k-means clustering

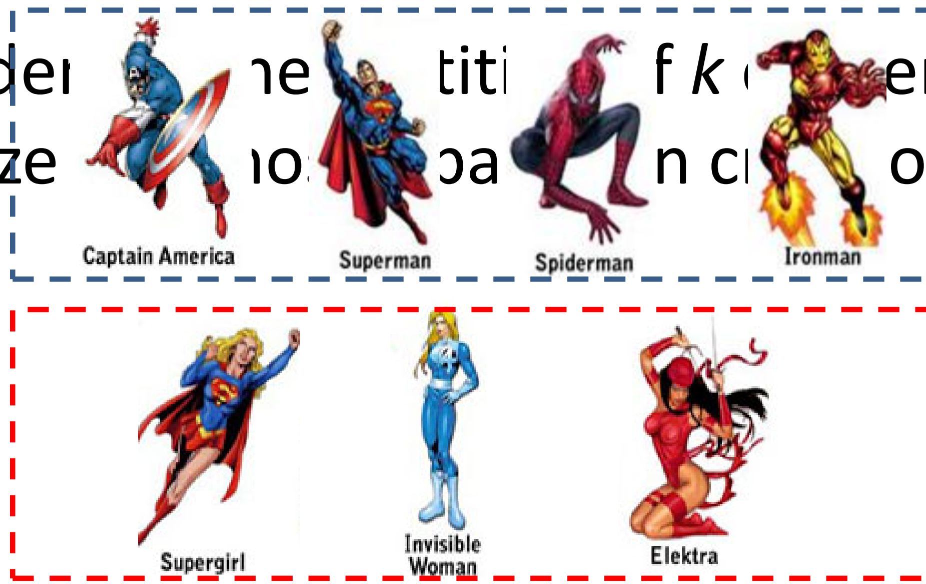
Hongning Wang
CS@UVa

Today's lecture

- *k*-means clustering
  – A typical partitional clustering algorithm
  – Convergence property
    - Expectation Maximization algorithm
  – Gaussian mixture model

Partitional clustering algorithms

- Partition instances into exactly *k* non-overlapping clusters
  - Flat structure clustering
  - Users need to specify the cluster size *k*
  - Task: ide[illegible] f *k* [illegible]ers that optimize [illegible] on



Partitional clustering algorithms

- Partition instances into exactly *k* non-overlapping clusters
  - Typical criterion
    - $\max \sum_{i \neq \mathrm{j}} d\left(c_i, c_j\right) - C \sum_i \sigma_i$

Inter-cluster distance

Optimize this in an alternative way

Intra-cluster distance

  - Optimal solution: enumerate every possible partition of size *k* and return the one optimizing the criterion

Let's approximate this!

Unfortunately, this is NP-hard!

k-means algorithm

Input: cluster size k, instances $\{x_i\}_{i=1}^N$, distance metric $d(x, y)$

Output: cluster membership assignments $\{z_i\}_{i=1}^N$

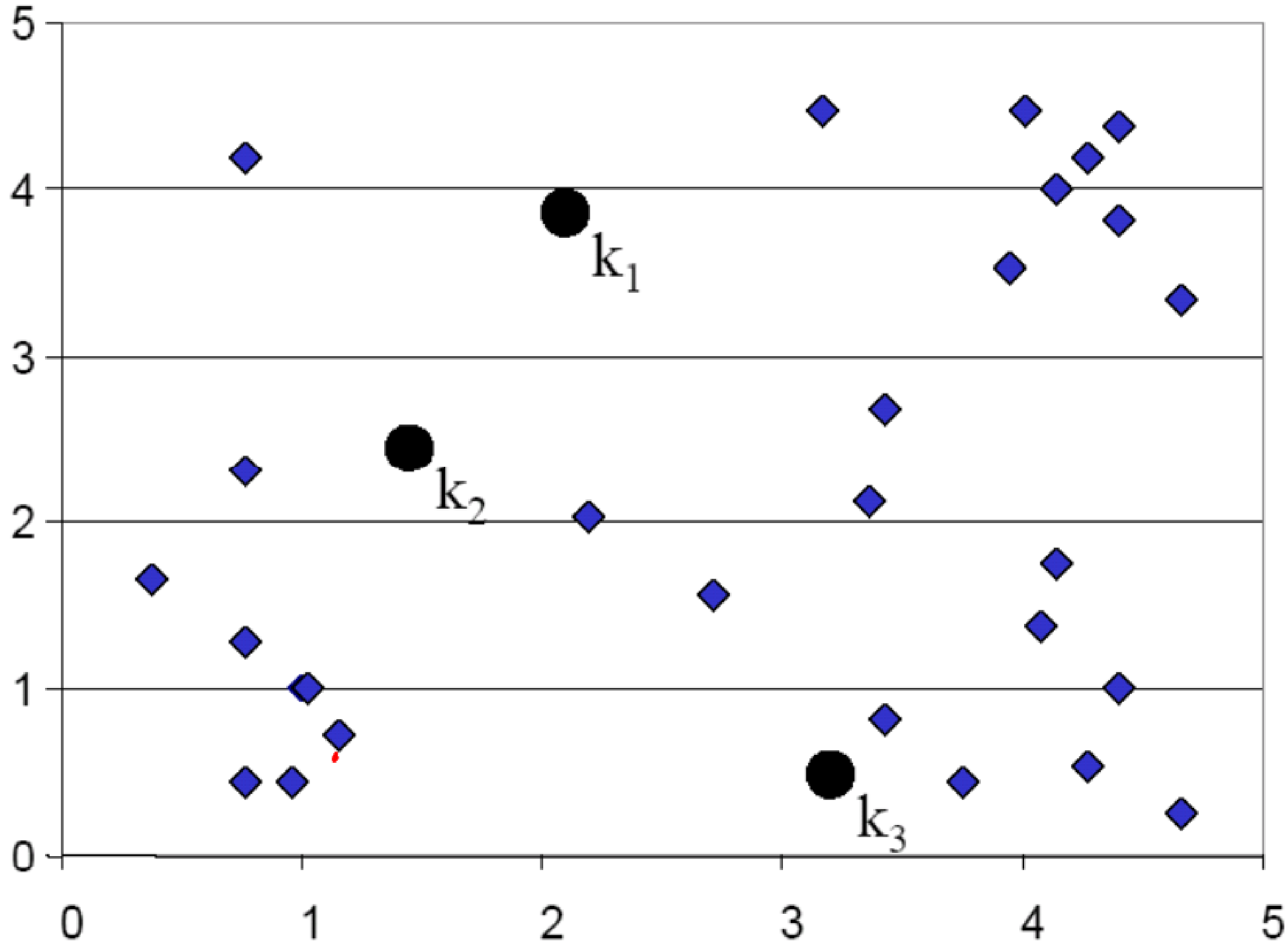
1. Initialize k cluster centroids $\{c_i\}_{i=1}^k$ (randomly if no domain knowledge available)
2. Repeat until no instance changes its cluster membership:
   – Decide the cluster membership of instances by assigning them to the nearest cluster centroid

     $$z_i = argmin_k d(c_k, x_i)$$ *Minimize intra distance*

   – Update the k cluster centroids based on the assigned cluster membership

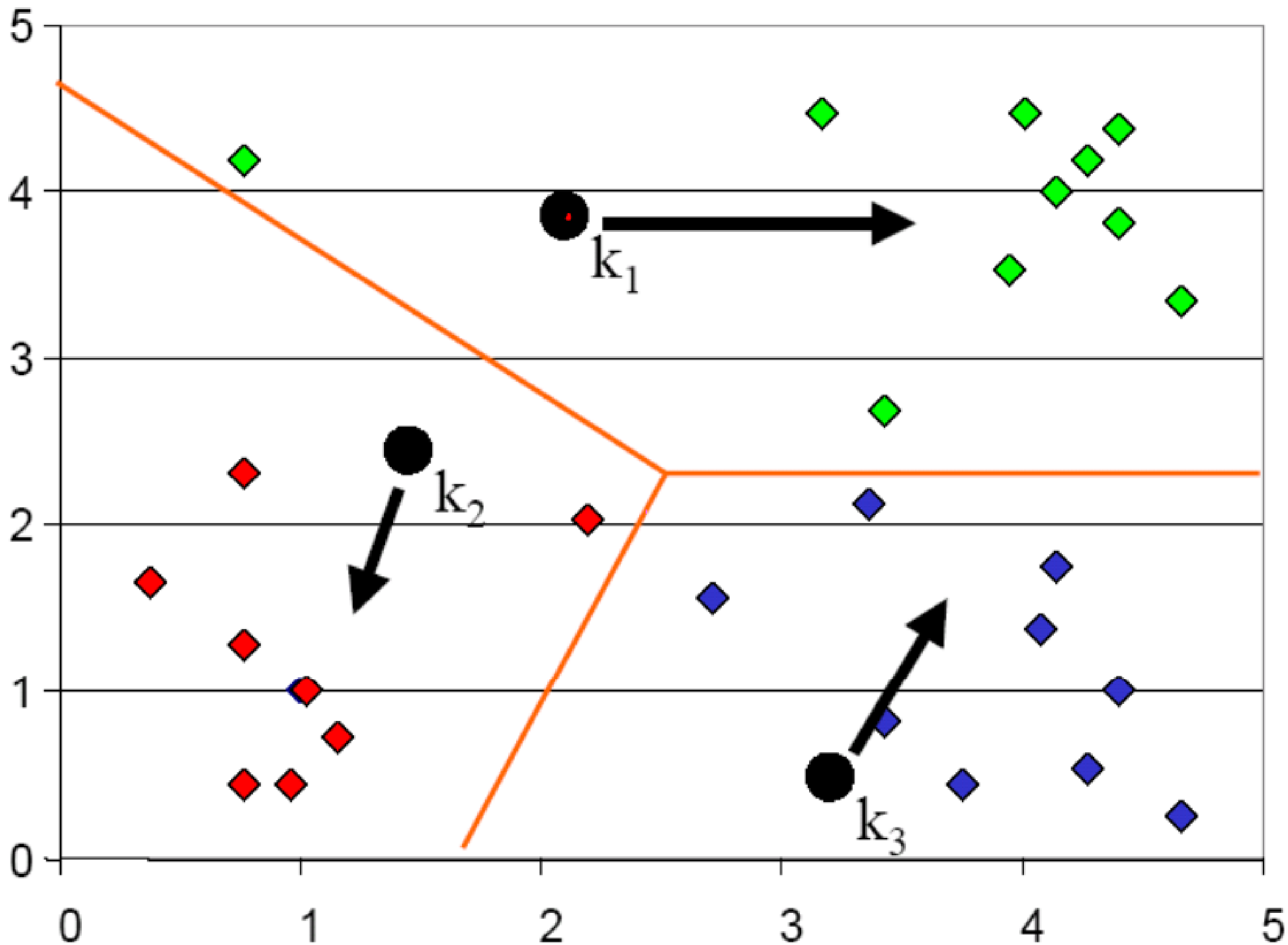
     $$c_k = \frac{\sum_i \delta(z_i = c_k) x_i}{\sum_i \delta(z_i = c_k)}$$ *Maximize inter distance*

k-means illustration

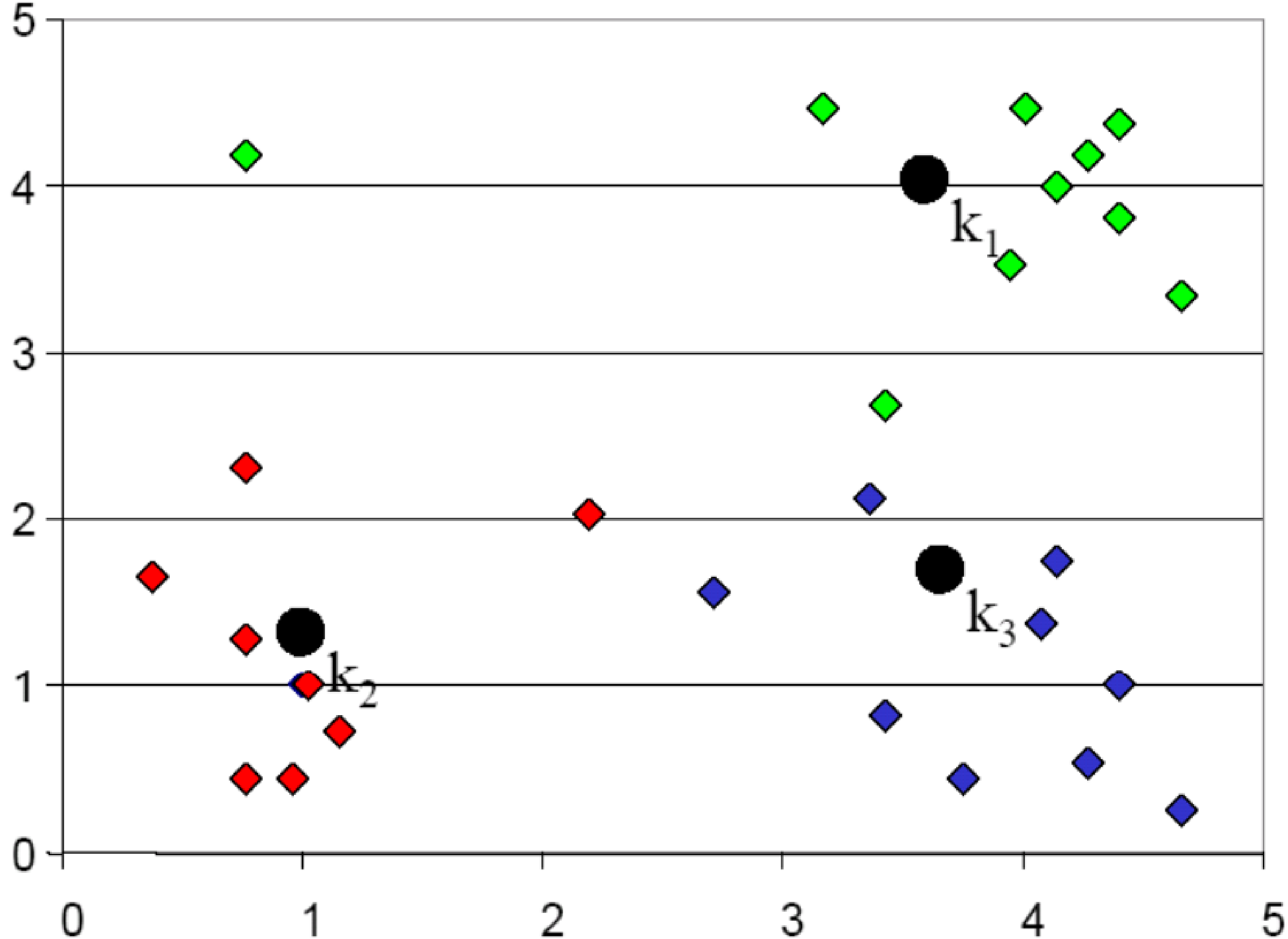


k-means illustration

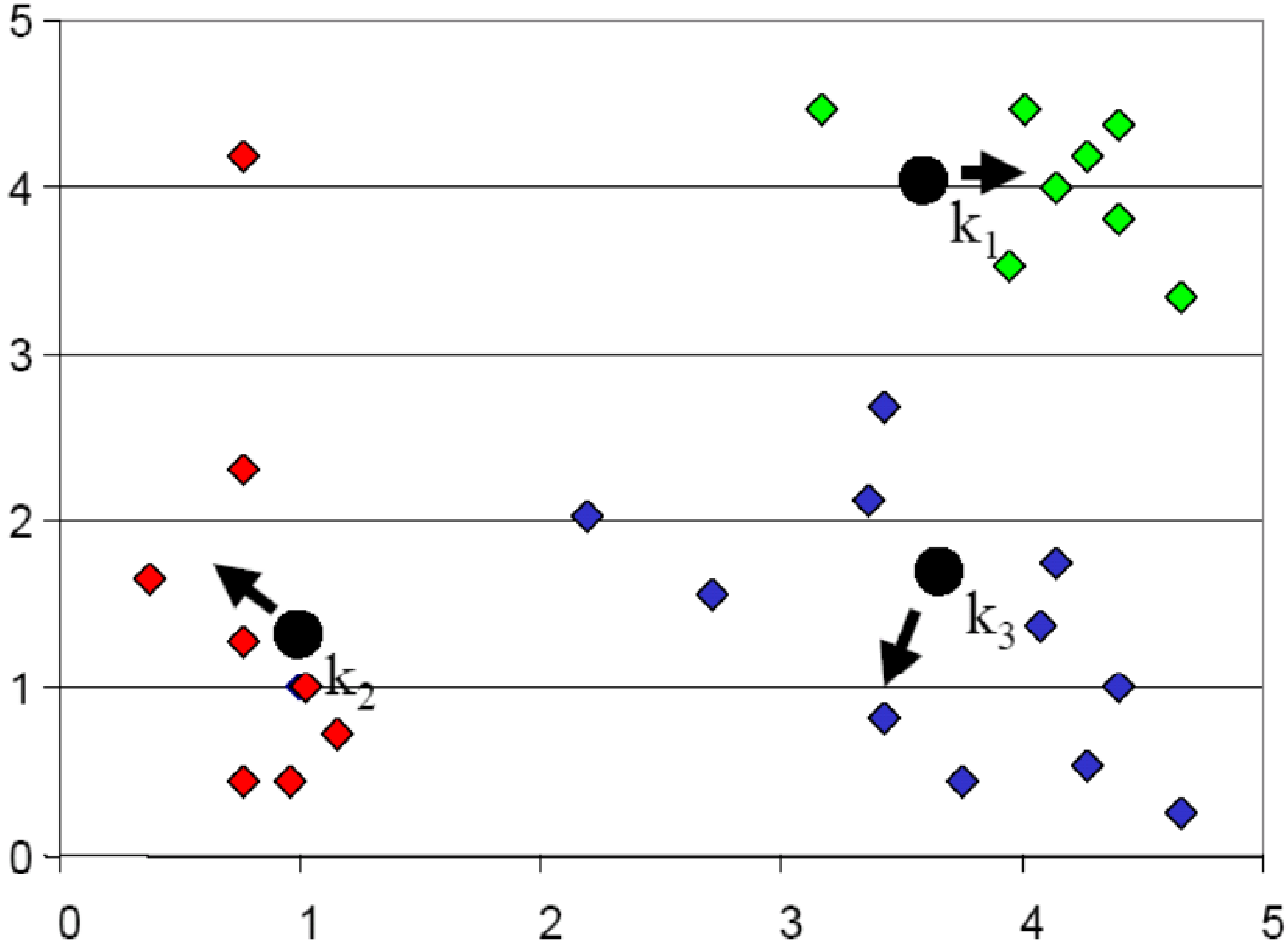
Voronoi diagram



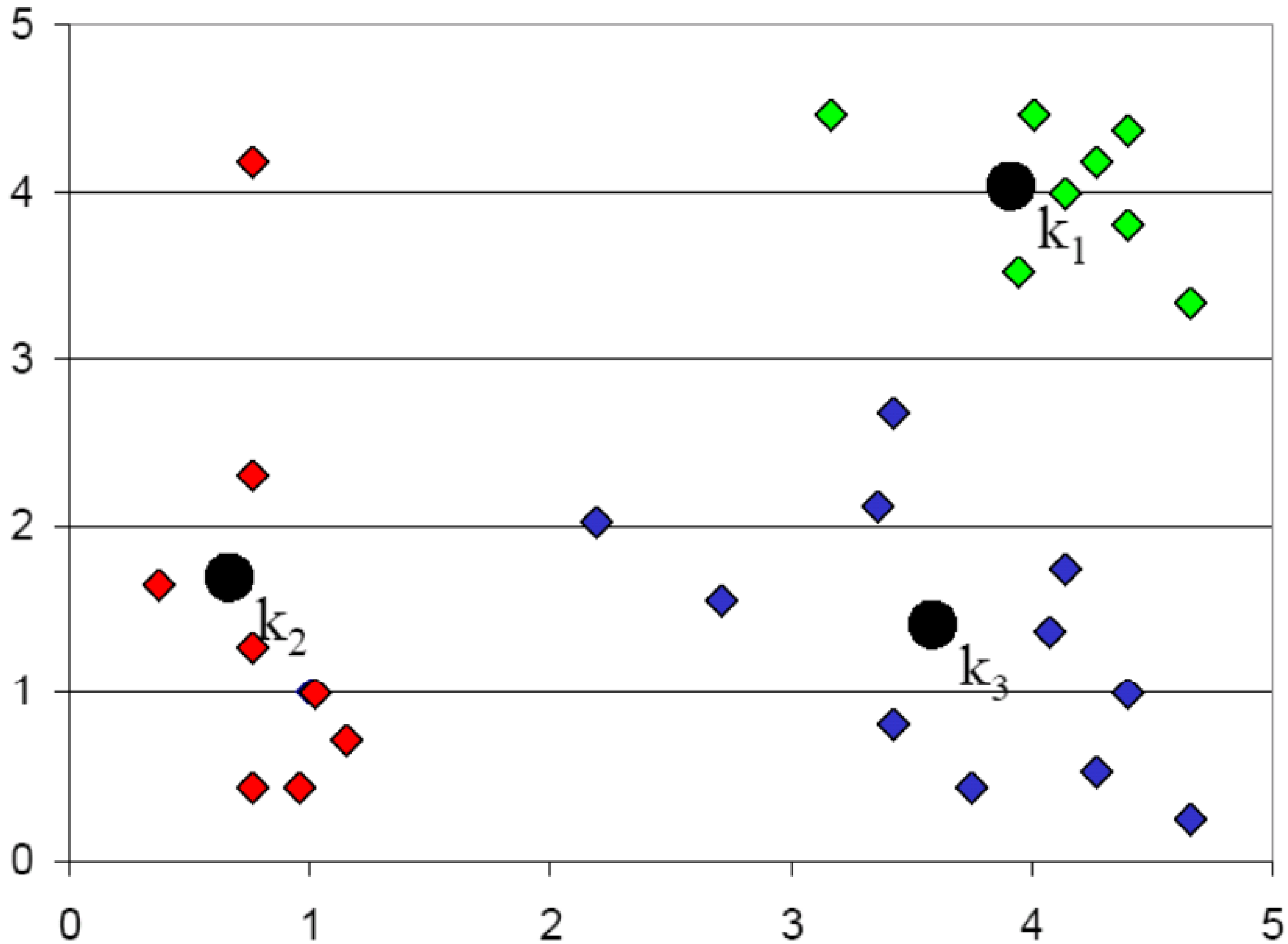
k-means illustration



k-means illustration



k-means illustration



Complexity analysis

- Decide cluster membership
  - $O(kn)$
- Compute cluster centroid
  - $O(n)$
- Assume k-means stops after l iterations
  - $O(knl)$

Don't forget the complexity of distance computation, e.g., $O(V)$ for Euclidean distance

Convergence property

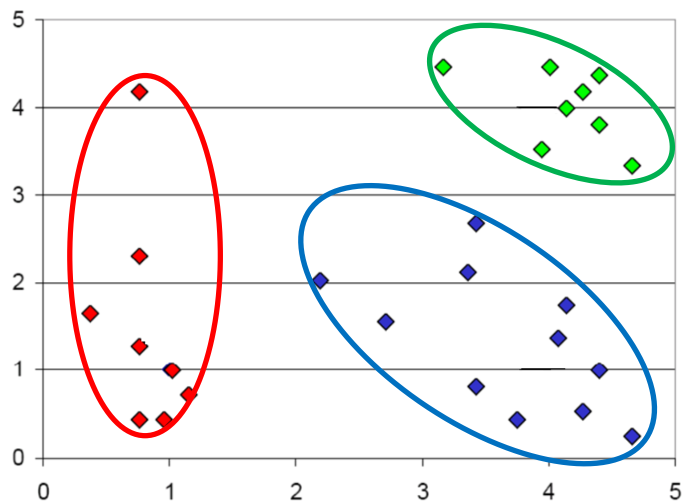
- Why *k*-means will stop?
  - Answer: it is a special version of Expectation Maximization (EM) algorithm, and EM is guaranteed to converge
  - However, it is only guaranteed to converge to local optimal, since *k*-means (EM) is a greedy algorithm

Probabilistic interpretation of clustering

- The density model of $p(x)$ is multi-modal
- Each mode represents a sub-population
  - E.g., unimodal Gaussian for each group

$p(x|z=2)$

$p(x|z=1)$



$p(x|z=3)$

Mixture model

$$p(x) = \sum_z p(x|z)p(z)$$

Unimodal distribution

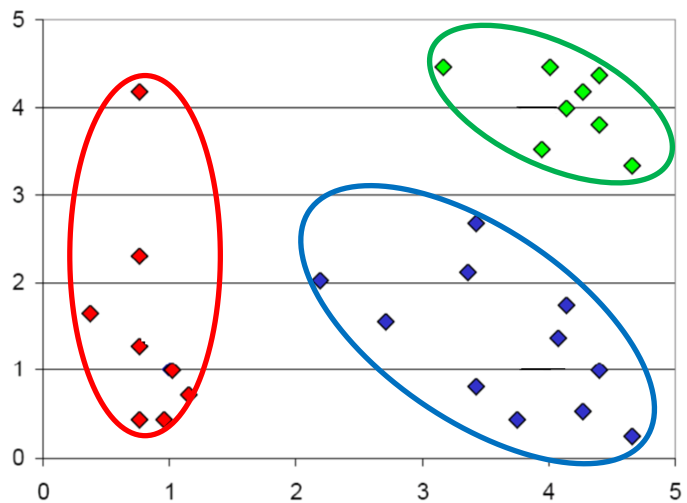
Mixing proportion

Probabilistic interpretation of clustering

- If z is known for every x
  - Estimating $p(z)$ and $p(x|z)$ is easy
    - Maximum likelihood estimation
    - This is Naïve Bayes

$p(x|z=2)$

$p(x|z=1)$



$p(x|z=3)$

Mixture model

$$p(x) = \sum_z p(x|z)p(z)$$

Unimodal distribution

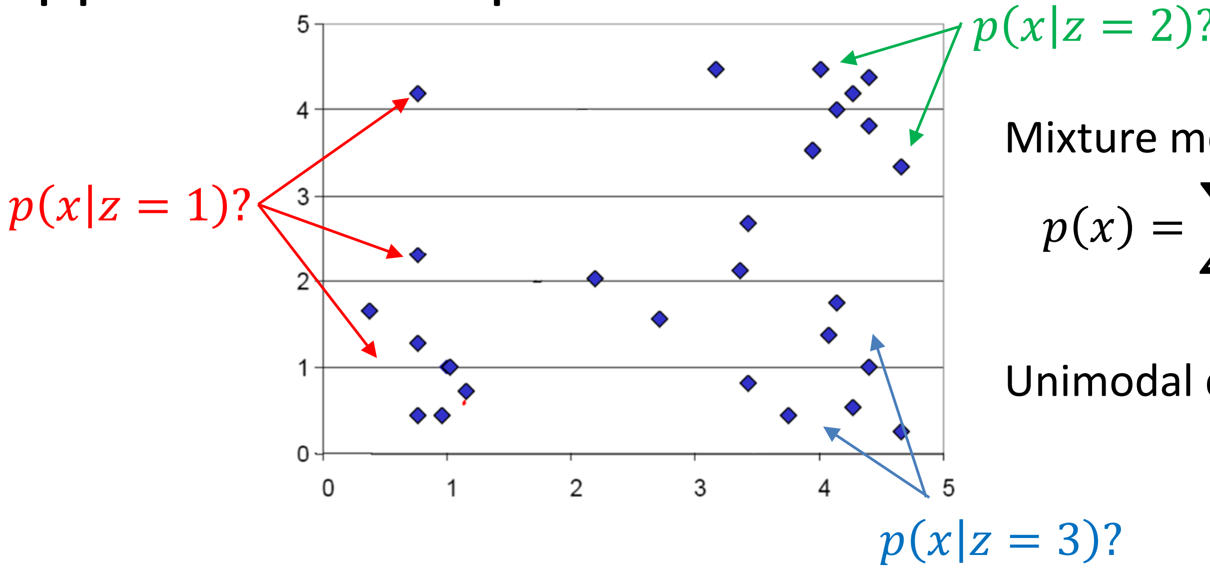
Mixing proportion

Probabilistic interpretation of clustering

- But z is unknown for all x
  - Estimating $p(z)$ and $p(x|z)$ is generally hard
    - $\max_{\alpha,\beta} \sum_i \log \sum_{z_i} p(x_i|z_i,\beta)p(z_i|\alpha)$

Usually a constrained optimization problem

  - Appeal to the Expectation Maximization algorithm



Mixture model

$$p(x) = \sum_z p(x|z)p(z)$$

Unimodal distribution

Mixing proportion

Introduction to EM

- Parameter estimation
  - All data is observable
    - Maximum likelihood method
    - Optimize the analytic form of $L(\theta) = \log p(X|\theta)$
  - Missing/unobservable data

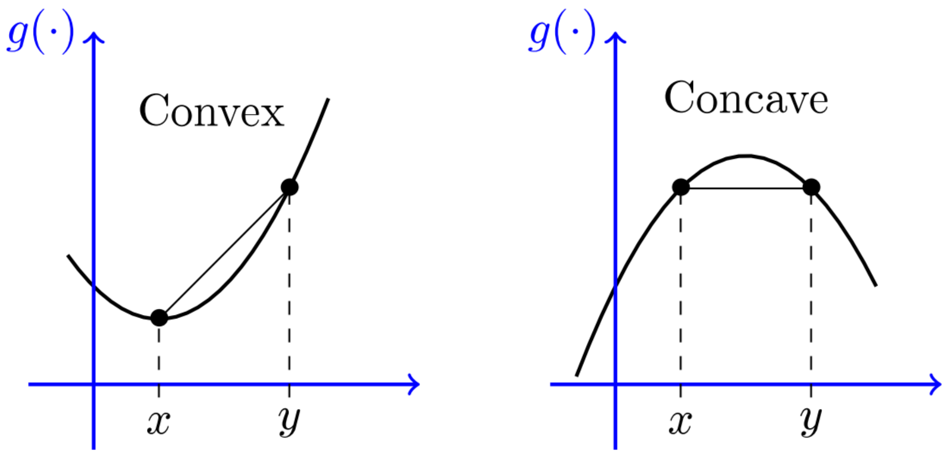
    E.g. cluster membership
    - Data: X (observed) + Z(hidden)
    - Likelihood: $L(\theta) = \log \sum_z p(X, Z|\theta)$
    - Approximate it!

Most of cases are intractable

Background knowledge

- Jensen's inequality
  - For any convex function $f(x)$ and positive weights λ,

$$f\left(\sum_i \lambda_i x_i\right) \leq \sum_i \lambda_i f(x_i) \qquad \sum_i \lambda_i = 1$$



Expectation Maximization

- Maximize data likelihood function by pushing the lower bound

Proposal distributions for Z

$$-L(\theta) = \log \sum_Z p(X, Z|\theta) = \log \sum_Z \frac{q(Z)\boxed{p(X, Z|\theta)}}{\boxed{q(Z)}}$$

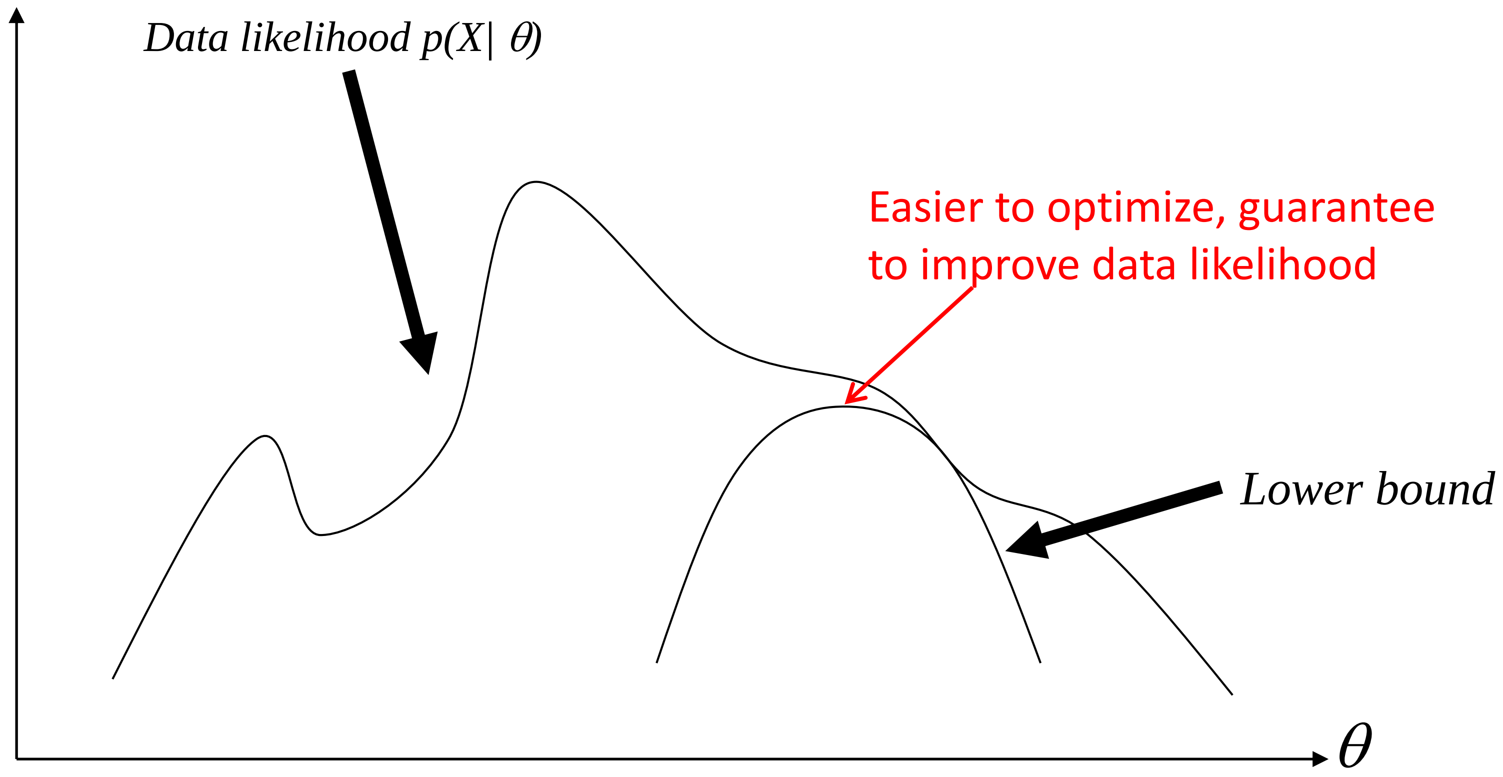
Jensen's inequality
$f(E[x]) \geq E[f(x)]$

$$\geq \sum_Z q(Z) \log p(X, Z|\theta) - \sum_Z q(Z) \log q(Z)$$

Lower bound: easier to compute, many good properties!

Components we need to tune when optimizing $L(\theta)$: $q(Z)$ and θ!

Intuitive understanding of EM



Expectation Maximization (cont)

- Optimize the lower bound w.r.t. $q(Z)$
  - $L(\theta) \geq \sum_Z q(Z) \, log \, p(X,Z|\theta) - \sum_Z q(Z) \, log \, q(Z)$

$$= \sum_Z q(Z)[\log p(Z|X,\theta) + \log p(X|\theta)] - \sum_Z q(Z) \log q(Z)$$

$$= \sum_Z q(Z) \log \frac{p(Z|X,\theta)}{q(Z)} + \log p(X|\theta)$$

KL-divergence between $q(Z)$ and $p(Z|X,\theta)$ Constant with respect to $q(Z)$

$$KL(P||Q) = \int P(x) \log \frac{P(x)}{Q(x)} dx$$

Expectation Maximization (cont)

- Optimize the lower bound w.r.t. $q(Z)$
  - $L(\theta) \geq -KL\big(q(Z)||p(Z|X,\theta)\big) + L(\theta)$
  - KL-divergence is non-negative, and equals to zero i.f.f. $q(Z) = p(Z|X,\theta)$
  - A step further: when $q(Z) = p(Z|X,\theta)$, we will get $L(\theta) \geq L(\theta)$, i.e., the lower bound is tight!
  - Other choice of $q(Z)$ cannot lead to this tight bound, but might reduce computational complexity
  - **Note**: calculation of $q(Z)$ is based on current θ

Expectation Maximization (cont)

- Optimize the lower bound w.r.t. $q(Z)$
  - Optimal solution: $q(Z) = p(Z|X, \theta^t)$

Posterior distribution of Z given current model θ^t

In k-means: this corresponds to assigning instance x_i to its closest cluster centroid c_k

$z_i = argmin_k d(c_k, x_i)$

Expectation Maximization (cont)

- Optimize the lower bound w.r.t. θ
  - $L(\theta) \geq \sum_Z p(Z|X,\theta^t) \log p(X,Z|\theta) - \cancel{\sum_Z p(Z|X,\theta^t) \log p(Z|X,\theta^t)}$ Constant w.r.t. θ
  - $\theta^{t+1} = argmax_\theta \sum_Z p(Z|X,\theta^t)\, log\, p(X,Z|\theta)$

$$= argmax_\theta E_{Z|X,\theta^t}[\log p(X,Z|\theta)]$$

Expectation of complete data likelihood

In k-means, we are *<u>not</u>* *computing the expectation, but the most probable configuration, and then* $c_k = \frac{\sum_i \delta(z_i=c_k)x_i}{\sum_i \delta(z_i=c_k)}$

Expectation Maximization

- EM tries to iteratively maximize likelihood
  - "Complete" likelihood: $L^c(\theta) = \log p(X, \mathrm{Z} | \theta)$
  - Starting from an initial guess $\theta^{(0)}$,
    1. **E-step**: compute the expectation of the complete likelihood

$$Q(\theta; \theta^t) = \mathrm{E}_{Z|X,\theta^t}[L^c(\theta)] = \sum_Z p(Z|X, \theta^t) \log \mathrm{p}(\mathrm{X}, \mathrm{Z}|\theta^t)$$

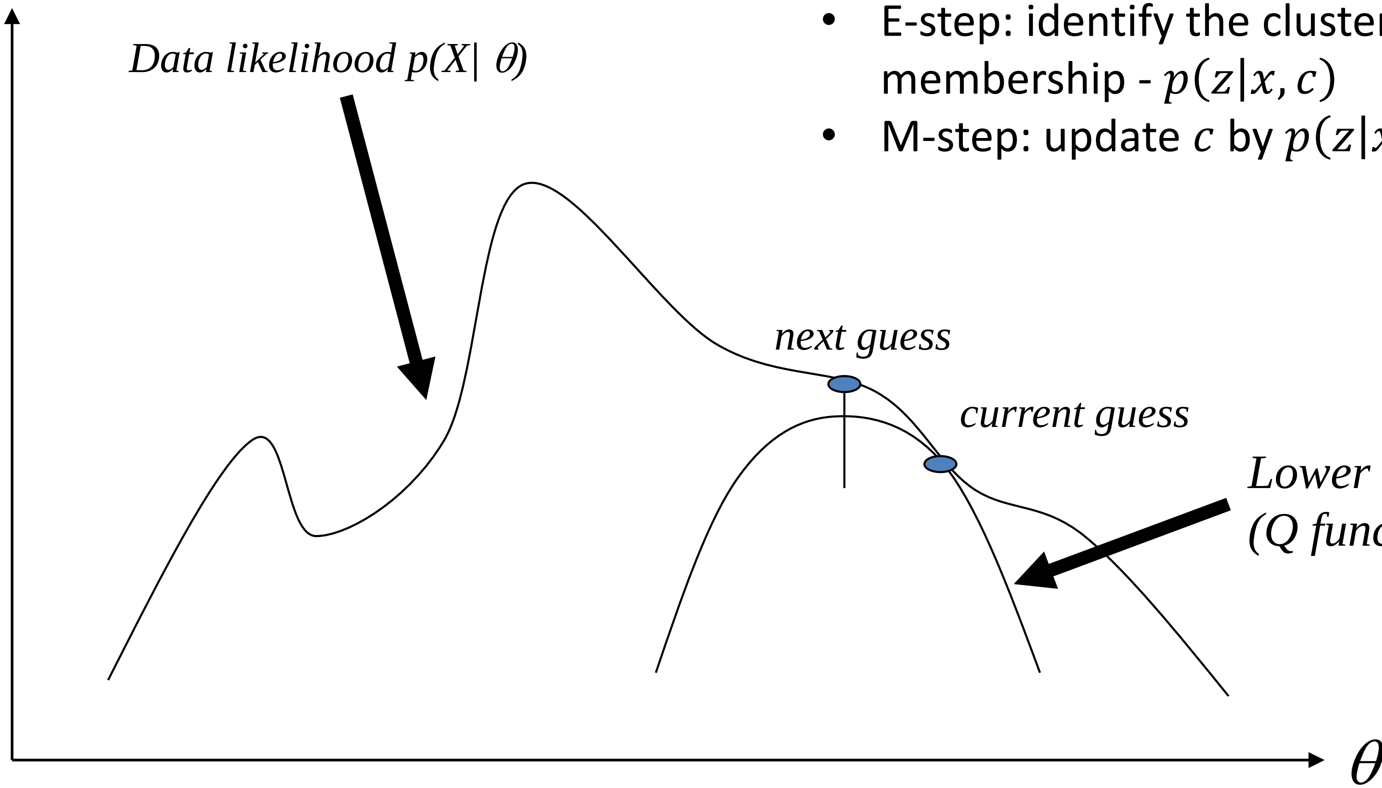
    2. **M-step**: compute $\theta^{(t+1)}$ by maximizing the Q-function

$$\theta^{t+1} = argmax_\theta Q(\theta; \theta^t)$$

Key step!

Intuitive understanding of EM

In *k*-means
- E-step: identify the cluster membership - $p(z|x,c)$
- M-step: update c by $p(z|x,c)$



E-step = computing the lower bound
M-step = maximizing the lower bound

Convergence guarantee

- Proof of EM

$$\log p(X|\theta) = \log p(Z,X|\theta) - \log p(Z|X,\theta)$$

Taking expectation with respect to $p(Z|X,\theta^t)$ of both sides:

$$\log p(X|\theta) = \sum_Z p(Z|X,\theta^t) \log p(Z,X|\theta) - \sum_Z p(Z|X,\theta^t) \log p(Z|X,\theta)$$

$$= Q(\theta;\theta^t) + \underline{H(\theta;\theta^t)} \longleftarrow \text{Cross-entropy}$$

Then the change of log data likelihood between EM iteration is:

$$\log p(X|\theta) - \log p(X|\theta^t) = Q(\theta;\theta^t) + H(\theta;\theta^t) - Q(\theta^t;\theta^t) - H(\theta^t;\theta^t)$$

By Jensen's inequality, we know $H(\theta;\theta^t) \geq H(\theta^t;\theta^t)$, that means

$$\log p(X|\theta) - \log p(X|\theta^t) \geq Q(\theta;\theta^t) - Q(\theta^t;\theta^t) \underline{\geq 0}$$

M-step guarantee this

What is not guaranteed

- Global optimal is not guaranteed!
  - Likelihood: $L(\theta) = \log \sum_Z p(X, \mathrm{Z}|\theta)$ is non-convex in most of case
  - EM boils down to a <u>greedy</u> algorithm
    - Alternative ascent
- Generalized EM
  - E-step: $\hat{q}(Z) = \mathrm{argmin}_{q(Z)} KL\big(q(Z)||p(Z|X, \theta^t)\big)$
  - M-step: choose θ that improves $Q(\theta; \theta^t)$

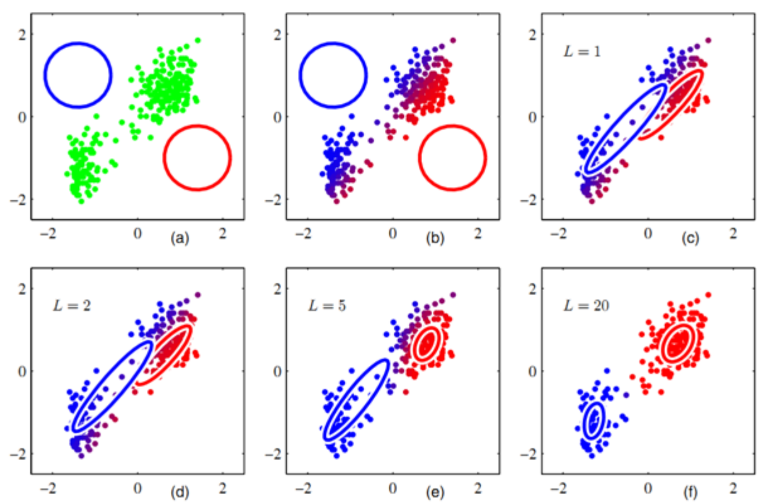
k-means v.s. Gaussian Mixture

- If we use Euclidean distance in *k*-means
  - We have explicitly assumed $p(x|z)$ is Gaussian
  - Gaussian Mixture Model (GMM)
    - $p(x|z) = N(\mu_z, \Sigma_z)$
    - $p(z) = \alpha_z$ ← Multinomial

$$P(x|z) = \frac{1}{\sqrt{(2\pi)^k \Sigma_z}} e^{-\frac{1}{2}(x-\mu_z)^T \Sigma_z^{-1}(x-\mu_z)}$$

$$\frac{1}{\delta\sqrt{2\pi}} e^{-\frac{(x-\mu_z)^T(x-\mu_z)}{2\delta^2}}$$

We do not consider cluster size in *k*-means

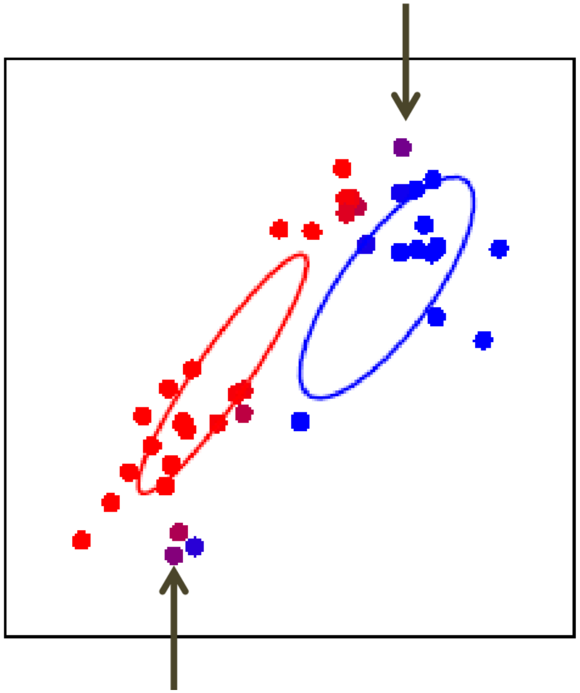


In *k*-means, we assume equal variance across clusters, so we don't need to estimate them

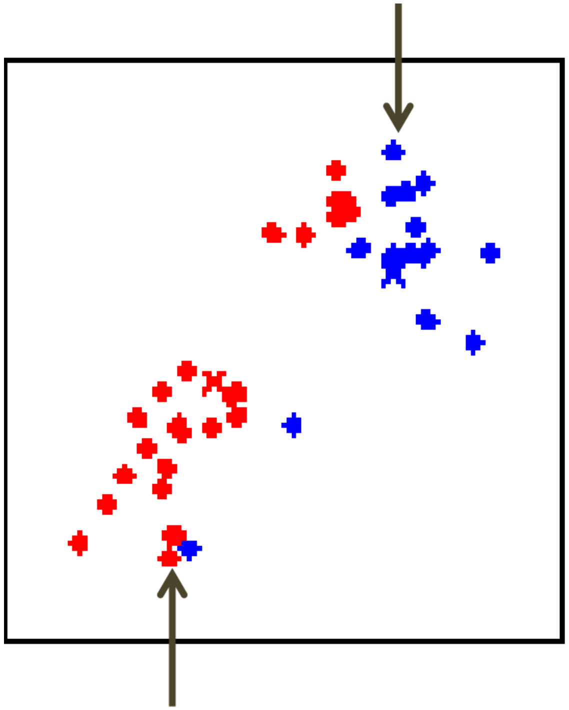
k-means v.s. Gaussian Mixture

- Soft v.s., hard posterior assignment

GMM



k-means



k-means in practice

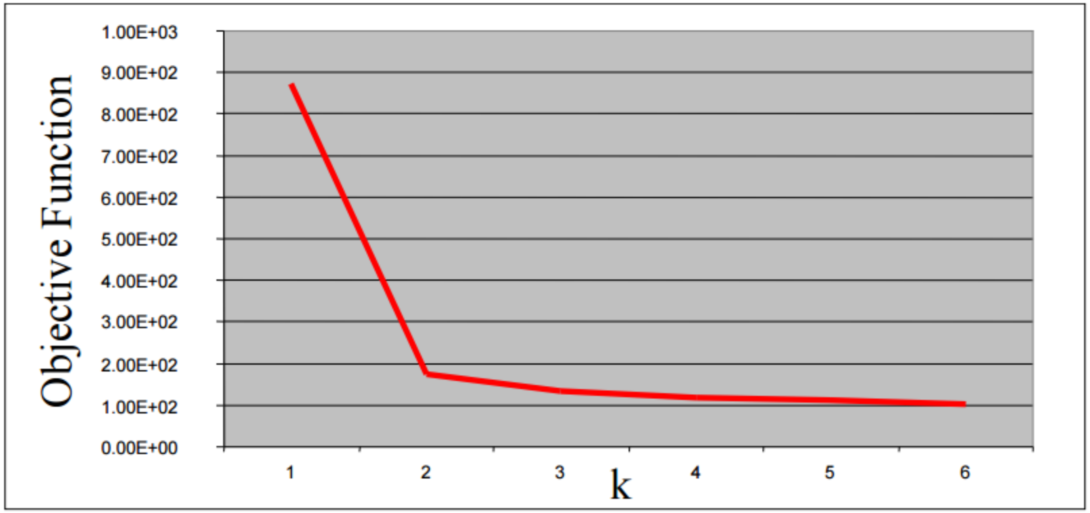
- Extremely fast and scalable
  - One of the most popularly used clustering methods
    - Top 10 data mining algorithms – ICDM 2006
  - Can be easily parallelized
    - Map-Reduce implementation
      - Mapper: assign each instance to its closest centroid
      - Reducer: update centroid based on the cluster membership
  - Sensitive to initialization
    - Prone to local optimal

Better initialization: *k*-means++

1. Choose the first cluster center at uniformly random
2. Repeat until all *k* centers have been found
   – For each instance compute $\mathrm{D_x} = \min_{\mathrm{k}} d(x, c_k)$
   – Choose a new cluster center with probability $p(x) \propto D_x^2$ ← *new center should be far away from existing centers*
3. Run *k*-means with selected centers as initialization

How to determine k

- Vary k to optimize clustering criterion
  - Internal v.s. external validation
  - Cross validation
    - Abrupt change in objective function



How to determine k

- Vary k to optimize clustering criterion
  - Internal v.s. external validation
  - Cross validation
    - Abrupt change in objective function
    - Model selection criterion – penalizing too many clusters
      - AIC, BIC

What you should know

- *k*-means algorithm
  - An alternative greedy algorithm
  - Convergence guarantee
    - EM algorithm
  - Hard clustering v.s., soft clustering
    - *k*-means v.s., GMM

Today’s reading

- Introduction to Information Retrieval
  - Chapter 16: Flat clustering
    - 16.4 *k*-means
    - 16.5 Model-based clustering