Data Mining

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Acknowledgements

- E. Frank
- I. Witten
- ... and others

Outline

- k-Means
- Probability-based/model-based clustering: the EM algorithm

K-Means

Partitioning Algorithms: Basic Concept

- *Partitioning method*: construct a partition of a database D of n objects into a set of k clusters such that the sum of the squared distances is minimized

$$\Sigma_{m=1}^{k}\Sigma_{t_{mi}\in Km}(C_m - t_{mi})^2$$

- Given a k, find a partition of k *clusters* that optimizes the chosen partitioning criterion
  - globally optimal: exhaustively enumerate all partitions
  - heuristic methods: *k-means* and *k-medoids* algorithms
  - *k-means* (MacQueen 67): each cluster is represented by the center of the cluster
  - *k-medoids* or PAM (partition around medoids) (Kaufman & Rousseeuw 87): each cluster is represented by one of the objects in the cluster

Goal of Clustering 1

- Total sum of pairwise distances:

$$T(C) = W(C) + B(C)$$

- Within cluster distances:

$$W(C) = \frac{1}{2} \sum_{k=1}^{K} \sum_{C(i)=k} \sum_{C(i')=k} d(x_i, x_{i'})$$

- Between cluster distances:

$$B(C) = \frac{1}{2} \sum_{k=1}^{K} \sum_{C(i)=k} \sum_{C(i')\neq k} d(x_i, x_{i'})$$

Goal of Clustering 2

- *Assuming* K *is fixed* in this simple setting, *maximizing* B(C) *and minimizing* W(C) *is the same!*
  - we assume real-valued data and use the ***squared** Euclidean distance*

$$d(x_i, x_{i'}) = \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2 = \left\| x_i - x_{i'} \right\|^2$$

$$T = \frac{1}{2}\sum_{i=1}^{N}\sum_{i'=1}^{N} d(x_i, x_{i'}) = \frac{1}{2}\sum_{k=1}^{K}\sum_{C(i)=k}\left(\sum_{C(i')=k} d(x_i, x_{i'}) + \sum_{C(i')\neq k} d(x_i, x_{i'})\right)$$

Goal of Clustering 3

- Thus, the goal is to minimize:

$$W(C) = \frac{1}{2} \sum_{k=1}^{K} \sum_{C(i)=k} \sum_{C(i')=k} \left\| x_i - x_{i'} \right\|^2 = \sum_{k=1}^{K} \sum_{C(i)=k} \left\| x_i - \bar{x}_k \right\|^2$$

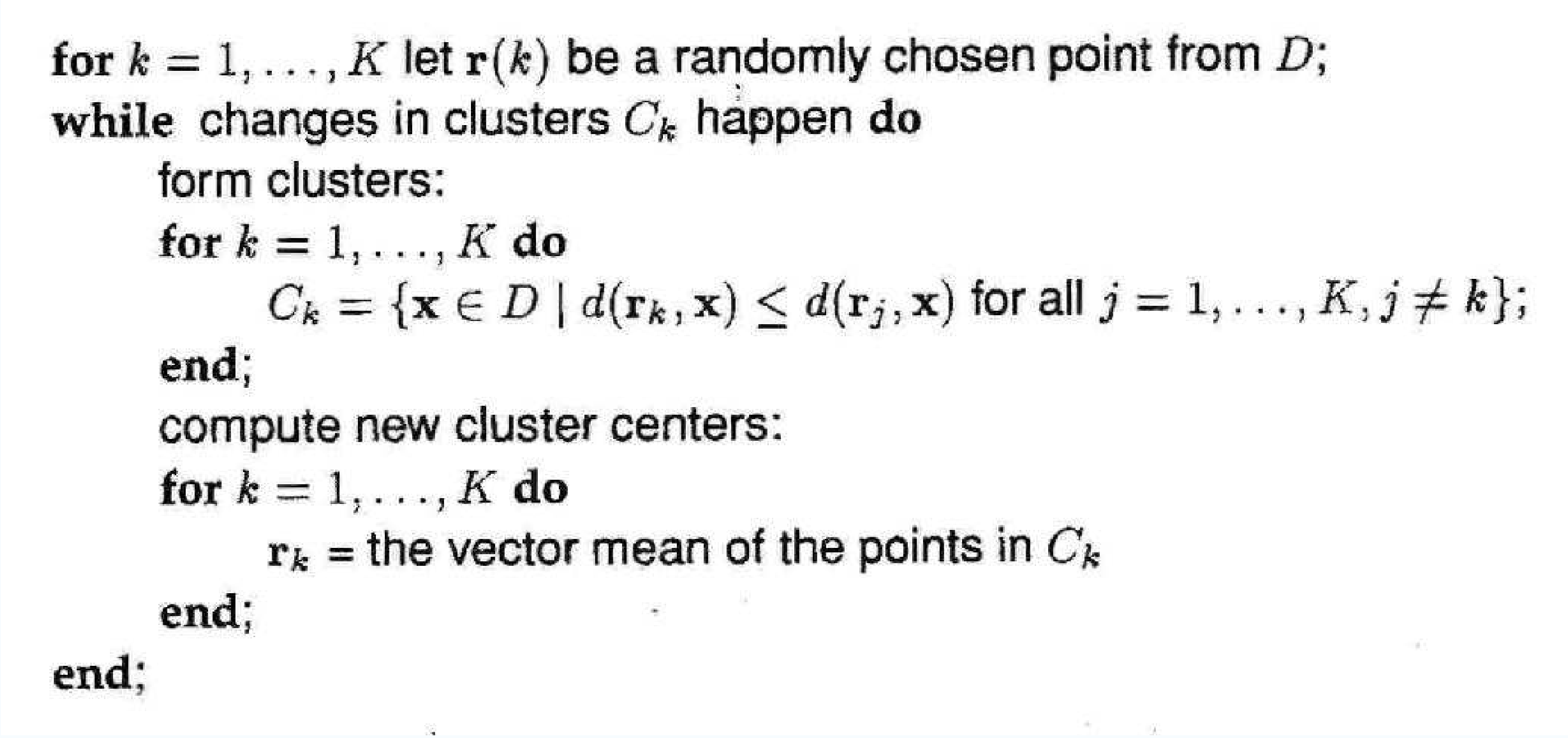
$$\min_{C} \sum_{k=1}^{K} \sum_{C(i)=k} \left\| x_i - \bar{x}_k \right\|^2$$

$$\min_{C,\{m_k\}_1^K} \sum_{k=1}^{K} \sum_{C(i)=k} \left\| x_i - m_k \right\|^2$$

- *Alternating optimization procedure…*

K-Means Algorithm

Given data points D ={$\mathbf{x}_1,\ldots,\mathbf{x}_n$} , find K clusters {$C_1,\ldots,C_K$}

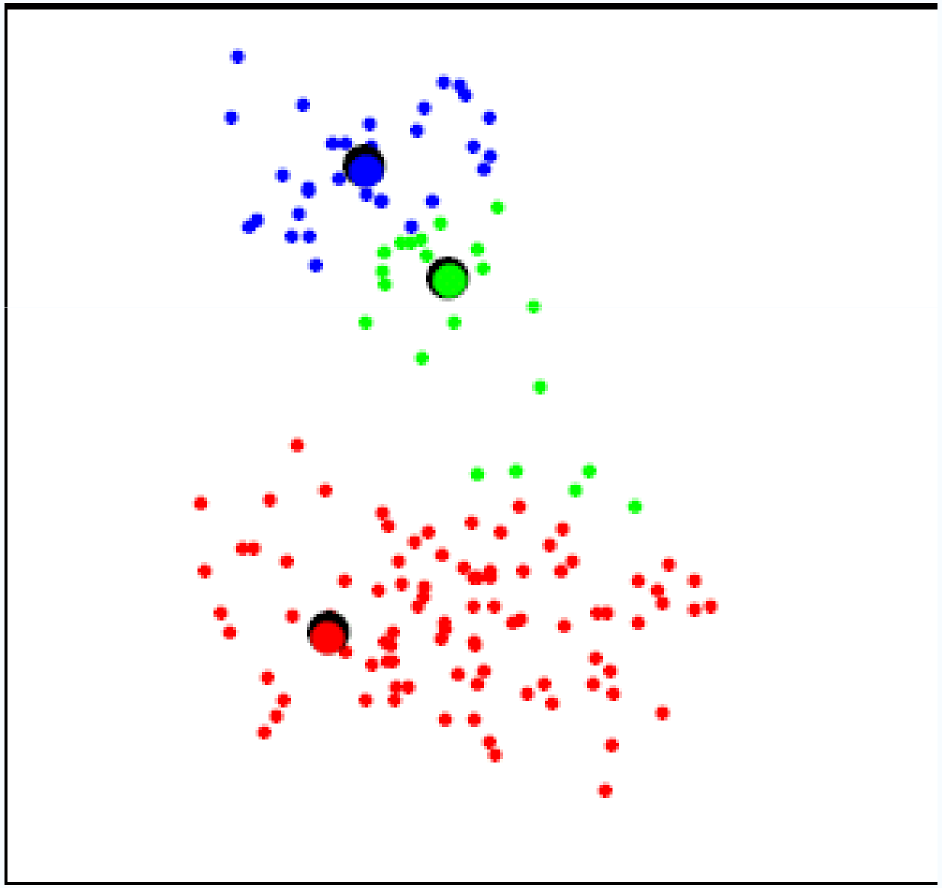


```
for $k = 1, \ldots, K$ let $\mathbf{r}(k)$ be a randomly chosen point from $D$;
while changes in clusters $C_k$ happen do
    form clusters:
    for $k = 1, \ldots, K$ do
        $C_k = \{\mathbf{x} \in D \mid d(\mathbf{r}_k, \mathbf{x}) \leq d(\mathbf{r}_j, \mathbf{x})$ for all $j = 1, \ldots, K, j \neq k\}$;
    end;
    compute new cluster centers:
    for $k = 1, \ldots, K$ do
        $\mathbf{r}_k$ = the vector mean of the points in $C_k$
    end;
end;
```

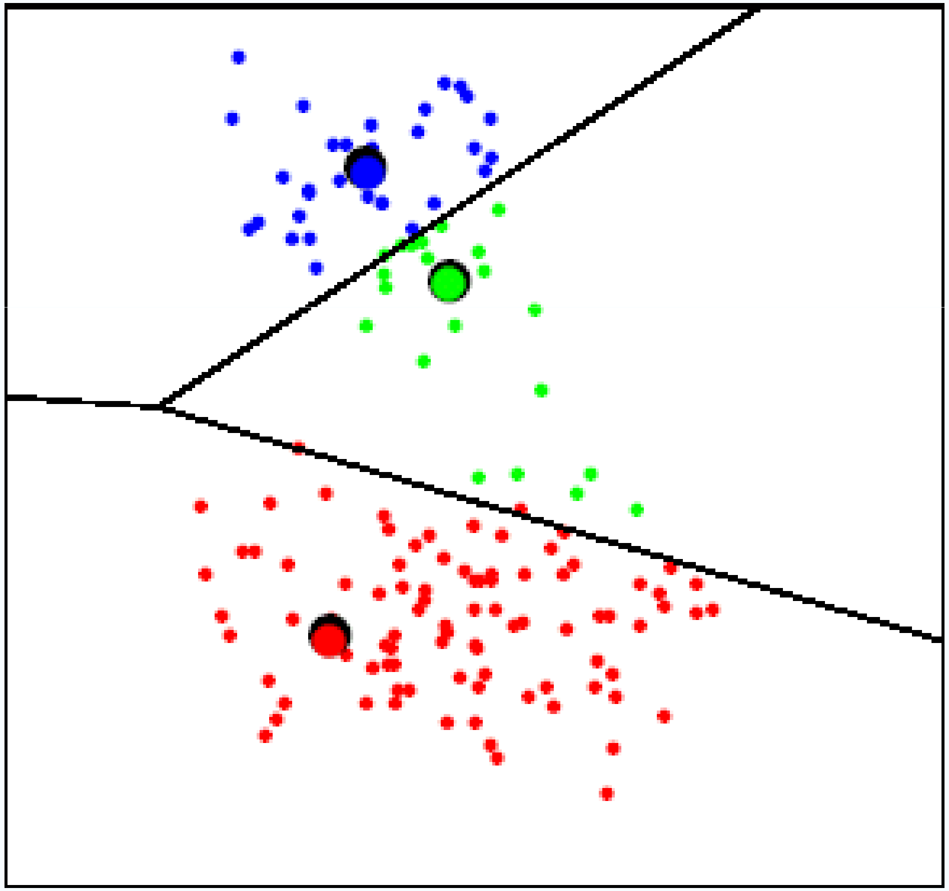
Complexity

- K number of cluster centers
- n sample size
- I number of iterations
- *Suggestions?*

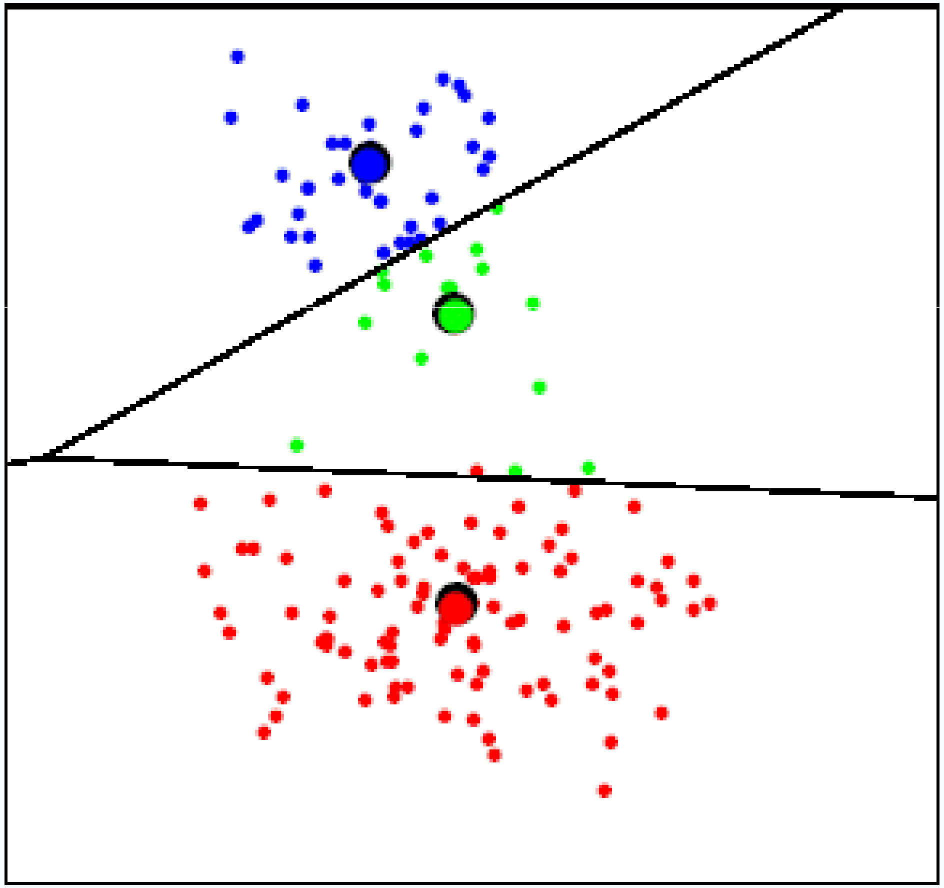
K-Means: Initial Centroids



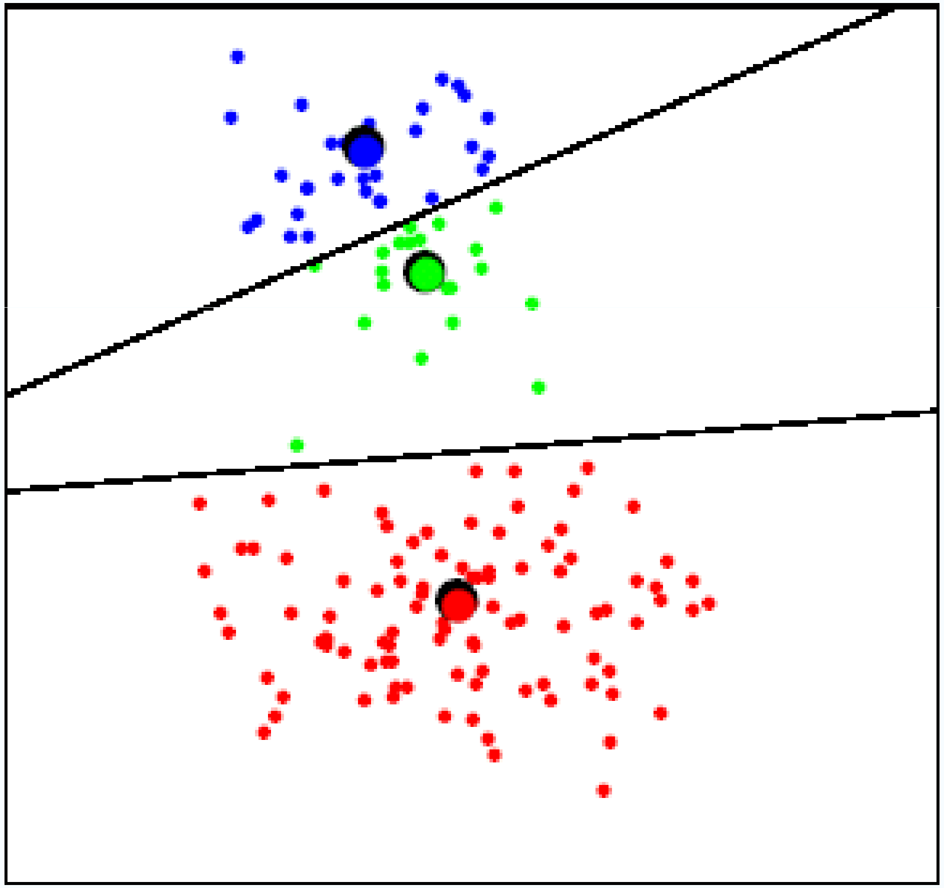
K-Means: Initial Partition



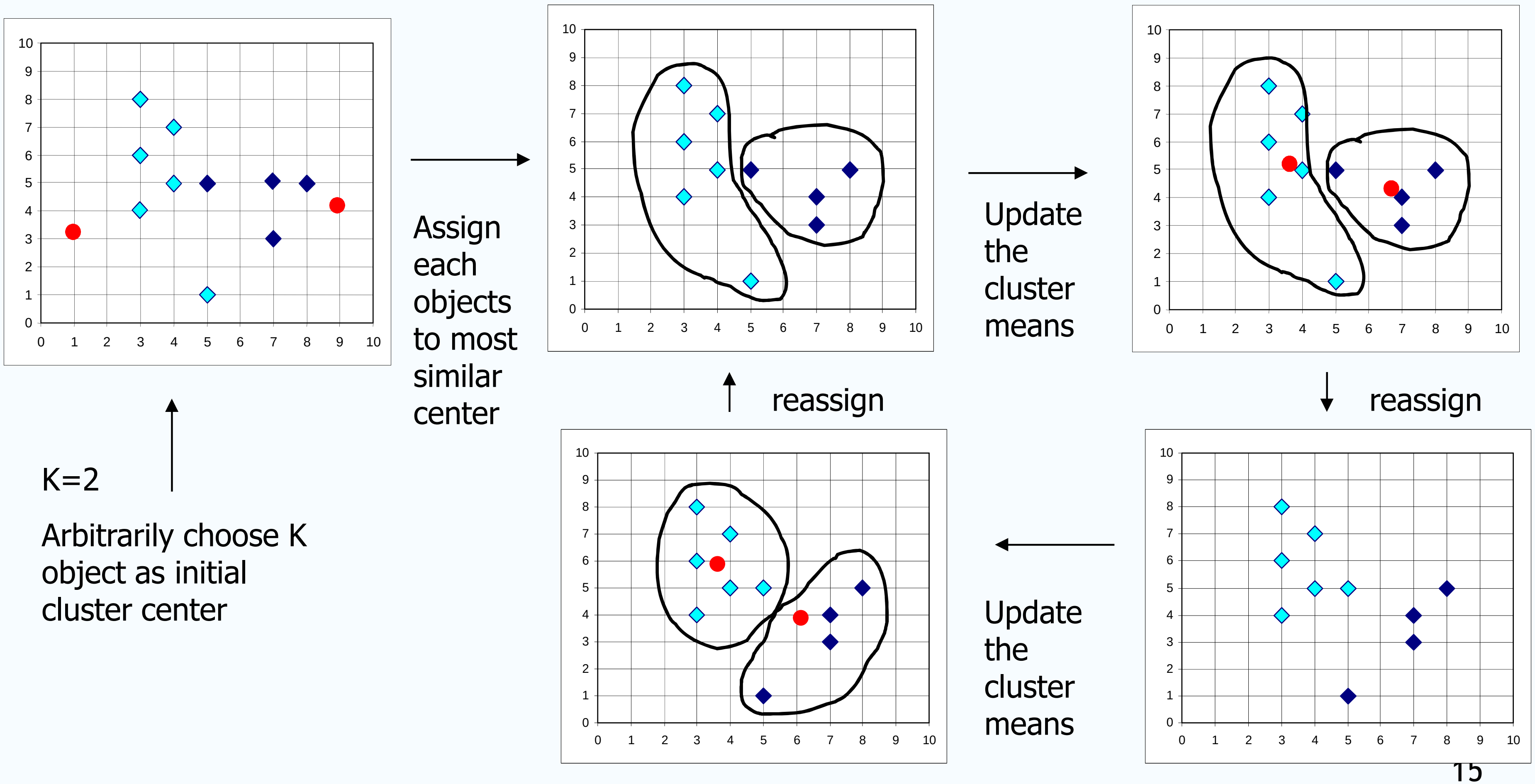
K-Means: Iteration 2



K-Means: Iteration 20



Another Example: K-Means At Work



K=2

Arbitrarily choose K object as initial cluster center

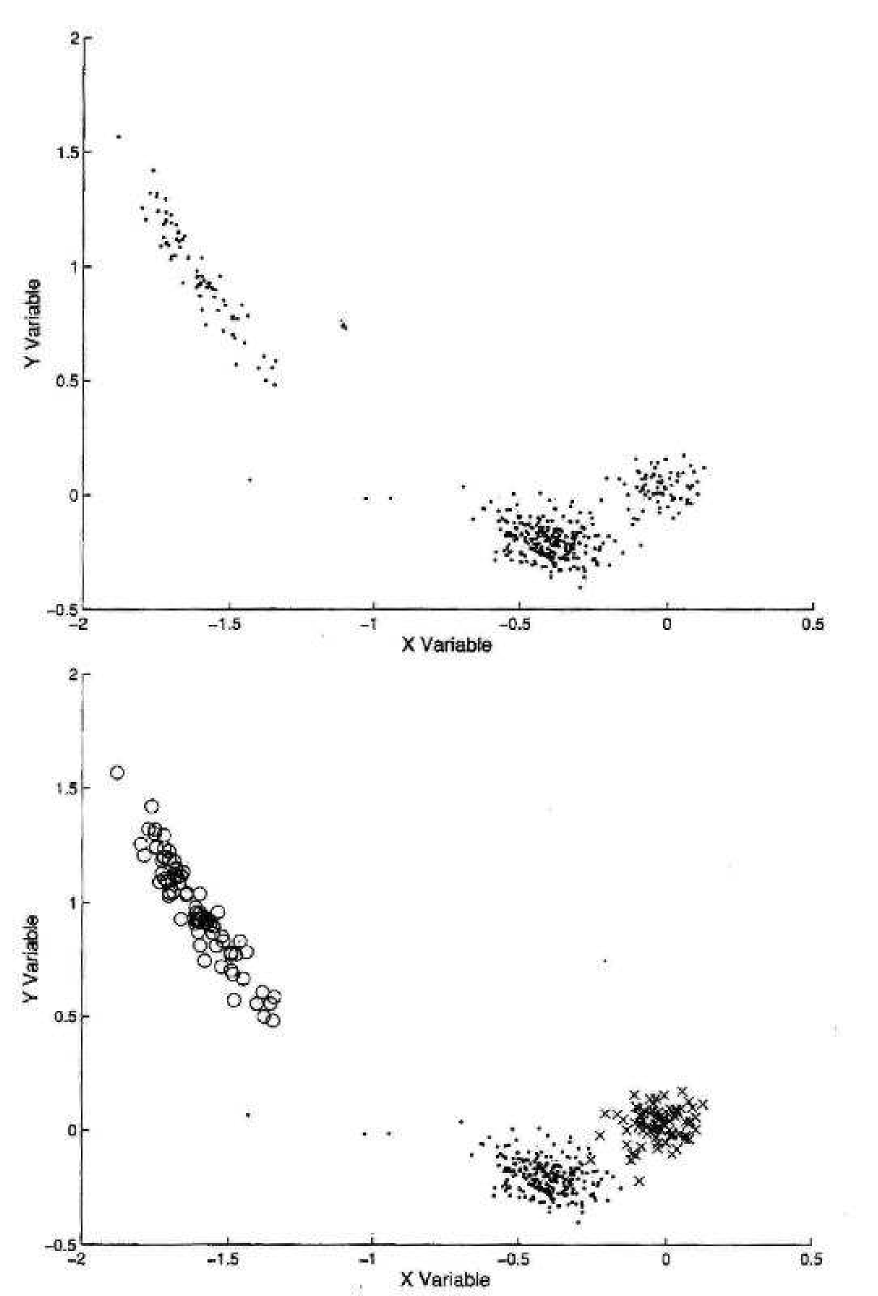
Assign each objects to most similar center

Update the cluster means

reassign

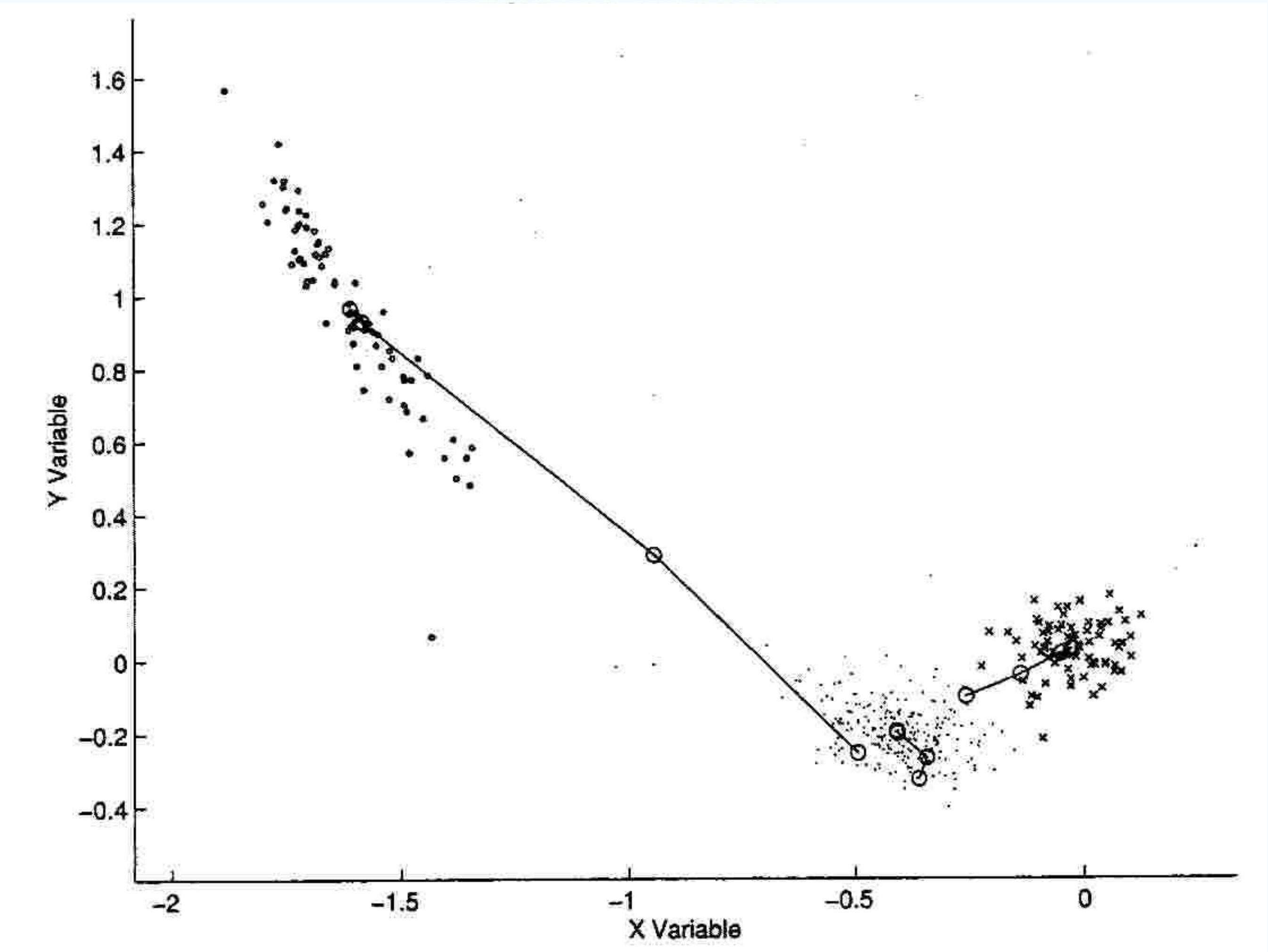
reassign

Update the cluster means

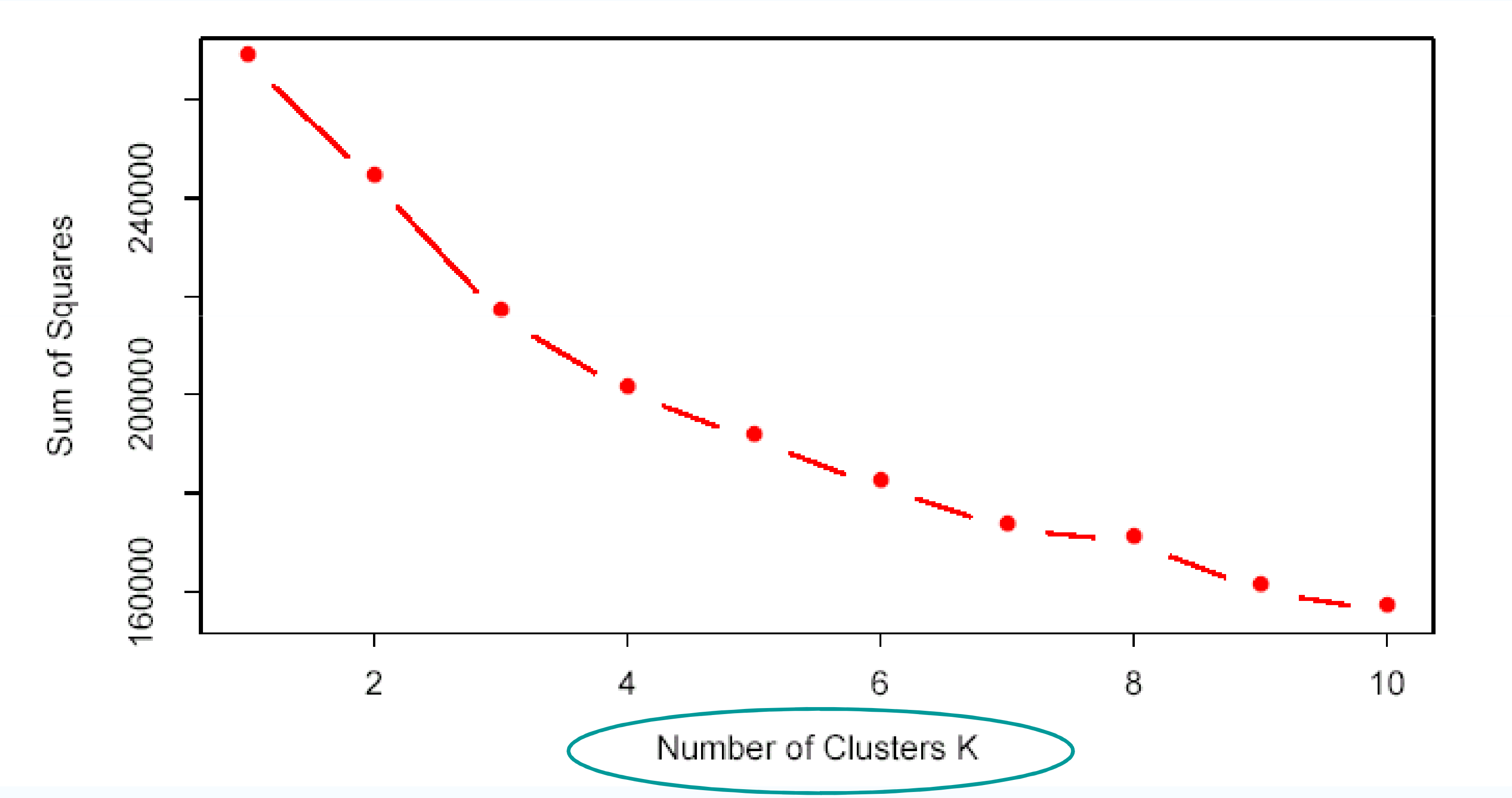


Antenna Data with/without Class Labels

Trajectory of Cluster Means on Antenna Data



K-Means Applied to Microarray Data



Y axis: total within-cluster sum of squares

K-Means Discussion 1

- Most suitable for real-valued data
- Prefers small, spherical clusters, unable to discover clusters with *non-convex shapes*
- Converges to a local optimum („trapped in local minimum“)
- *Not too many theoretical results on convergence*
- Example for local minimum:
    - four instances at the vertices of a two-dimensional rectangle
    - two cluster centers at the midpoints of the rectangle’s long sides

K-Means Discussion 2

- Result can vary significantly based on initial choice of seeds
- Simple way to increase chance of finding a global optimum: restarts with different random seeds (“random restarts”)
- Linear in the examples - suitable for *large datasets*
- K has to be specified by the user - extensions as X-Means possible

Probability-Based/Model-Based Clustering: The EM Algorithm

Probability-Based Clustering

- Problem with previous approaches:
    - *ad hoc*: what are actually the clusters that are obtained? ("semantics")
    - instances are "deterministically" assigned to one cluster
- From a probabilistic perspective, we want to find the *most likely clusters given the data*
- Also: instance only has certain *probability of belonging to a particular cluster*

Finite Mixtures

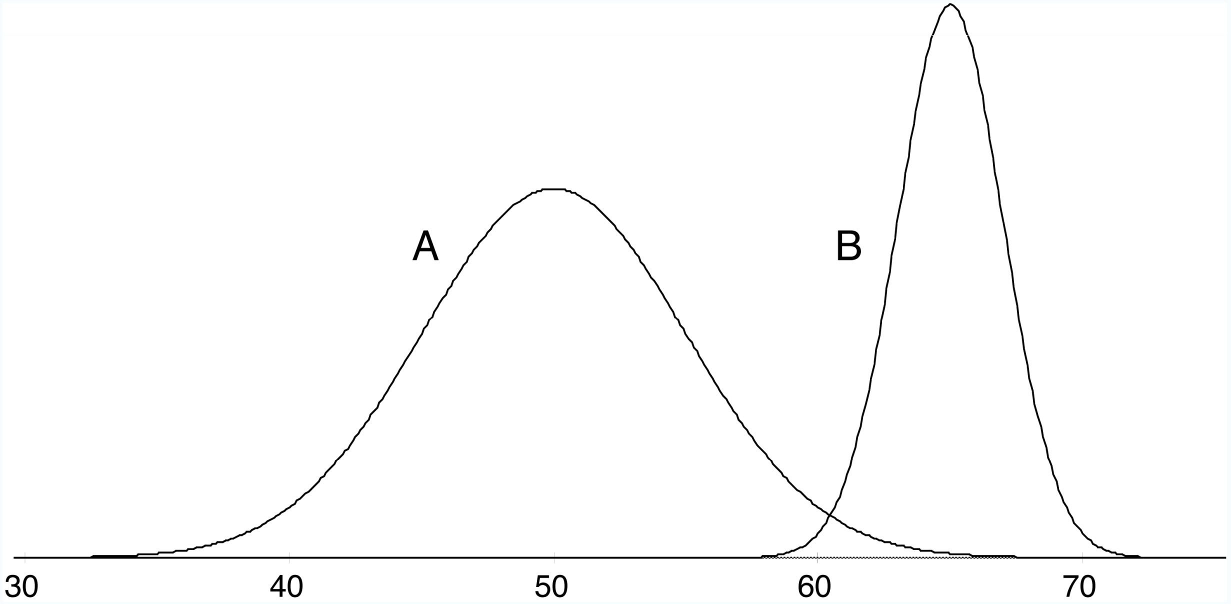
- Probabilistic clustering algorithms model the data as a mixture of distributions
- They are called *finite mixtures* because there is only a finite number of clusters being represented
- *Each cluster* is represented by *one distribution*
  - distribution governing the probabilities of attribute values in the clusters
- Usually individual distributions are normal distributions
- Distributions are combined using cluster weights

A Two-Class Mixture Model

data

A	51	B	62	B	64	A	48	A	39	A	51
A	43	A	47	A	51	B	64	B	62	A	48
B	62	A	52	A	52	A	51	B	64	B	64
B	64	B	64	B	62	B	63	A	52	A	42
A	45	A	51	A	49	A	43	B	63	A	48
A	42	B	65	A	48	B	65	B	64	A	41
A	46	A	48	B	62	B	66	A	48		
A	45	A	49	A	43	B	65	B	64		
A	45	A	46	A	40	A	46	A	48		

model



μ_A=50, σ_A =5, p_A=0.6 μ_B=65, σ_B =2, p_B=0.4

Using the Mixture Model

- The probability of an instance x belonging to cluster A is:

$$\Pr[A \mid x] = \frac{\Pr[x \mid A]\Pr[A]}{\Pr[x]} = \frac{f(x;\mu_A,\sigma_A)p_A}{\Pr[x]}$$

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

- The *likelihood* of a *single instance* x given *all clusters* is:

$$\Pr[x \mid \text{the distributions}] = \sum_i \Pr[x \mid \text{cluster}_i]\Pr[\text{cluster}_i]$$

Learning the Clusters

- Assume we know that there are k clusters
- To learn the clusters we need to determine their *parameters*, i.e., their means and standard deviations
- We actually have a *performance criterion*: *likelihood of training data* given the clusters
- Fortunately, there exists an algorithm that finds a local maximum of the likelihood

EM Algorithm for Clustering

- EM algorithm: expectation-maximization algorithm
- In a sense, generalization of k-means to *probabilistic setting*
- Similar iterative procedure:
  1. Calculate cluster probability for each instance (**E**xpectation step)
  2. Estimate distribution parameters based on the cluster probabilities (**M**aximization step)
- Cluster probabilities are stored as instance weights

More on EM

- Estimating parameters from weighted instances:

$$\mu_A = \frac{w_1 x_1 + w_2 x_2 + \ldots + w_n x_n}{w_1 + w_2 + \ldots + w_n}$$

$$\sigma_A{}^2 = \frac{w_1 (x_1 - \mu)^2 + w_2 (x_2 - \mu)^2 + \ldots + w_n (x_n - \mu)^2}{w_1 + w_2 + \ldots + w_n}$$

Log-Likelihood

- Procedure stops when *log-likelihood* saturates

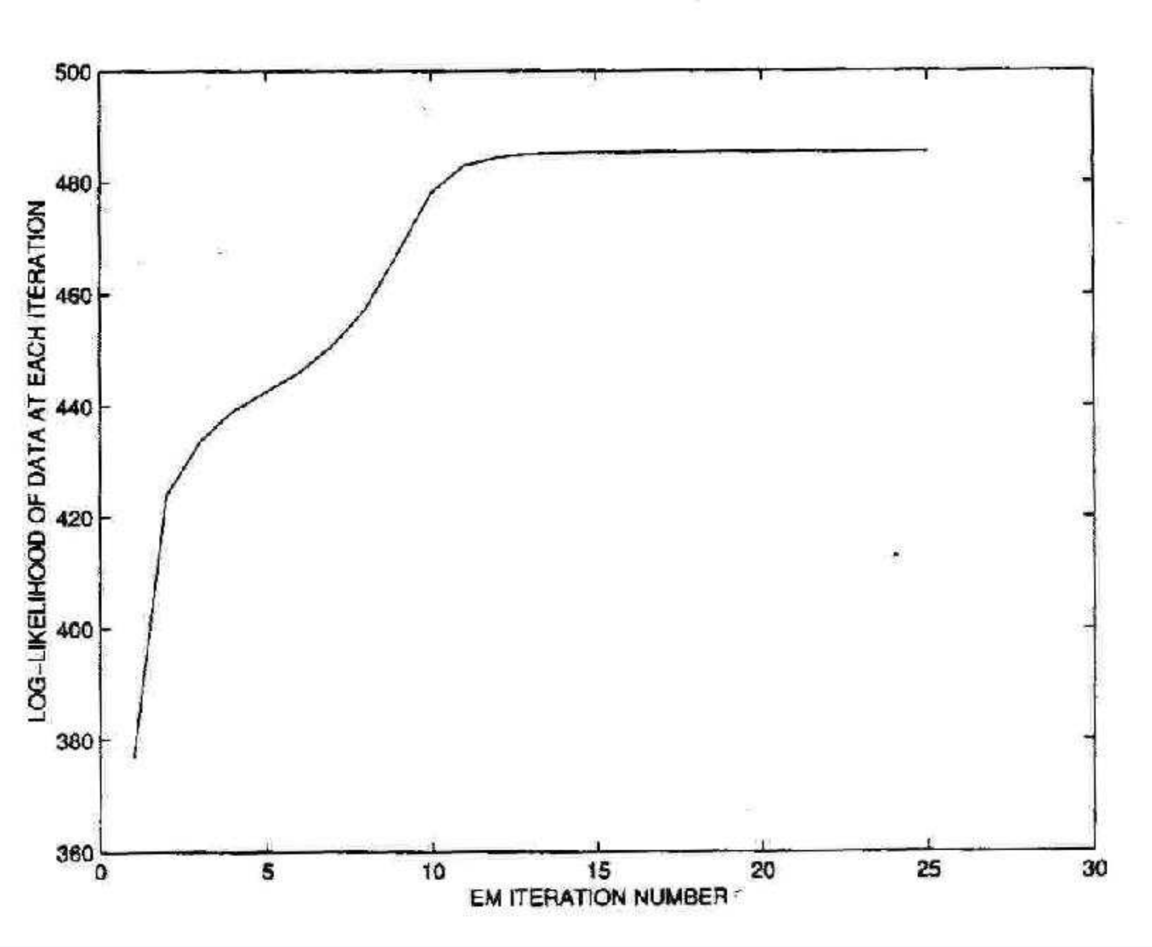
$$\log \prod_{x_i \in D} likelihood(x_i) = \log \prod_{x_i \in D} \sum_{k \in Cluster} p_k P(x_i \mid C_k) =$$

$$\sum_{x_i \in D} \log \sum_{k \in Cluster} p_k P(x_i \mid C_k)$$

- For two clusters A and B:

$$\sum_{x_i \in D} \log(p_A P(x_i \mid A) + p_B P(x_i \mid B))$$

EM: Log-Likelihood over a Few Iterations



Special Case of EM: Putting it All Together

```
while log likelihood changes do
  % calculate cluster probability
  % for each instance (E-step)
  for each instance $x_i$ do
    $w_i = f(x_i; \mu_A, \sigma_A)p_A / P[x_i]$
  % estimate distribution parameters based
  % on the cluster probabilities (M-step)
  $\mu_A = \Sigma w_i x_i / \Sigma w_i$
  $\sigma_A^2 = \Sigma w_i(x_i - \mu_A)^2 / \Sigma w_i$
   % analogously for $\mu_B$ and $\sigma_B^2$ with $(1-w_i)$
```

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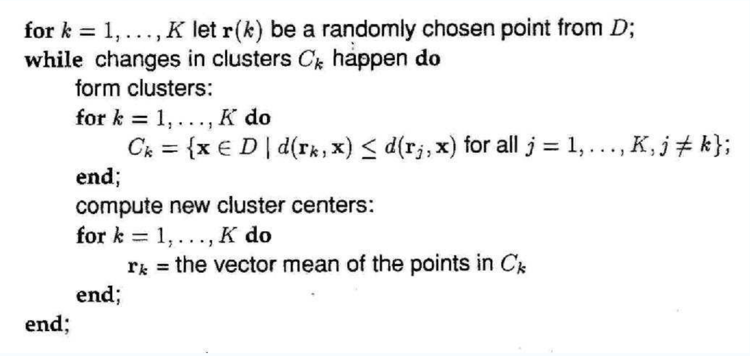

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    end;
    compute new cluster centers:
    for $k = 1, \ldots, K$ do
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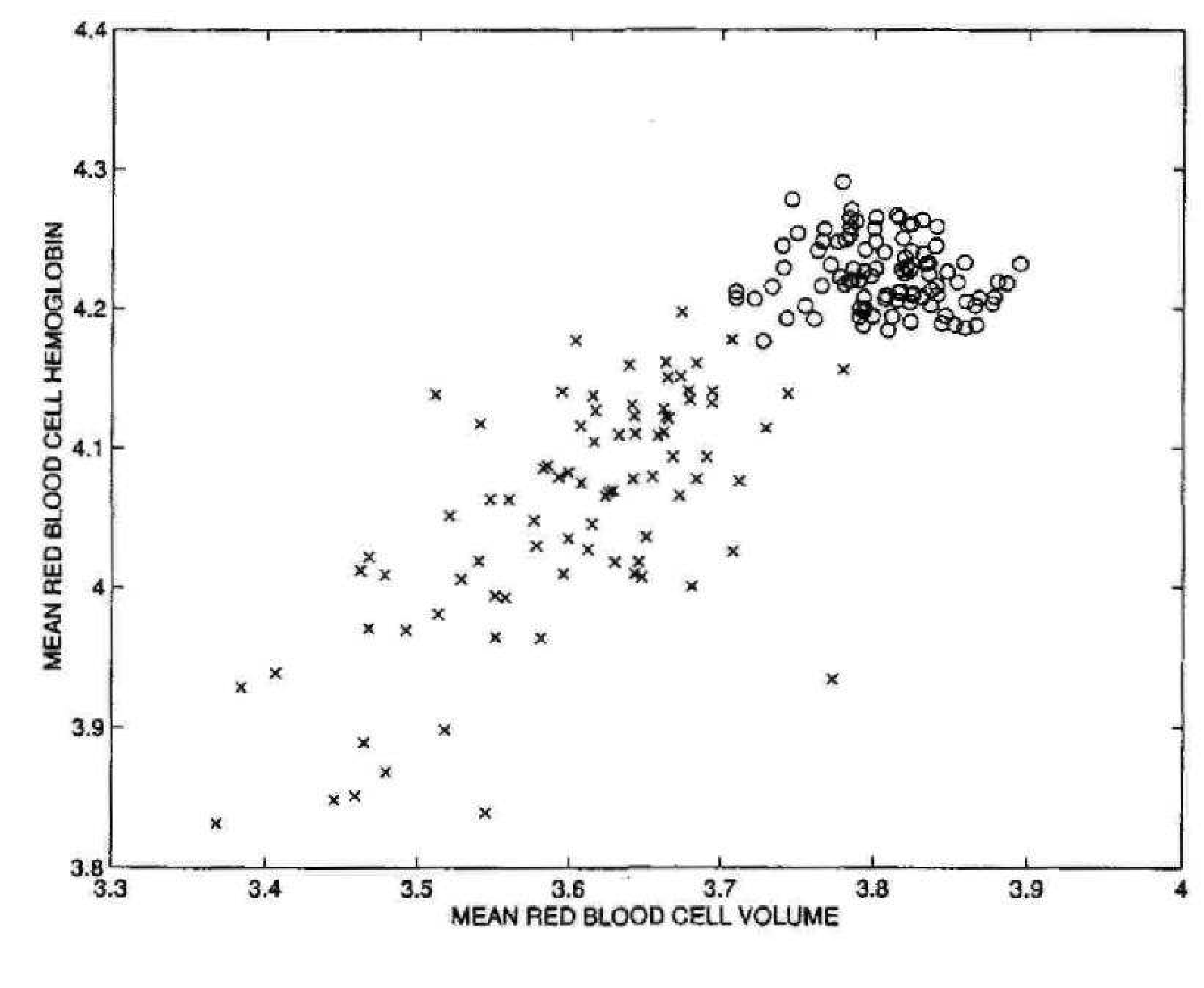
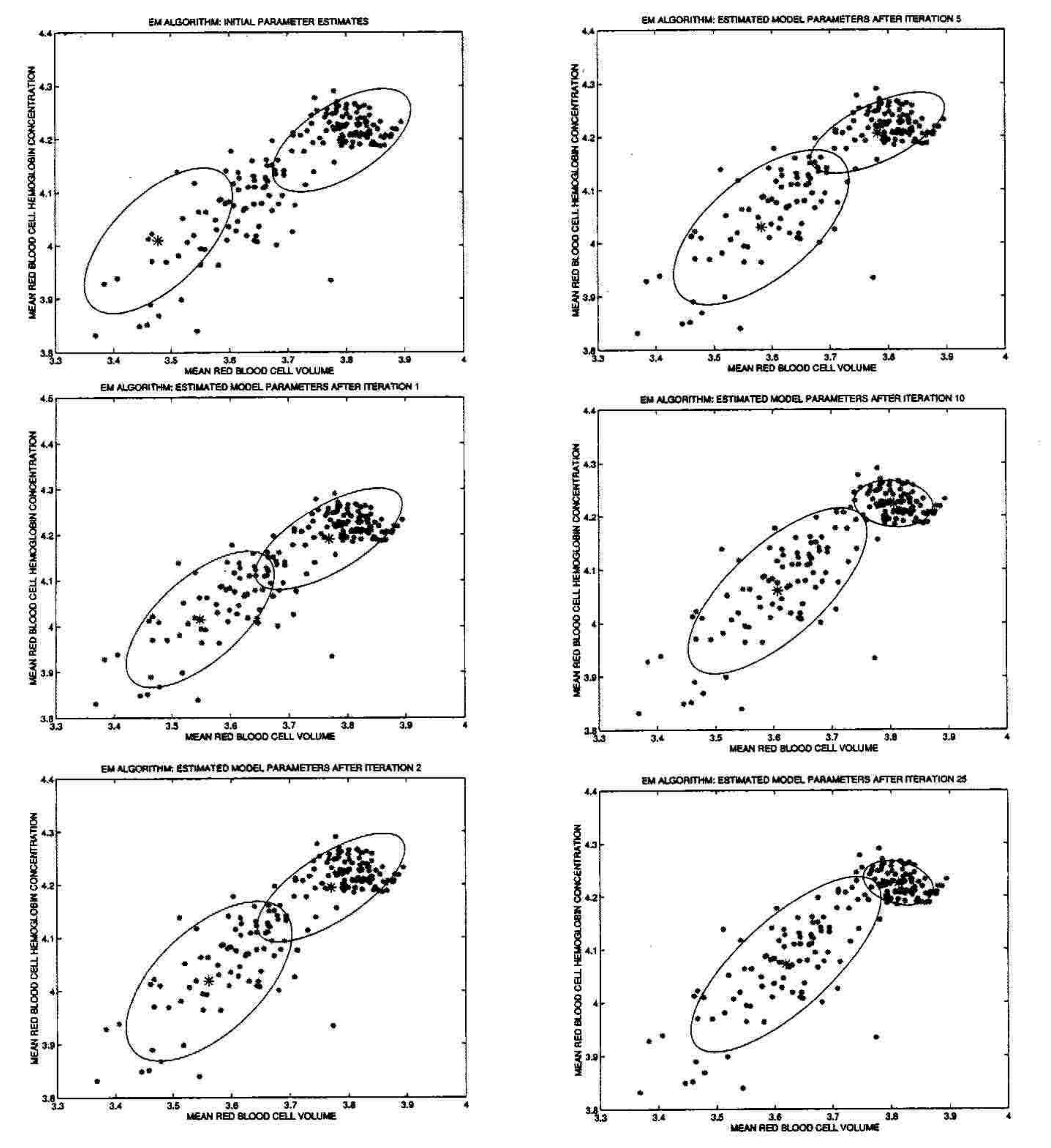
    end;
end;
```

Red Blood Cell Data



Circles: healthy, crosses: iron deficient anemia



Example Run EM on Red Blood Cell Data

3σ covariance ellipses and means for iterations 1, 2, 5, 10, 25

Extensions 1

- Using more than two distributions: easy
- Several attributes: easy if independence is assumed
- Correlated attributes: difficult
  - Modeled jointly using a bivariate normal distribution with a covariance matrix
  - With n attributes this requires estimating n + n(n+1)/2 parameters
- Nominal attributes: easy if independent

Extensions 2

- Correlated nominal attributes: difficult
  - two correlated attributes result in v1 x v2 parameters
- Missing values: easy
- Distributions other than the normal distribution can be used:
  - log-normal if predetermined minimum is given
  - log-odds if bounded from above and below
  - Poisson for attributes that are integer counts
- Cross-validation can be used to estimate k

Discussion

- Can be used to fill in missing values
- Big advantage of probabilistic clustering schemes: likelihood of data can be estimated and used to compare different clusterings