal{D}|\Theta) \geq \sum_{n=1}^{N} \sum_{\mathbf{z}_n} q(\mathbf{z}_n) \log \left(\frac{p(\mathbf{x}_n, \mathbf{z}_n)}{q(\mathbf{z}_n)} \right) \triangleq \mathcal{L}(\Theta, q(\mathbf{Z}))$$

- What's the GAP?

$$\log p(\mathcal{D}|\Theta) - \mathcal{L}(\Theta, q(\mathbf{Z})) = \mathrm{KL}(q(\mathbf{Z}) \| p(\mathbf{Z}|\mathcal{D}))$$

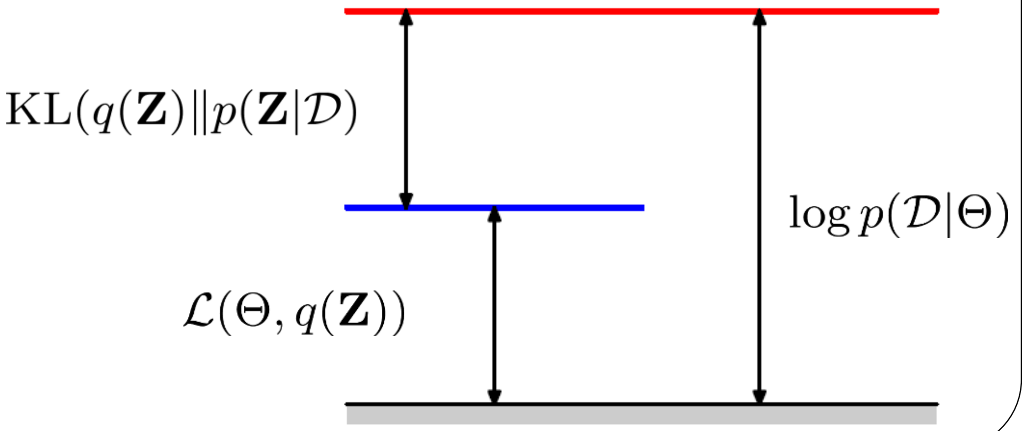


EM-algorithm

- Maximize the lower bound or minimize the gap:

$$\log p(\mathcal{D}|\Theta) \geq \sum_{n=1}^{N} \sum_{\mathbf{z}_n} q(\mathbf{z}_n) \log \left(\frac{p(\mathbf{x}_n, \mathbf{z}_n)}{q(\mathbf{z}_n)} \right) \triangleq \mathcal{L}(\Theta, q(\mathbf{Z}))$$

  - Maximize over $q(\mathrm{Z})$ => E-step
  - Maximize over Θ => M-step



Convergence of EM

- Local optimum is guaranteed under mild conditions (Depster et al., 1977)
  - alternating minimization for a bi-convex problem

$$\mathcal{L}(\Theta_{t+1}) \geq \mathcal{L}(\Theta_t)$$

- Some special cases with global optimum (Wu, 1983)

- First-order gradient descent for log-likelihood
  - for comparison with other gradient ascent methods, see (Xu & Jordan, 1995)

Relation between GMM and K-Means

- Small variance asymptotics:
  - The EM algorithm for GMM reduces to K-Means under certain conditions:

E-step:

$$\gamma(z_{nk}) = \frac{\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \Sigma_k)}{\sum_j \pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j, \Sigma_j)}$$

M-step:

$$\boldsymbol{\mu}_k = \frac{1}{N_k}\sum_{n=1}^{N} \gamma(z_{nk})\mathbf{x}_n$$

$$\Sigma_k = \frac{1}{N_k}\sum_{n=1}^{N} \gamma(z_{nk})(\mathbf{x}_n - \boldsymbol{\mu}_k)(\mathbf{x}_n - \boldsymbol{\mu}_k)^\top$$

$$\pi_k = \frac{N_k}{N}$$

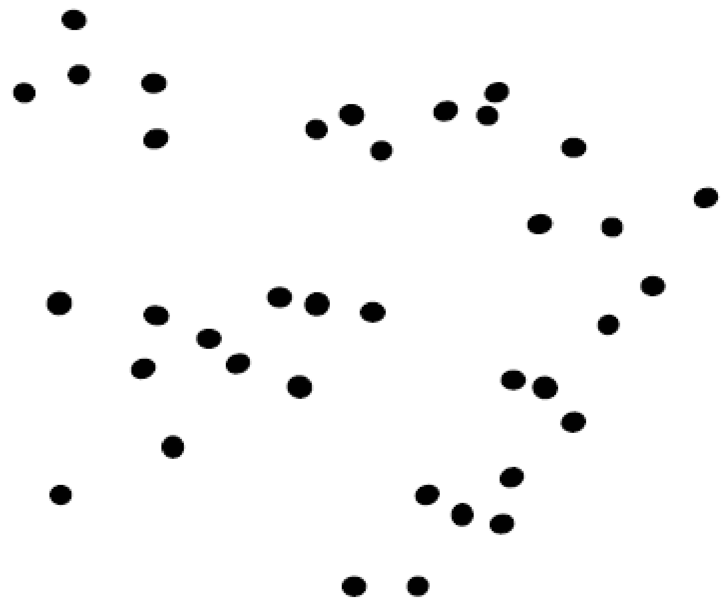
$$\text{let } \Sigma_k = \sigma I \text{ and } \sigma \to 0$$

$$\gamma(z_{nk}) = \frac{\pi_k \exp(-\frac{1}{2\sigma}\|\mathbf{x}_n - \boldsymbol{\mu}_k\|_2^2)}{\sum_j \pi_j \exp(-\frac{1}{2\sigma}\|\mathbf{x}_n - \boldsymbol{\mu}_j\|_2^2)}$$

$$= k^*, \text{ where } k^* = \mathrm{argmin}_k \|\mathbf{x}_n - \boldsymbol{\mu}_k\|_2^2$$

Single Linkage Hierarchical Clustering

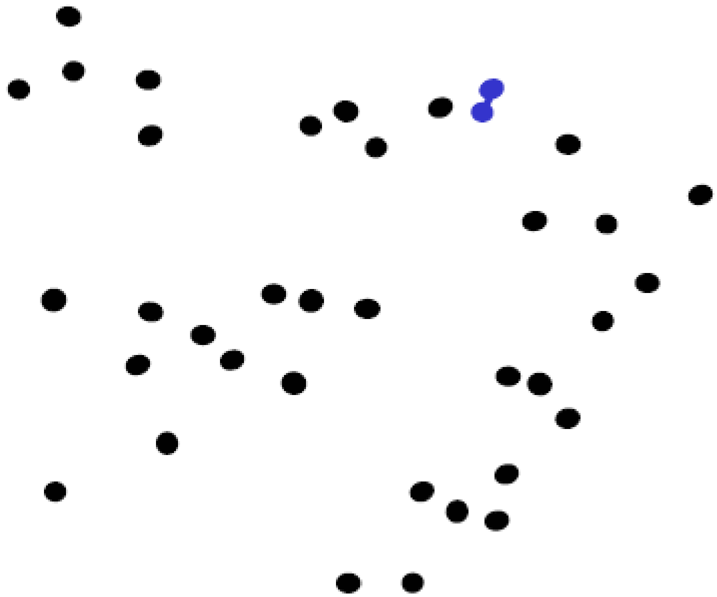
- Start with "every point is its own cluster"



[Slide courtesy: Andrew Moore]

Single Linkage Hierarchical Clustering

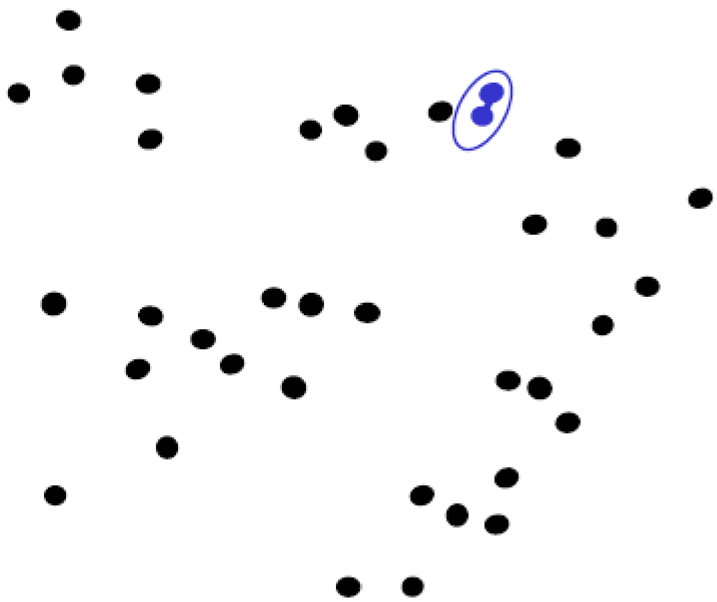
- Start with "every point is its own cluster"
- Find "most similar" pairs of clusters



[Slide courtesy: Andrew Moore]

Single Linkage Hierarchical Clustering

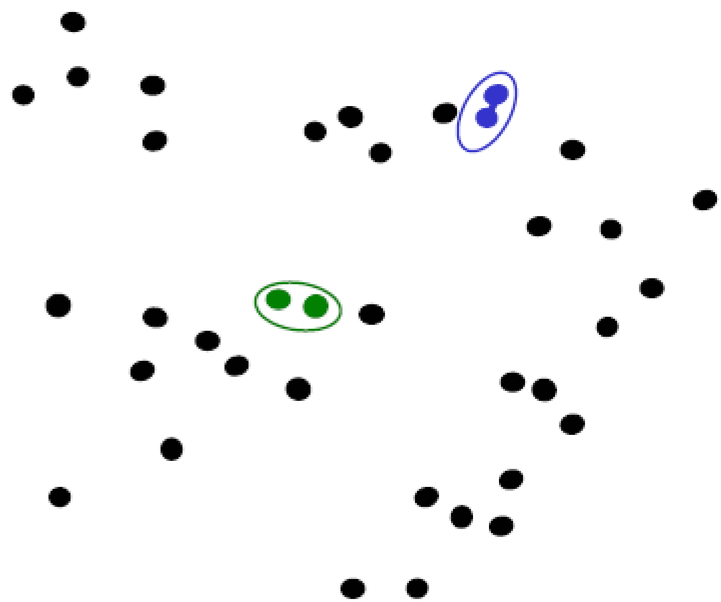
- Start with "every point is its own cluster"
- Find "most similar" pairs of clusters
- Merge it into a parent cluster



[Slide courtesy: Andrew Moore]

Single Linkage Hierarchical Clustering

- Start with "every point is its own cluster"
- Find "most similar" pairs of clusters
- Merge it into a parent cluster
- Repeat



[Slide courtesy: Andrew Moore]

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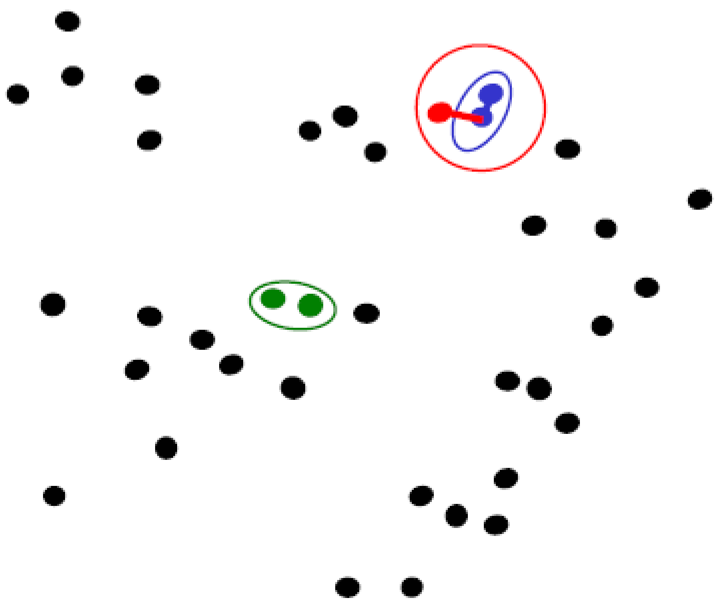

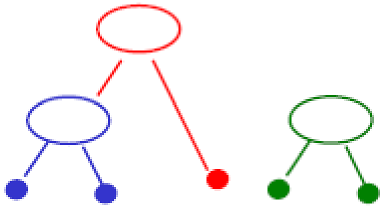

[Slide courtesy: Andrew Moore]

Single Linkage Hierarchical Clustering

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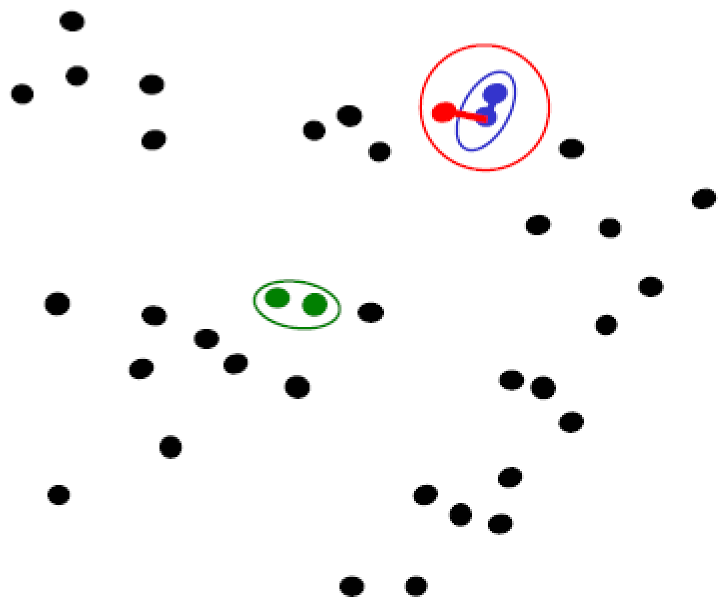
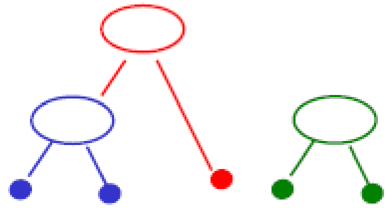


Key Question:

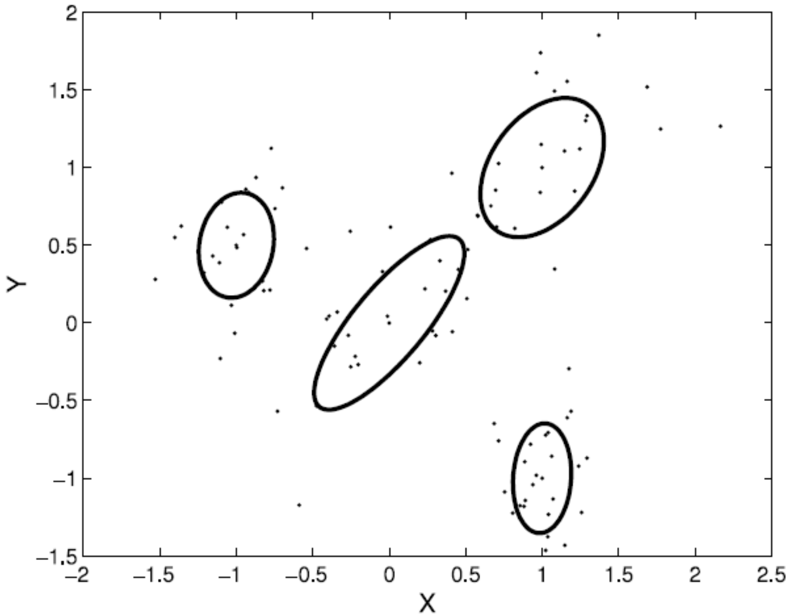
How do we define similarity between clusters?

=> minimum, maximum, or average distance between points in clusters



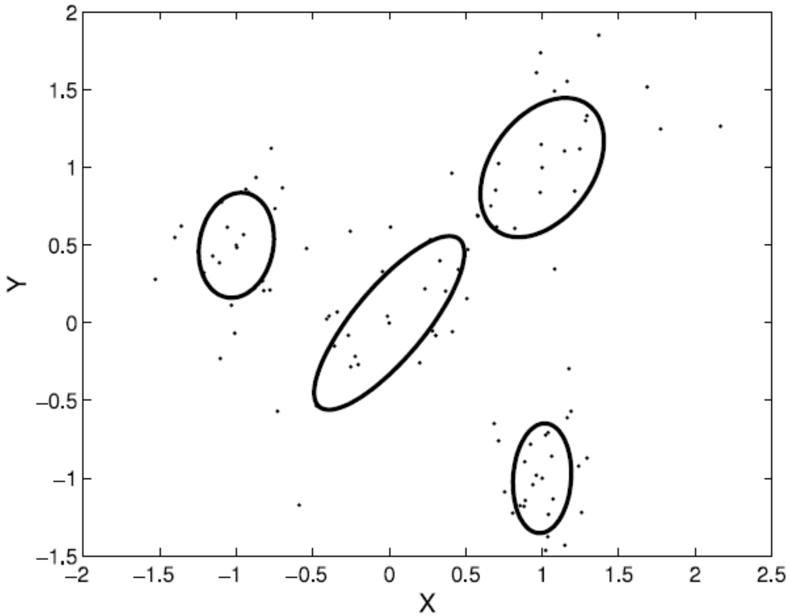
[Slide courtesy: Andrew Moore]

How many components are good?



- Can we let the data speak for themselves?
  - let data determine model complexity (e.g., the number of components in mixture models)
  - allow model complexity to grow as more data observed

How many components are good?



- Can we let the data speak for themselves?
  - we will talk about Dirichlet Process (DP) Mixtures
  - and nonparametric Bayesian models

Summary

- Gaussian Mixtures and K-means are effective tools to discover clustering structures
- EM algorithms can be applied to do MLE for GMMs
- Relationships between GMMs and K-means are discussed

- Unresolved issues
  - How to determine the number of components for mixture models?
  - How to determine the number of components for K-means?

Materials to Read

- Chap. 9 of Bishop's PRML book
- Bottou, L. & Bengio, Y. Convergence Properties of the K-means Algorithms, NIPS 1995.