Clustering Techniques for Information Retrieval

Berlin Chen
Department of Computer Science & Information Engineering
National Taiwan Normal University

References:

1. Christopher D. Manning, Prabhakar Raghavan and Hinrich Schütze, Introduction to Information Retrieval, Cambridge University Press, 2008. (Chapters 16 & 17)
2. *Modern Information Retrieval*, Chapters 5 & 7
3. "*A Gentle Tutorial of the EM Algorithm and its Application to Parameter Estimation for Gaussian Mixture and Hidden Markov Models*," Jeff A. Bilmes, U.C. Berkeley TR-97-021

Clustering

- Place similar objects in the same group and assign dissimilar objects to different groups
  - **Word clustering**
    - Neighbor overlap: words occur with the similar left and right neighbors (such as *in* and *on*)
  - **Document clustering**
    - Documents with the similar topics or concepts are put together
- But clustering cannot give a comprehensive description of the object
  - How to label objects shown on the visual display is a difficult problem

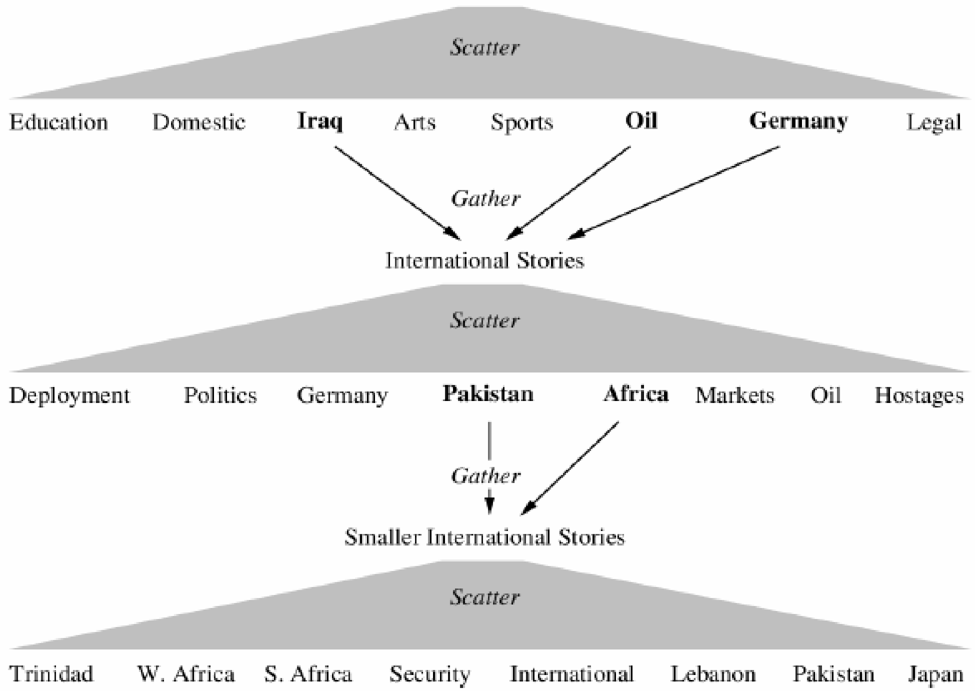
Clustering vs. Classification

- Classification is supervised and requires a set of labeled training instances for each group (class)
  - Learning with a teacher

- Clustering is unsupervised and learns without a teacher to provide the labeling information of the training data set
  - Also called automatic or unsupervised classification

Why Cluster Documents for IR (1/4)

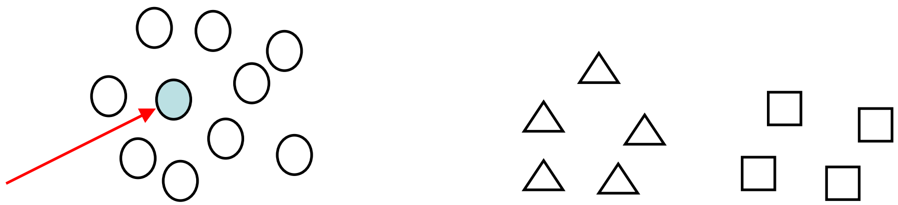
1. Whole corpus analysis/navigation
   - Better user interface (users prefer browsing over searching since they are unsure about which search terms to use)
   - E.g., the *scatter-gather* approach



► **Figure 16.3** The Scatter-Gather user interface. A collection of New York Times news stories is clustered ("scattered") into eight clusters (top row). The user manually *gathers* three of these into a smaller collection *International Stories* and performs another scattering operation. This process repeats until a small cluster with relevant documents is found (e.g., *Trinidad*).

Why Cluster Documents for IR (2/4)

2. Improve recall in search applications
   - Achieve better search results by
     - Alleviating the term-mismatch (synonym) problem facing the vector space model



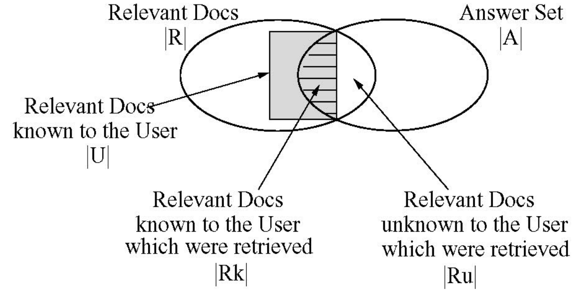
found relevant document

     - Estimating the collection model of the language modeling (LM) retrieval approach more accurately

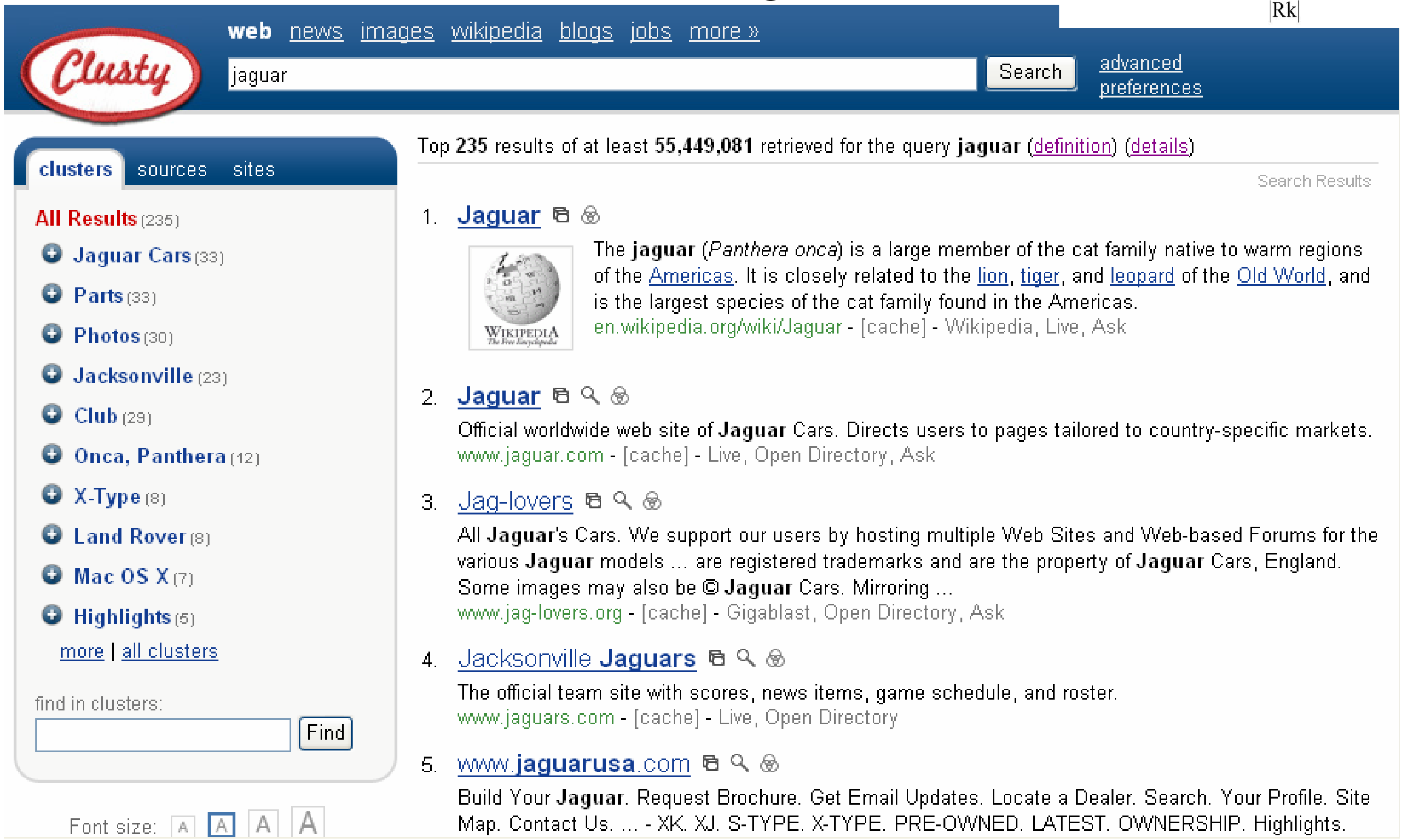
$$P(Q|M_D) = \prod_{i=1}^{N} \left[\lambda \cdot P(w_i|M_D) + (1-\lambda) \cdot P(w_i|M_C)\right]$$

The collection model can be estimated from the cluster the document *D* belongs to, instead of the entire collection

Why Cluster Documents for IR (3/4)



3. Better navigation of search results
   - Result set clustering
   - Effective "user recall" will be higher



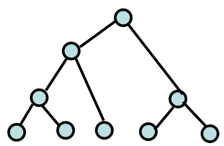
http://clusty.com

Why Cluster Documents for IR (4/4)

4. Speech up the search process
   - For retrieval models using exhaustive matching (computing the similarity of the query to every document) without efficient inverted index supports
     - E.g., latent semantic analysis (LSA), language modeling (LM) ?
   - Solution: cluster-based retrieval
     - First find the clusters that are closet to the query and then only consider documents from these clusters

Types of Clustering Algorithms

- Two types of structures produced by clustering algorithms
  - Flat or non-hierarchical clustering
  - Hierarchical clustering
- **Flat clustering**
  - Simply consisting of a certain number of clusters and the relation between clusters is often undetermined
  - Measurement: construction error minimization or probabilistic optimization
- **Hierarchical clustering**
  - A hierarchy with usual interpretation that each node stands for a subclass of its mother's node
    - The leaves of the tree are the single objects
    - Each node represents the cluster that contains all the objects of its descendants
  - Measurement: similarities of instances



Hard Assignment vs. Soft Assignment (1/2)

- Another important distinction between clustering algorithms is whether they perform soft or hard assignment
- **Hard Assignment**
  – Each object (or document in the context of IR) is assigned to one and only one cluster
- **Soft Assignment (probabilistic approach)**
  – Each object may be assigned to multiple clusters
  – An object x_i has a probability distribution $P(\cdot|x_i)$ over clusters c_j where $P(x_i|c_j)$ is the probability that x_i is a member of c_j
  – Is somewhat more appropriate in many tasks such as NLP, IR, …

Hard Assignment vs. Soft Assignment (2/2)

- Hierarchical clustering usually adopts hard assignment
- While in flat clustering, both types of assignments are common

Summarized Attributes of Clustering Algorithms (1/2)

- Hierarchical Clustering
  - Preferable for detailed data analysis
  - Provide more information than flat clustering
  - No single best algorithm (each of the algorithms only optimal for some applications)
  - Less efficient than flat clustering (minimally have to compute n x n matrix of similarity coefficients)

Summarized Attributes of Clustering Algorithms (2/2)

- Flat Clustering
  - Preferable if efficiency is a consideration or data sets are very large
  - *K*-means is the conceptually feasible method and should probably be used on a new data because its results are often sufficient
    - *K*-means assumes a simple Euclidean representation space, and so cannot be used for many data sets, e.g., nominal data like colors (or samples with features of different scales)
  - The EM algorithm is the most choice. It can accommodate definition of clusters and allocation of objects based on complex probabilistic models
    - Its extensions can be used to handle topological/hierarchical orders of samples
      - E.g., Probabilistic Latent Semantic Analysis (PLSA)

Flat Clustering

Flat Clustering

- Start out with a partition based on randomly selected seeds (one seed per cluster) and then refine the initial partition
  - In a multi-pass manner (recursion/iterations)

- **Problems** associated with non-hierarchical clustering
  - When to stop ? group average similarity, likelihood, mutual information
  - What is the right number of clusters (cluster cardinality) ?

    k-1 → k → k+1

- **Algorithms** introduced here
  - The *K*-means algorithm
  - The EM algorithm

Hierarchical clustering
also has to face this problem

The *K*-means Algorithm (1/10)

- Also called *Linde-Buzo-Gray* (LBG) in signal processing
  - A hard clustering algorithm
  - Define clusters by the **center of mass** of their members

- The K-means algorithm also can be regarded as
  - A kind of vector quantization
    - Map from a continuous space (high resolution) to a discrete space (low resolution)
  - E.g. color quantization
    - 24 bits/pixel (16 million colors) $\rightarrow$ 8 bits/pixel (256 colors)
    - A compression rate of 3

$$\boldsymbol{X} = \{\boldsymbol{x}^t\}_{t=1}^{n} \xrightarrow{\text{index } j} \boldsymbol{F} = \{\boldsymbol{m}_j\}_{j=1}^{k}$$

$\text{Dim}(\boldsymbol{x}^t)=24 \rightarrow |F|=2^8$

$\boldsymbol{m}_j$: cluster centriod or reference vector, code word, code vector

The *K*-means Algorithm (2/10)

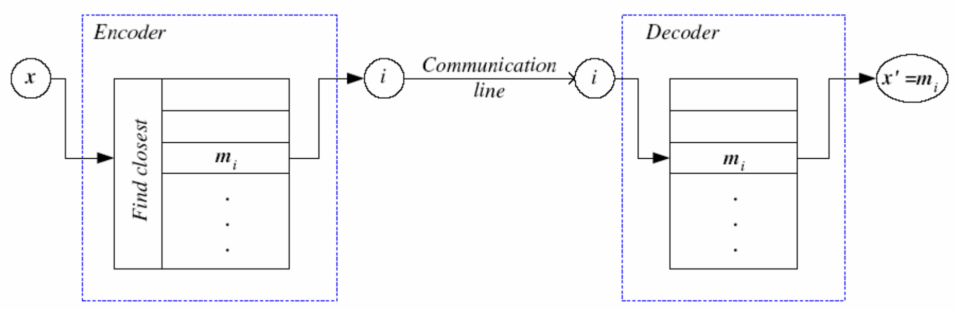


Figure 7.1: Given $\boldsymbol{x}$, the encoder sends the index of the closest code word and the decoder generates the code word with the received index as $\boldsymbol{x}'$. Error is $\|\boldsymbol{x}' - \boldsymbol{x}\|^2$.

Total reconstruction error (RSS : residual sum of squares)

label

$$E\left(\{\mathbf{m}_i\}_{i=1}^{k} \middle| \mathbf{X}\right) = \sum_{t=1}^{N} \sum_{i=1}^{k} b_i^t \left\|\mathbf{x}^t - \mathbf{m}_i\right\|^2, \text{ where } b_i^t = \begin{cases} 1 & \text{if} \left\|\mathbf{x}^t - \mathbf{m}_i\right\| = \min_j \left\|\mathbf{x}^t - \mathbf{m}_j\right\| \\ 0 & \text{otherwise} \end{cases}$$

- b_i^t and $\boldsymbol{m}_i$ are unknown
- b_i^t depends on $\boldsymbol{m}_i$ and this optimization problem can not be solved analytically

The *K*-means Algorithm (3/10)

- **Initialization**
  - A set of initial cluster centers is needed $\{\boldsymbol{m}_i\}_{i=1}^{k}$

- **Recursion**
  - Assign each object $\boldsymbol{x}^t$ to the cluster whose center is closest

$$b_i^t = \begin{cases} 1 & \text{if} \left\| \boldsymbol{x}^t - \boldsymbol{m}_i \right\| = \min_j \left\| \boldsymbol{x}^t - \boldsymbol{m}_j \right\| \\ 0 & \text{otherwise} \end{cases}$$

  - Then, re-compute the center of each cluster as the centroid or mean (average) of its members
    - Using the medoid as the cluster center ?

    (a medoid is one of the objects in the cluster)

$$\boldsymbol{m}_i = \frac{\sum_{t=1}^{N} b_i^t \cdot \boldsymbol{x}^t}{\sum_{t=1}^{N} b_i^t}$$

These two steps are repeated until $\boldsymbol{m}_i$ stabilizes

The *K*-means Algorithm (4/10)

- Algorithm

Initialize $\boldsymbol{m}_i, i = 1, \ldots, k$, for example, to k random $\boldsymbol{x}^t$

Repeat

For all $\boldsymbol{x}^t \in \mathcal{X}$

$$b_i^t \leftarrow \begin{cases} 1 & \text{if } \|\boldsymbol{x}^t - \boldsymbol{m}_i\| = \min_j \|\boldsymbol{x}^t - \boldsymbol{m}_j\| \\ 0 & \text{otherwise} \end{cases}$$

For all $\boldsymbol{m}_i, i = 1, \ldots, k$

$$\boldsymbol{m}_i \leftarrow \sum_t b_i^t \boldsymbol{x}^t / \sum_t b_i^t$$

Until $\boldsymbol{m}_i$ converge

The *K*-means Algorithm (5/10)

- Example 1

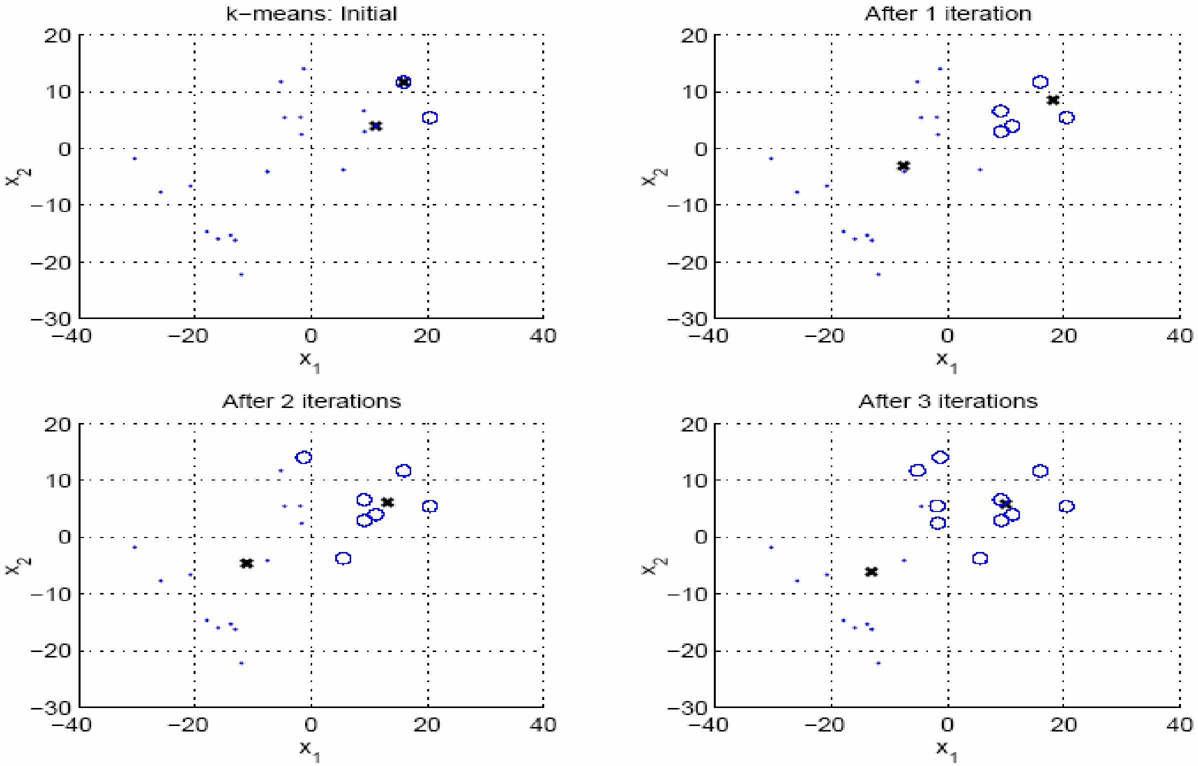


Figure 7.2: Evolution of k-means. Crosses indicate center positions. Data points are marked depending on the closest center.

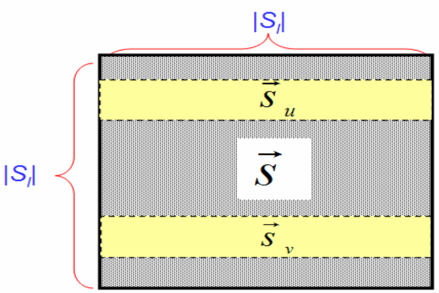
The *K*-means Algorithm (6/10)

- Example 2

Cluster	Members	
1	*ballot* (0.28), *polls* (0.28), *Gov* (0.30), *seats* (0.32)	government
2	*profit* (0.21), *finance* (0.21), *payments* (0.22)	finance
3	*NFL* (0.36), *Reds* (0.28), *Sox* (0.31), *inning* (0.33), *quarterback* (0.30), *scored* (0.30), *score* (0.33)	sports
4	*researchers* (0.23), *science* (0.23)	research
5	*Scott* (0.28), *Mary* (0.27), *Barbara* (0.27), *Edward* (0.29)	name

Table 14.4 An example of K-means clustering. Twenty words represented as vectors of co-occurrence counts were clustered into 5 clusters using K-means. The distance from the cluster centroid is given after each word.

$$s_{u,v} = \frac{\vec{s}_u \cdot \vec{s}_v}{|\vec{s}_u| \times |\vec{s}_u|}$$

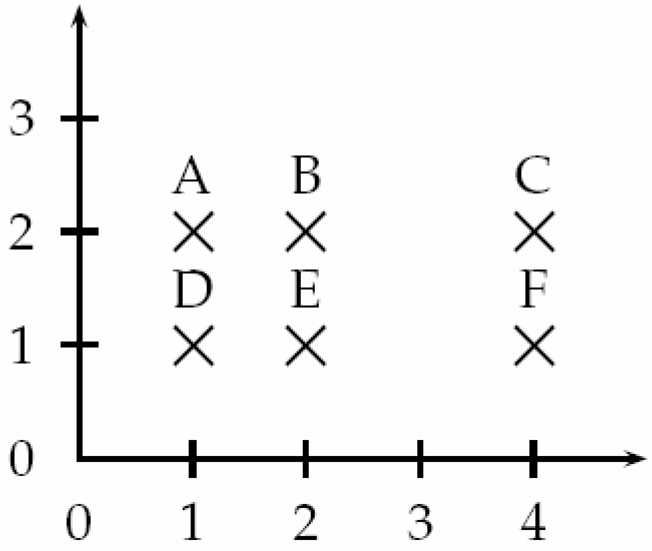


The *K*-means Algorithm (7/10)

- Complexity: O(*IKNM*)
  - I: Iterations; K: cluster number; N: object number; M: object dimensionality
- Choice of initial cluster centers (seeds) is important
  - Pick at random
  - Or, calculate the mean $\mathbf{m}$ of all data and generate *k* initial centers $\boldsymbol{m}_i$ by adding small random vector to the mean $\mathbf{m} \pm \boldsymbol{\delta}$
  - Or, project data onto the principal component (first eigenvector), divide it range into *k* equal interval, and take the mean of data in each group as the initial center $\boldsymbol{m}_i$
  - Or, use another method such as hierarchical clustering algorithm on a subset of the objects
    - E.g., buckshot algorithm uses the group-average agglomerative clustering to randomly sample of the data that has size square root of the complete set

The *K*-means Algorithm (8/10)

- Poor seeds will result in **sub-optimal** clustering

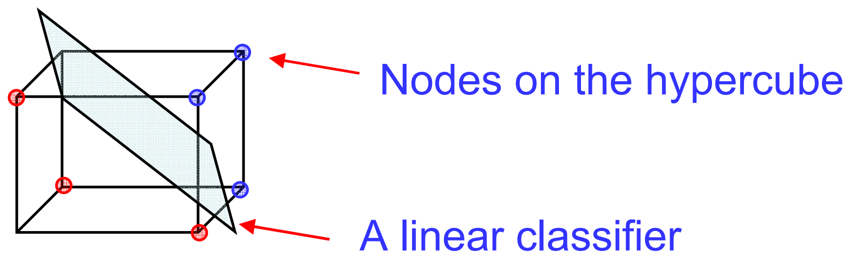


► **Figure 16.7** The outcome of clustering in k-means depends on the initial seeds. For seeds B and E, k-means converges to $\{A, B, C\}, \{D, E, F\}$, a suboptimal clustering. For seeds D and F, it converges to $\{A, B, D, E\}, \{C, F\}$, the global optimum for $K = 2$.

The *K*-means Algorithm (9/10)

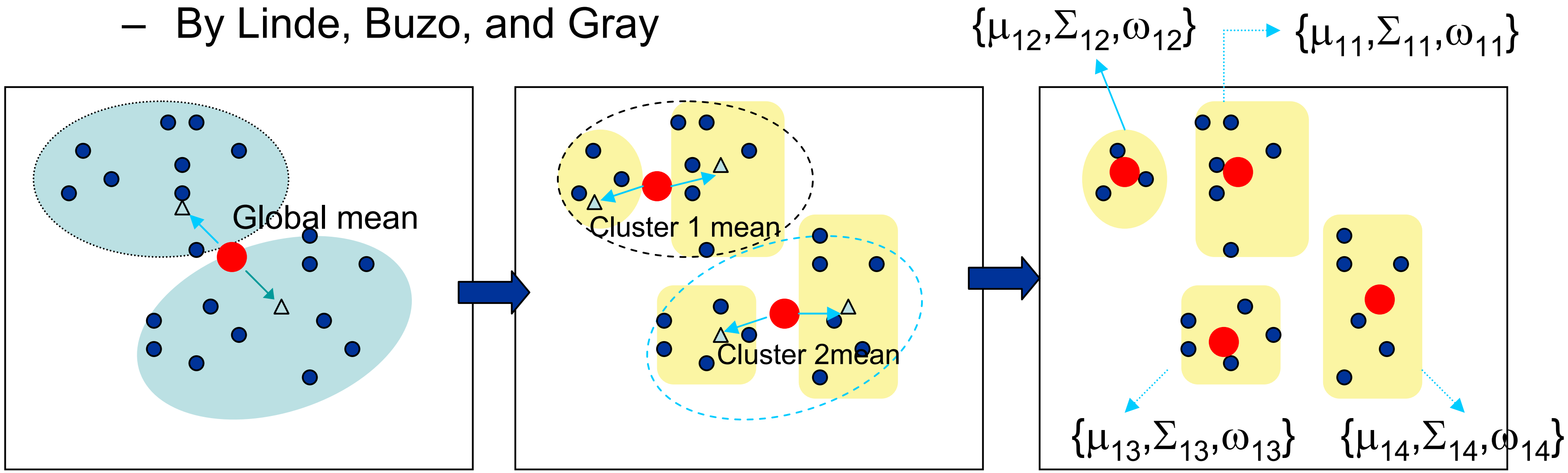
- How to break ties when in case there are several centers with the same distance from an object
  - E.g., randomly assign the object to one of the candidate clusters (or assign the object to the cluster with lowest index)
  - Or, perturb objects slightly
- Applications of the *K*-means Algorithm
  - Clustering
  - Vector quantization
  - A preprocessing stage before classification or regression
    - Map from the original space to l-dimensional space/hypercube

$l = \log_2 k$ (k clusters)



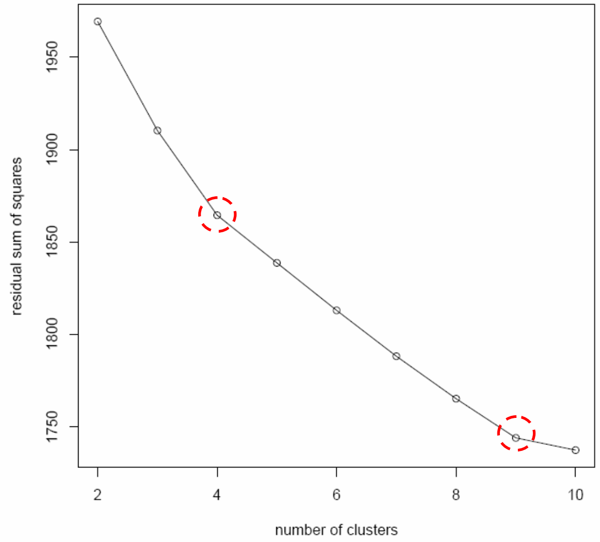
The K-means Algorithm (10/10)

- E.g., the LBG algorithm $M \rightarrow 2M$ at each iteration
  - By Linde, Buzo, and Gray



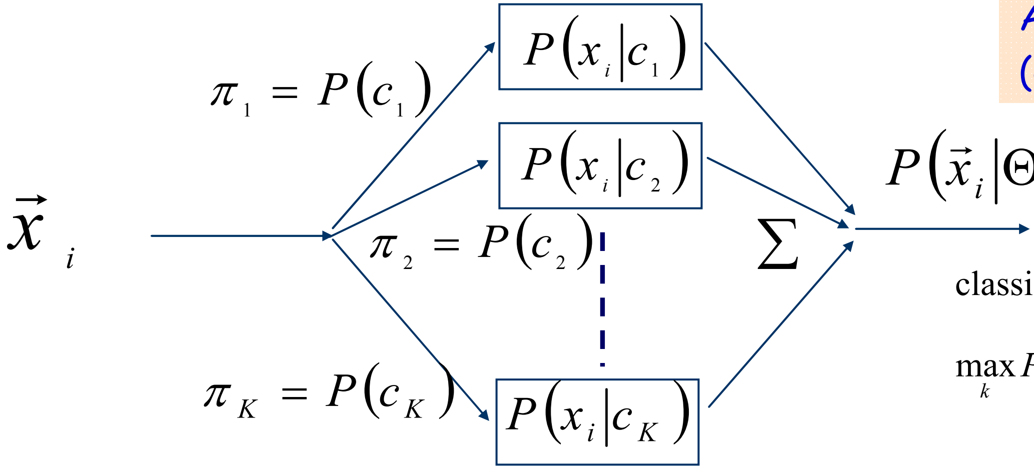
Total Reconstruction error
(residual sum of squares)

$$E\left(\{\mathbf{m}_i\}_{i=1}^{k} \middle| \mathbf{X}\right) = \sum_{t=1}^{N}\sum_{i=1}^{k} b_i^t \left\| \mathbf{x}^t - \mathbf{m}_i \right\|^2$$



The EM Algorithm (1/2)

- A **soft version** of the K-mean algorithm
  - Each object could be the member of multiple clusters
  - Clustering as estimating a mixture of (continuous) probability distributions



A Mixture Gaussian HMM
(or A Mixture of Gaussians)

$$P(\vec{x}_i|\Theta) = \sum_{k=1}^{K} P(\vec{x}_i|c_k;\Theta)P(c_k|\Theta)$$

classification:

$$\max_k P(c_k|\vec{x}_i,\Theta) = \max_k \frac{(\vec{x}_i|c_k;\Theta)P(c_k|\Theta)}{P(\vec{x}_i|\Theta)}$$
$$= \max_k (\vec{x}_i|c_k;\Theta)P(c_k|\Theta)$$

Likelihood function for data samples: $\boldsymbol{X} = \vec{x}_1, \vec{x}_2, \ldots, \vec{x}_n$

$$P(\boldsymbol{X}|\Theta) = \prod_{i=1}^{n} P(\vec{x}_i|\Theta)$$
$$= \prod_{i=1}^{n} \sum_{k_i=1}^{K} P(\vec{x}_i|c_{k_i};\Theta)P(c_{k_i}|\Theta)$$

Continuous case:

$$P(\vec{x}_i|c_k;\Theta) = \frac{1}{\sqrt{(2\pi)^m|\Sigma_k|}} \exp\left(-\frac{1}{2}(\vec{x}_i - \vec{\mu}_k)^T \Sigma_k^{-1}(\vec{x}_i - \vec{\mu}_k)\right)$$

$$\boldsymbol{X} = \{\vec{x}_1, \vec{x}_2, \cdots, \vec{x}_n\}$$

$\vec{x}_i$'s are independent identically distributed (i.i.d.)

The EM Algorithm (2/2)

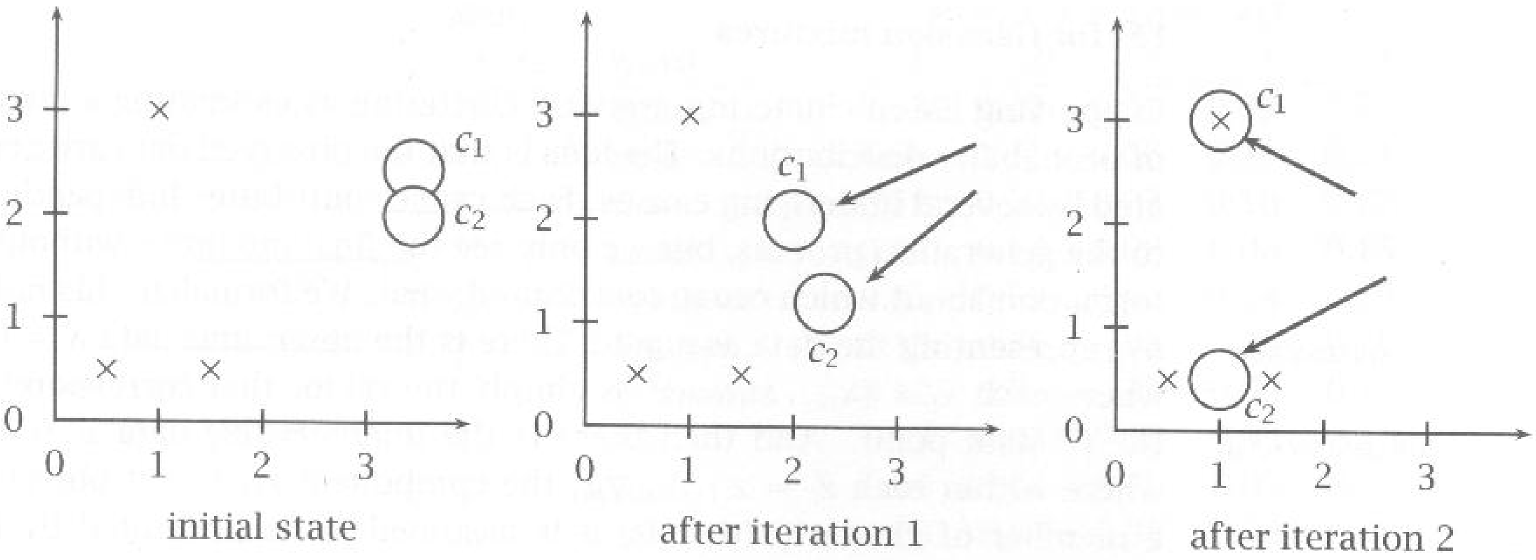
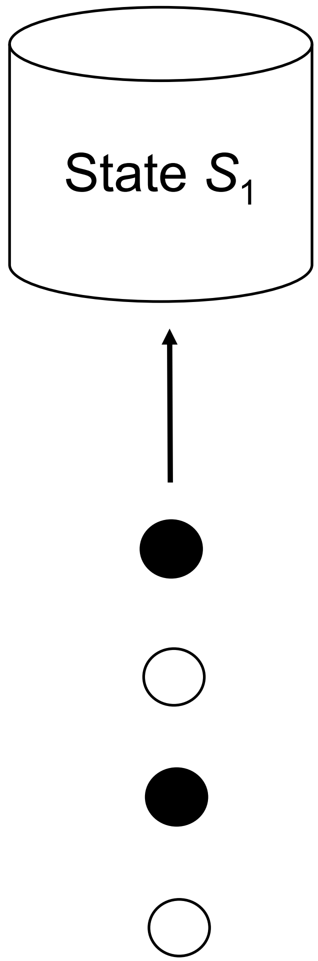


Figure 14.10 An example of using the EM algorithm for soft clustering.

Maximum Likelihood Estimation (1/2)

- Hard Assignment



P(B| S_1)=2/4=0.5

P(W| S_1)=2/4=0.5

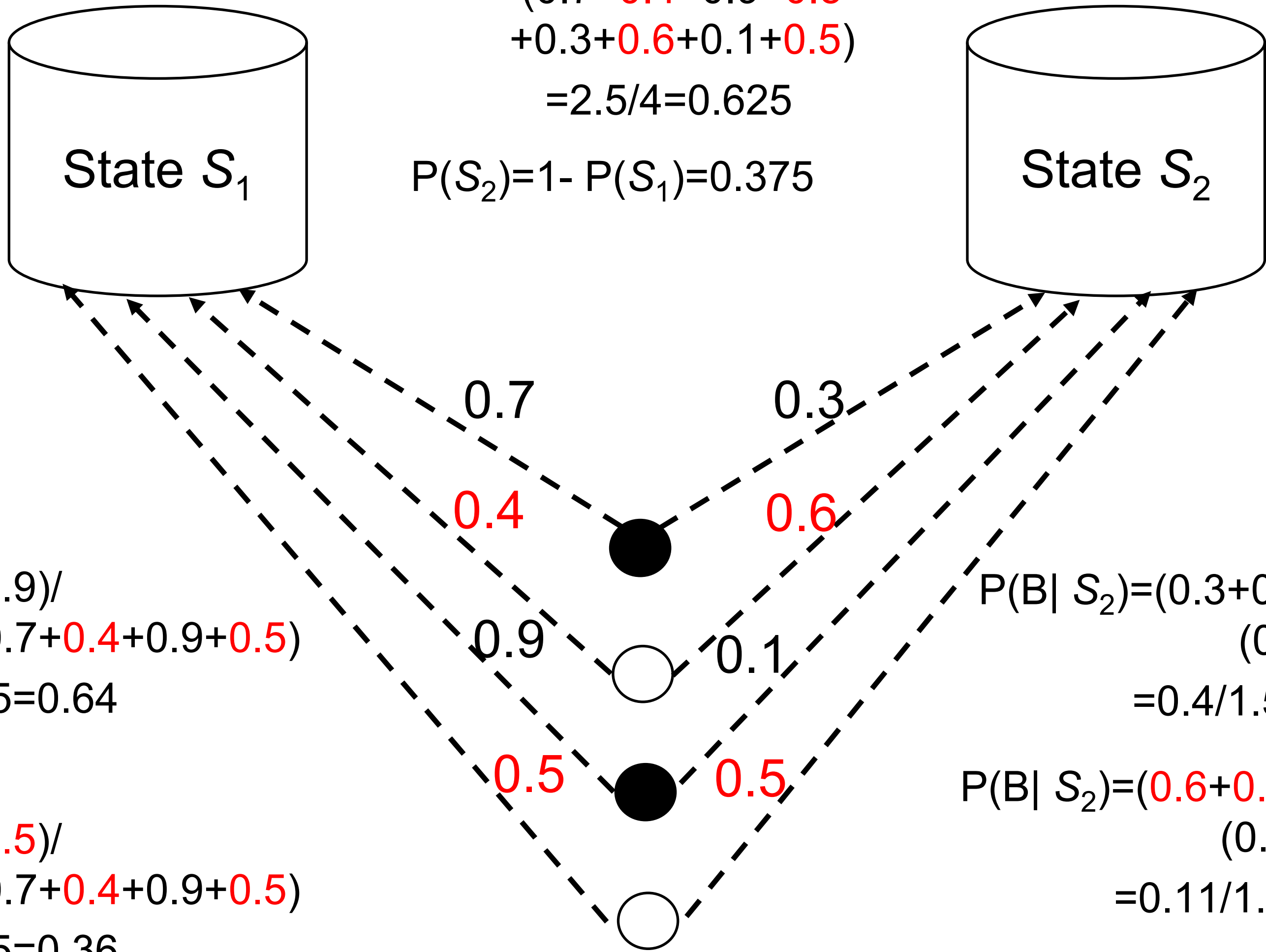
Maximum Likelihood Estimation (2/2)

- Soft Assignment

$P(S_1)=(0.7+0.4+0.9+0.5)/(0.7+0.4+0.9+0.5+0.3+0.6+0.1+0.5)$

$=2.5/4=0.625$

$P(S_2)=1-P(S_1)=0.375$



$P(B|S_1)=(0.7+0.9)/(0.7+0.4+0.9+0.5)$

$=1.6/2.5=0.64$

$P(B|S_1)=(0.4+0.5)/(0.7+0.4+0.9+0.5)$

$=0.9/2.5=0.36$

$P(B|S_2)=(0.3+0.1)/(0.3+0.6+0.1+0.5)$

$=0.4/1.5=0.27$

$P(B|S_2)=(0.6+0.5)/(0.3+0.6+0.1+0.5)$

$=0.11/1.5=0.73$

Expectation-Maximization Updating Formulas (1/2)

- Mixture Weight

$$\hat{\pi}_k = P\left(c_k \middle| \hat{\Theta}\right) = \frac{w_k}{\sum_{k=1}^{K} w_k} = \frac{\sum_{i=1}^{n} \frac{P\left(\vec{x}_i \middle| c_k, \Theta\right) P\left(c_k \middle| \Theta\right)}{\sum_{l=1}^{K} P\left(\vec{x}_i \middle| c_l, \Theta\right) P\left(c_l \middle| \Theta\right)}}{\sum_{k=1}^{K} \sum_{i=1}^{n} \frac{P\left(\vec{x}_i \middle| c_k, \Theta\right) P\left(c_k \middle| \Theta\right)}{\sum_{l=1}^{K} P\left(\vec{x}_i \middle| c_l, \Theta\right) P\left(c_l \middle| \Theta\right)}} = \frac{\sum_{i=1}^{n} \frac{P\left(\vec{x}_i \middle| c_k, \Theta\right) P\left(c_k \middle| \Theta\right)}{\sum_{l=1}^{K} P\left(\vec{x}_i \middle| c_l, \Theta\right) P\left(c_l \middle| \Theta\right)}}{n}$$

- Mean of Gaussian

$$\hat{\vec{\mu}}_k = \frac{\sum_{i=1}^{n} w_{k,i} \cdot \vec{x}_i}{\sum_{i=1}^{n} w_{k,i}} = \frac{\sum_{i=1}^{n} \frac{P\left(\vec{x}_i \middle| c_k, \Theta\right) P\left(c_k \middle| \Theta\right)}{\sum_{l=1}^{K} P\left(\vec{x}_i \middle| c_l, \Theta\right) P\left(c_l \middle| \Theta\right)} \cdot \vec{x}_i}{\sum_{i=1}^{n} \frac{P\left(\vec{x}_i \middle| c_k, \Theta\right) P\left(c_k \middle| \Theta\right)}{\sum_{l=1}^{K} P\left(\vec{x}_i \middle| c_l, \Theta\right) P\left(c_l \middle| \Theta\right)}}$$

Expectation-Maximization Updating Formulas (2/2)

- Covariance Matrix of Gaussian

$$\hat{\Sigma}_k = \frac{\sum_{i=1}^{n} w_{k,i} \cdot \left(\vec{x}_i - \hat{\vec{\mu}}_k\right)\left(\vec{x}_i - \hat{\vec{\mu}}_k\right)^T}{\sum_{i=1}^{n} w_{k,i}}$$

$$= \frac{\sum_{i=1}^{n} \frac{P\left(\vec{x}_i \middle| c_k, \Theta\right) P\left(c_k \middle| \Theta\right)}{\sum_{l=1}^{K} P\left(\vec{x}_i \middle| c_l, \Theta\right) P\left(c_l \middle| \Theta\right)} \cdot \left(\vec{x}_i - \hat{\vec{\mu}}_k\right)\left(\vec{x}_i - \hat{\vec{\mu}}_k\right)^T}{\sum_{i=1}^{n} \frac{P\left(\vec{x}_i \middle| c_k, \Theta\right) P\left(c_k \middle| \Theta\right)}{\sum_{l=1}^{K} P\left(\vec{x}_i \middle| c_l, \Theta\right) P\left(c_l \middle| \Theta\right)}}$$

More facts about The EM Algorithm

- The initial cluster distributions can be estimated using the *K*-means algorithm

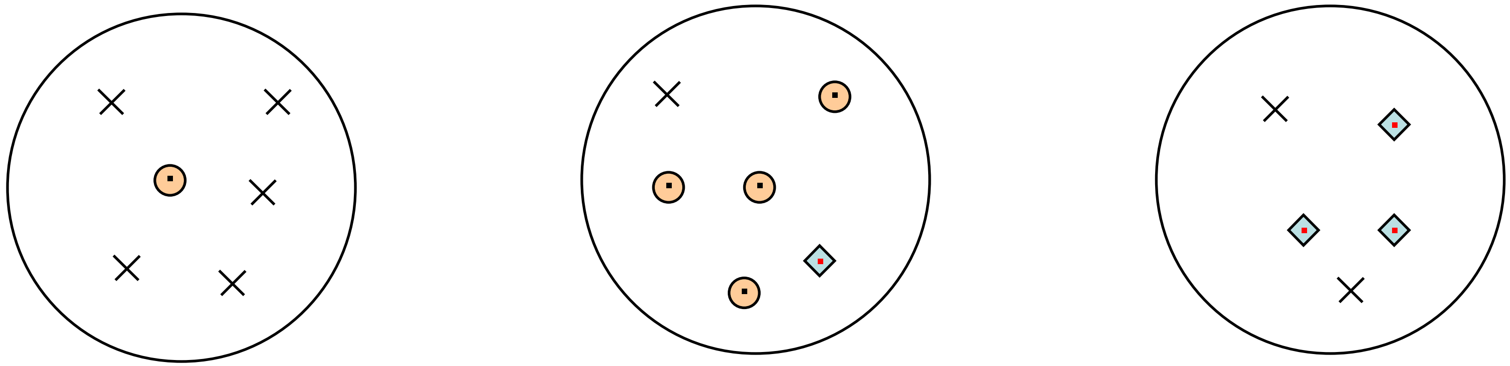
- The procedure terminates when the likelihood function $P(X|\Theta)$ is converged or maximum number of iterations is reached

Evaluation of Clustering (1/2)

- Internal criterion for the quality of a clustering result
  - The typical objective is to attain
    - High intra-cluster similarity (documents with a cluster are similar)
    - Low inter-cluster similarity (document from different clusters are dissimilar)
  - The measured quality depends on both the document representation and the similarity measure used
  - Good scores on an internal criterion do not necessarily translate into good effective in an application

Evaluation of Clustering (2/2)

- External criterion for the quality of a clustering result
  – Evaluate how well the clustering matches the gold standard classes produced by human judges
    - That is, the quality is measured by the ability of the clustering algorithm to discover some or all of the hidden patterns or latent (true) classes



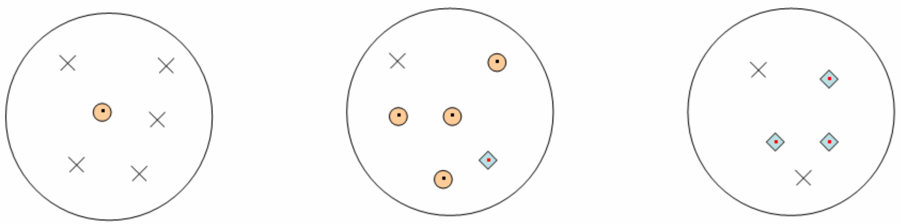
  – Two common criteria
    - Purity
    - Rand Index (RI)

Purity (1/2)

- Each cluster is first assigned to class which is most frequent in the cluster
- Then, the accuracy of the assignment is measured by counting the number of correctly assigned documents and dividing by the sample size

$$\text{Purity}\ (\Omega, \Gamma) = \frac{1}{N} \sum_k \max_j \left| \omega_j \cap c_k \right|$$

- $\Omega = \{\omega_1, \omega_2, \ldots, \omega_K\}$: the set of clusters
- $\Gamma = \{c_1, c_2, \ldots, c_J\}$: the set of classes
- N : the sample size



$$\text{Purity}(\Omega, \Gamma) = \frac{1}{17}(5+4+3) = 0.71$$

Purity (2/2)

- High purity is easy to achieve for a large number of clusters (?)
  - Purity will be 1 if each document gets its own cluster
  - Therefore, purity cannot be used to trade off the quality of the clustering against the number of clusters

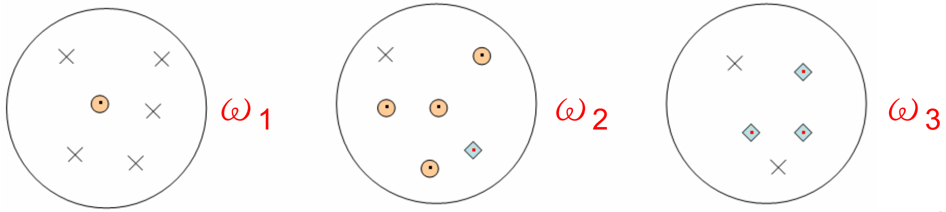
Rand Index (1/3)

- Measure the similarity between the clusters and the classes in ground truth
  - Consider the assignments of all possible pairs of distinct documents in the cluster and the true class

Number of points	Same cluster in clustering	Different clusters in clustering
Same class in ground truth	**TP (True Positive)**	**FN (False Negative)**
Different classes in ground truth	**FP (False Positive)**	**TN (True Negative)**

$$\mathrm{RI} = \frac{\mathrm{TP} + \mathrm{TN}}{\mathrm{TP} + \mathrm{FP} + \mathrm{FN} + \mathrm{TN}}$$

Rand Index (2/3)



$$\mathrm{TP} = \underbrace{\overset{\times}{\binom{5}{2}}}_{\omega_1} + \underbrace{\overset{\odot}{\binom{4}{2}}}_{\omega_2} + \underbrace{\left[\overset{\diamond}{\binom{3}{2}} + \overset{\times}{\binom{2}{2}}\right]}_{\omega_3} = 20$$

$$\mathrm{FP} = \underbrace{\overset{\times}{\binom{5}{1}}\overset{\odot}{\binom{1}{1}}}_{\omega_1} + \underbrace{\left[\overset{\odot}{\binom{4}{1}}\overset{\times}{\binom{1}{1}} + \overset{\odot}{\binom{4}{1}}\overset{\diamond}{\binom{1}{1}} + \overset{\times}{\binom{1}{1}}\overset{\diamond}{\binom{1}{1}}\right]}_{\omega_2} + \underbrace{\overset{\diamond}{\binom{3}{1}}\overset{\times}{\binom{2}{1}}}_{\omega_3}$$

$$= 20$$

$$\left(= \left[\underbrace{\binom{6}{2}}_{\omega_1} + \underbrace{\binom{6}{2}}_{\omega_2} + \underbrace{\binom{5}{2}}_{\omega_3}\right] - \mathrm{TP} \right)$$

all positive pairs

$$\mathrm{TN} = \underbrace{\left[\overset{\times}{\binom{5}{1}}\overset{\odot}{\binom{4}{1}} + \overset{\times}{\binom{5}{1}}\overset{\diamond}{\binom{1}{1}} + \overset{\odot}{\binom{1}{1}}\overset{\times}{\binom{1}{1}} + \overset{\odot}{\binom{1}{1}}\overset{\diamond}{\binom{1}{1}}\right]}_{\omega_1\omega_2}$$

$$+ \underbrace{\left[\overset{\times}{\binom{5}{1}}\overset{\diamond}{\binom{3}{1}} + \overset{\odot}{\binom{1}{1}}\overset{\diamond}{\binom{3}{1}} + \overset{\diamond}{\binom{1}{1}}\overset{\times}{\binom{2}{1}}\right]}_{\omega_1\omega_3}$$

$$+ \underbrace{\left[\overset{\odot}{\binom{4}{1}}\overset{\diamond}{\binom{3}{1}} + \overset{\odot}{\binom{4}{1}}\overset{\times}{\binom{2}{1}} + \overset{\times}{\binom{1}{1}}\overset{\diamond}{\binom{3}{1}} + \overset{\diamond}{\binom{1}{1}}\overset{\times}{\binom{2}{1}}\right]}_{\omega_2\omega_3} = 72$$

	Same cluster	Different clusters
Same class	TP=20	FN=24
Different classes	FP=20	TN=72

$$\mathrm{FN} = \underbrace{\left[\overset{\times}{\binom{5}{1}}\overset{\times}{\binom{1}{1}} + \overset{\odot}{\binom{1}{1}}\overset{\odot}{\binom{4}{1}}\right]}_{\omega_1\omega_2} + \underbrace{\overset{\times}{\binom{5}{1}}\overset{\times}{\binom{2}{1}}}_{\omega_1\omega_3} + \underbrace{\left[\overset{\times}{\binom{1}{1}}\overset{\times}{\binom{2}{1}} + \overset{\diamond}{\binom{1}{1}}\overset{\diamond}{\binom{3}{1}}\right]}_{\omega_2\omega_3}$$

$$= 24$$

$$\left(= \left[\underbrace{\binom{6}{1}\binom{6}{1}}_{\omega_1\omega_2} + \underbrace{\binom{6}{1}\binom{5}{1}}_{\omega_1\omega_3} + \underbrace{\binom{6}{1}\binom{5}{1}}_{\omega_2\omega_3}\right] - \mathrm{TN} \right)$$

all negative pairs

$$\mathrm{RI} = \frac{20 + 72}{20 + 20 + 24 + 72} = 0.68$$

all pairs

$$N(N-1)/2 = 17 \times 16 / 2 = 136$$

Rand Index (3/3)

- The rand index has a value between 0 and 1
  - 0 indicates that the clusters and the classes in ground truth do not agree on any pair of points
  - 1 indicates that the clusters and the classes in ground truth are exactly the same

F-Measure Based on Rand Index

- F-Measure: harmonic mean of precision (P) and recall (R)

$$P = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FP}}, \qquad R = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FN}}$$

	Same cluster	Different clusters
Same class	TP	FN
Different classes	FP	TN

$$\mathrm{F}_b = \frac{b^2 + 1}{\frac{b^2}{R} + \frac{1}{P}} = \frac{\left(b^2 + 1\right)PR}{b^2 P + R}$$

  – If we want to penalize false negatives (FN) more strongly than false positives (FP), then we can set $b > 1$
    - That is, giving more weight to recall (R)

Hierarchical Clustering

Hierarchical Clustering

- Can be in either bottom-up or top-down manners
  - **Bottom-up** (agglomerative) 凝集的
    - Start with individual objects and grouping the most similar ones
      - E.g., with the minimum distance apart

$$sim(x, y) = \frac{1}{1 + d(x, y)}$$

distance measures will be discussed later on

    - The procedure terminates when one cluster containing all objects has been formed
  - **Top-down** (divisive) 分裂的
    - Start with all objects in a group and divide them into groups so as to maximize within-group similarity

Hierarchical Agglomerative Clustering (HAC)

- A bottom-up approach
- Assume a similarity measure for determining the similarity of two objects
- Start with all objects in a separate cluster (a singleton) and then repeatedly joins the two clusters that have the most similarity until there is one only cluster survived
- The history of merging/clustering forms a binary tree or hierarchy

HAC: Algorithm

Given: a set $\mathcal{X} = \{x_1, \ldots x_n\}$ of objects

a function sim: $\mathcal{P}(\mathcal{X}) \times \mathcal{P}(\mathcal{X}) \rightarrow \mathbb{R}$

for $i := 1$ **to** n **do**

$c_i := \{x_i\}$ **end**

Initialization (for tree leaves): Each object is a cluster

$C := \{c_1, \ldots, c_n\}$

$j := n + 1$

while $|C| > 1$

cluster number

$(c_{n_1}, c_{n_2}) := \arg\max_{(c_u, c_v) \in C \times C} \mathrm{sim}(c_u, c_v)$

$c_j = c_{n_1} \cup c_{n_2}$

merged as a new cluster

$C := C \backslash \{c_{n_1}, c_{n_2}\} \cup \{c_j\}$

The original two clusters are removed

$j := j + 1$

Figure 14.2 Bottom-up hierarchical clustering.

Distance Metrics

- Euclidian Distance (*L_2* norm)

$$L_2(\vec{x},\vec{y})=\sum_{i=1}^{m}(x_i-y_i)^2$$

  – Make sure that all attributes/dimensions have the same scale (or the same variance)

- *L_1* Norm (City-block distance)

$$L_1(\vec{x},\vec{y})=\sum_{i=1}^{m}\left|x_i-y_i\right|$$

- Cosine Similarity (transform to a distance by subtracting from 1)

$$1-\frac{\vec{x}\bullet\vec{y}}{|\vec{x}|\cdot|\vec{y}|}$$

ranged between 0 and 1

Measures of Cluster Similarity (1/7)

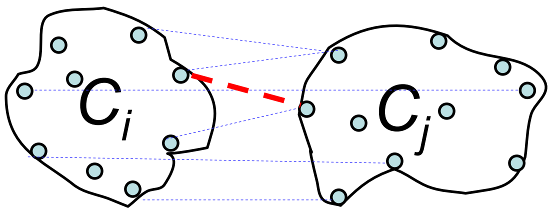
- Especially for the bottom-up approaches

- **Single-link** clustering
  – The similarity between two clusters is the similarity of the two closest objects in the clusters

  – Search over all pairs of objects that are from the two different clusters and select the pair with the greatest similarity

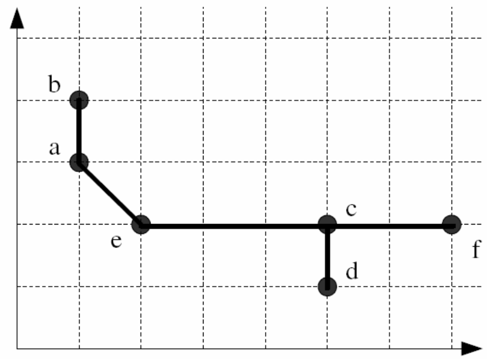
  – Elongated clusters are achieved

$$sim(c_i, c_j) = \max_{\vec{x} \in c_i, \vec{y} \in c_j} sim(\vec{x}, \vec{y})$$



greatest similarity

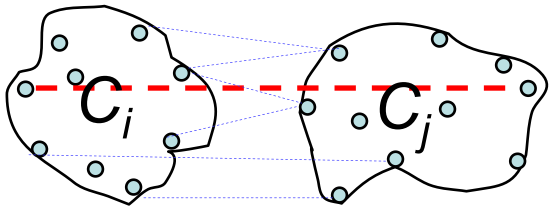
cf. the minimal spanning tree



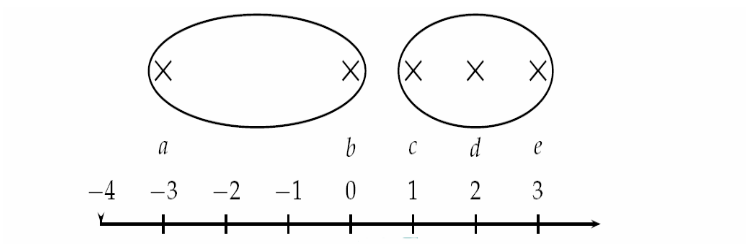
Measures of Cluster Similarity (2/7)

- **Complete-link** clustering
  - The similarity between two clusters is the similarity of their two most dissimilar members
  - Sphere-shaped clusters are achieved
  - Preferable for most IR and NLP applications

$$sim\left(c_i, c_j\right) = \min_{\vec{x} \in c_i, \vec{y} \in c_j} sim\left(\vec{x}, \vec{y}\right)$$



  - More sensitive to outliers



▶ **Figure 17.6** Outliers in complete-link clustering. The four points have the coordinates $-3+2\times\epsilon, 0, 1+2\times\epsilon, 2$ and $3-\epsilon$. Complete-link clustering creates the two clusters shown as ellipses. Intuitively, $\{b, c, d, e\}$ should be one cluster, but it is split by outlier a.

Measures of Cluster Similarity (3/7)

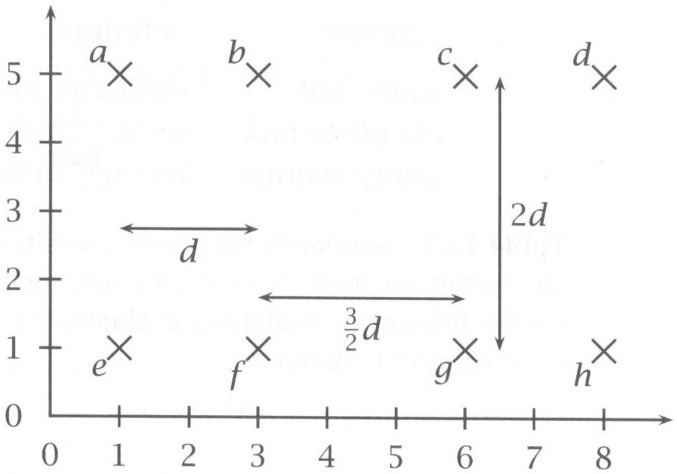


Figure 14.4 A cloud of points in a plane.

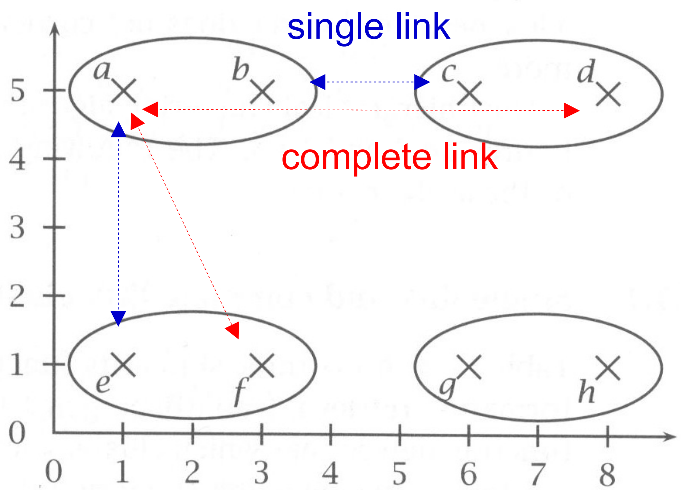


Figure 14.5 Intermediate clustering of the points in figure 14.4.

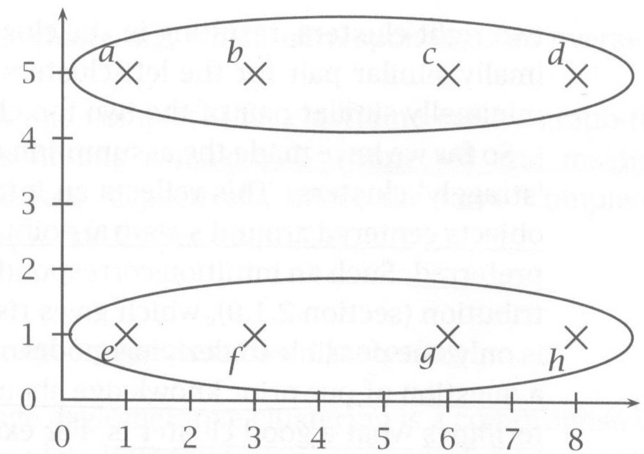


Figure 14.6 Single-link clustering of the points in figure 14.4.

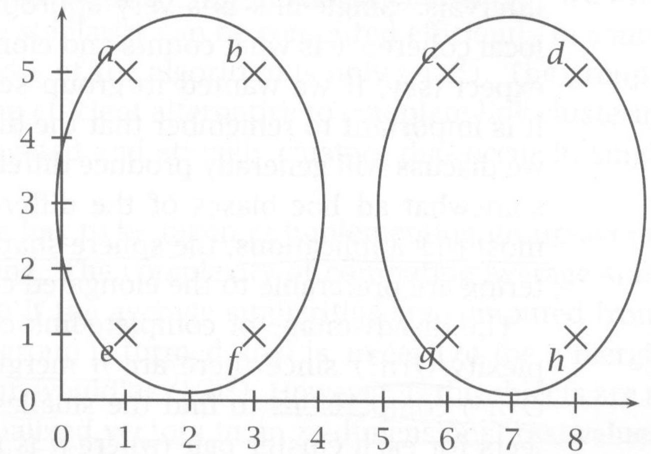
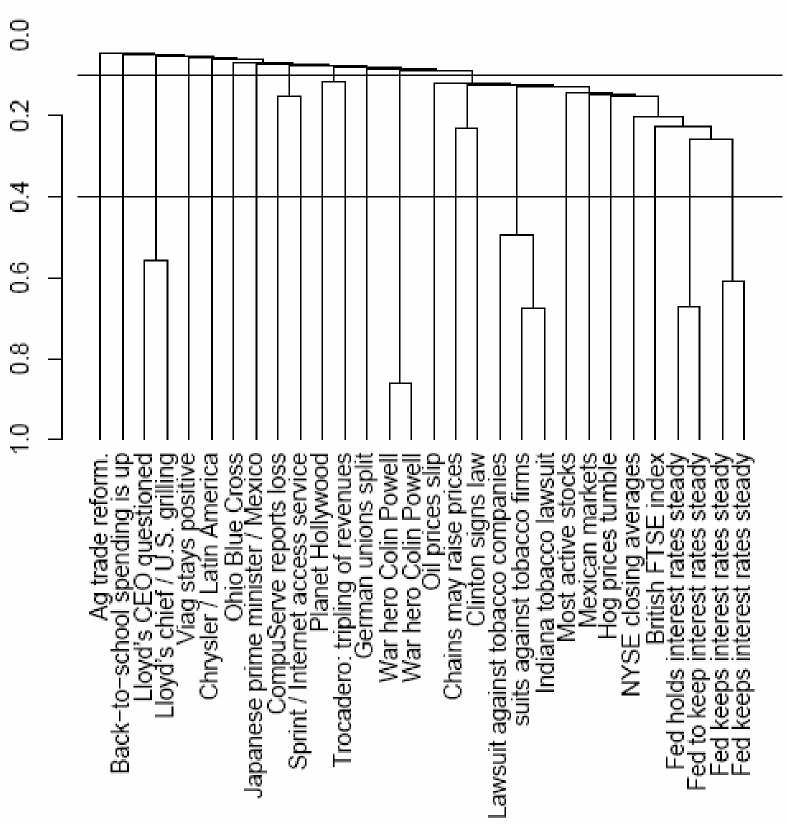
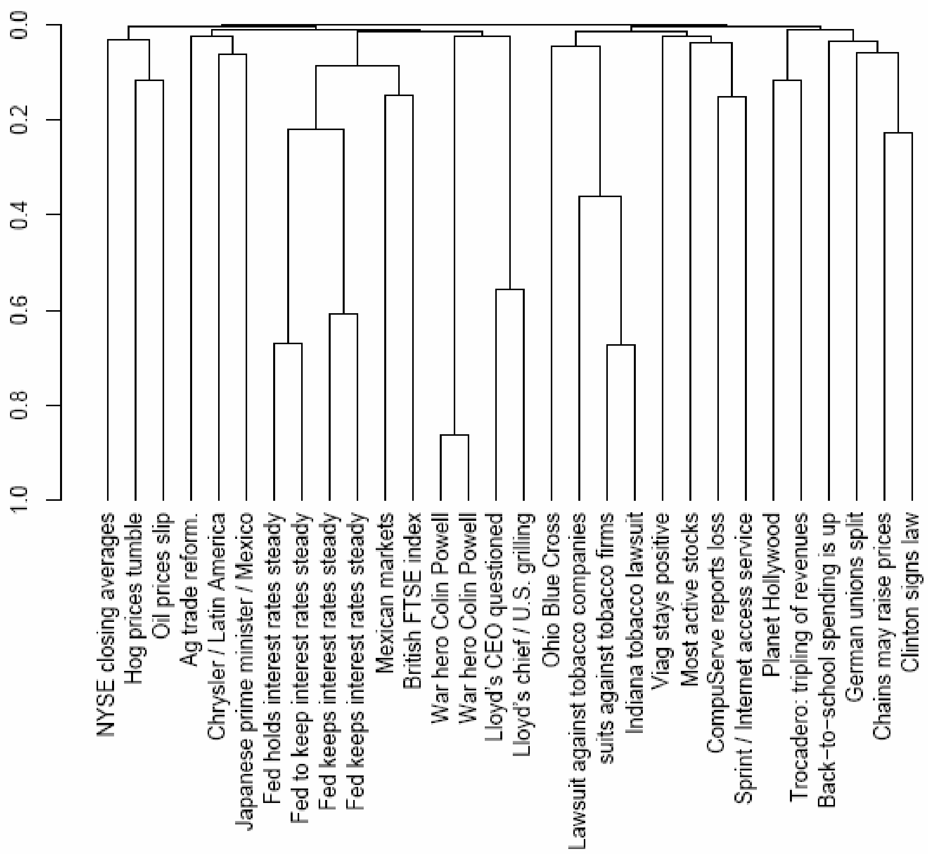


Figure 14.7 Complete-link clustering of the points in figure 14.4.

Measures of Cluster Similarity (4/7)



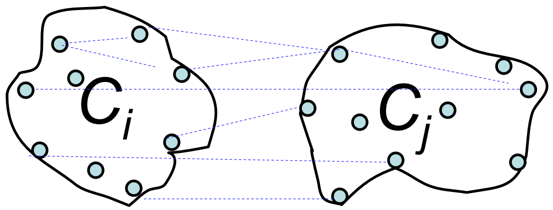
► **Figure 17.1** A dendrogram of a single-link clustering of 30 documents from Reuters-RCV1. The y-axis represents combination similarity, the similarity of the two component clusters that gave rise to the corresponding merge. For example, the combination similarity of *Lloyd's CEO questioned* and *Lloyd's chief / U.S. grilling* is ≈ 0.56. Two possible cuts of the dendrogram are shown: at 0.4 into 24 clusters and at 0.1 into 12 clusters.



► **Figure 17.4** A dendrogram of a complete-link clustering of 30 documents from Reuters-RCV1. This complete-link clustering is more balanced than the single-link clustering of the same documents in Figure 17.1. When cutting the last merger, we obtain two clusters of similar size (documents 1–16 and documents 17–30). The y-axis represents combination similarity.

Measures of Cluster Similarity (5/7)

- **Group-average** agglomerative clustering
  - A compromise between single-link and complete-link clustering
  - The similarity between two clusters is the average similarity between members



  - If the objects are represented as length-normalized vectors and the similarity measure is the cosine
    - There exists an fast algorithm for computing the average similarity

$$sim(\vec{x}, \vec{y}) = \cos(\vec{x}, \vec{y}) = \frac{\vec{x} \cdot \vec{y}}{|\vec{x}||\vec{y}|} = \vec{x} \cdot \vec{y}$$

length-normalized vectors

Measures of Cluster Similarity (6/7)

- **Group-average** agglomerative clustering (cont.)
  - The average similarity *SIM* between vectors in a cluster c_j is defined as

$$SIM(c_j) = \frac{1}{|c_j|(|c_j|-1)} \sum_{\vec{x}\in c_j} \sum_{\substack{\vec{y}\in c_j\\ \vec{y}\neq\vec{x}}} sim(\vec{x},\vec{y}) = \frac{1}{|c_j|(|c_j|-1)} \sum_{\vec{x}\in c_j} \sum_{\substack{\vec{y}\in c_j\\ \vec{y}\neq\vec{x}}} \vec{x}\cdot\vec{y}$$

  - The sum of members in a cluster c_j : $\vec{s}(c_j) = \sum_{\vec{x}\in c_j} \vec{x}$
  - Express $SIM(c_j)$ in terms of $\vec{s}(c_j)$

$$\vec{s}(c_j)\cdot\vec{s}(c_j) = \sum_{\vec{x}\in c_j} \vec{x}\cdot\vec{s}(c_j) = \sum_{\vec{x}\in c_j}\sum_{\vec{y}\in c_j} \vec{x}\cdot\vec{y}$$

length-normalized vector

$$= |c_j|(|c_j|-1)\,SIM(c_j) + \sum_{\vec{x}\in c_j} \boxed{\vec{x}\cdot\vec{x}}$$

=1

$$= |c_j|(|c_j|-1)\,SIM(c_j) + |c_j|$$

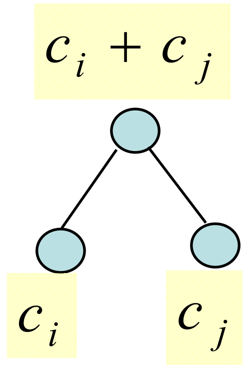
$$\therefore\ SIM(c_j) = \frac{\vec{s}(c_j)\cdot\vec{s}(c_j) - |c_j|}{|c_j|(|c_j|-1)}$$

Measures of Cluster Similarity (7/7)

- **Group-average** agglomerative clustering (cont.)

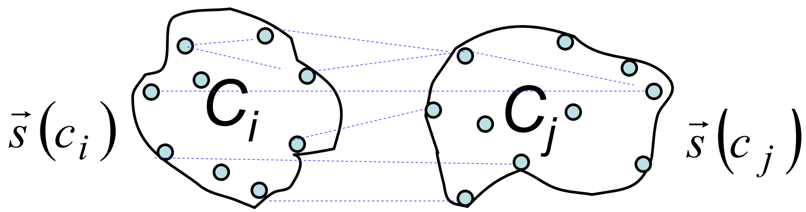
-As merging two clusters c_i and c_j, the cluster sum vectors $\vec{s}(c_i)$ and $\vec{s}(c_j)$ are known in advance

$$\Rightarrow \vec{s}(c_{New}) = \vec{s}(c_i) + \vec{s}(c_j), \quad |c_{New}| = |c_i| + |c_j|$$



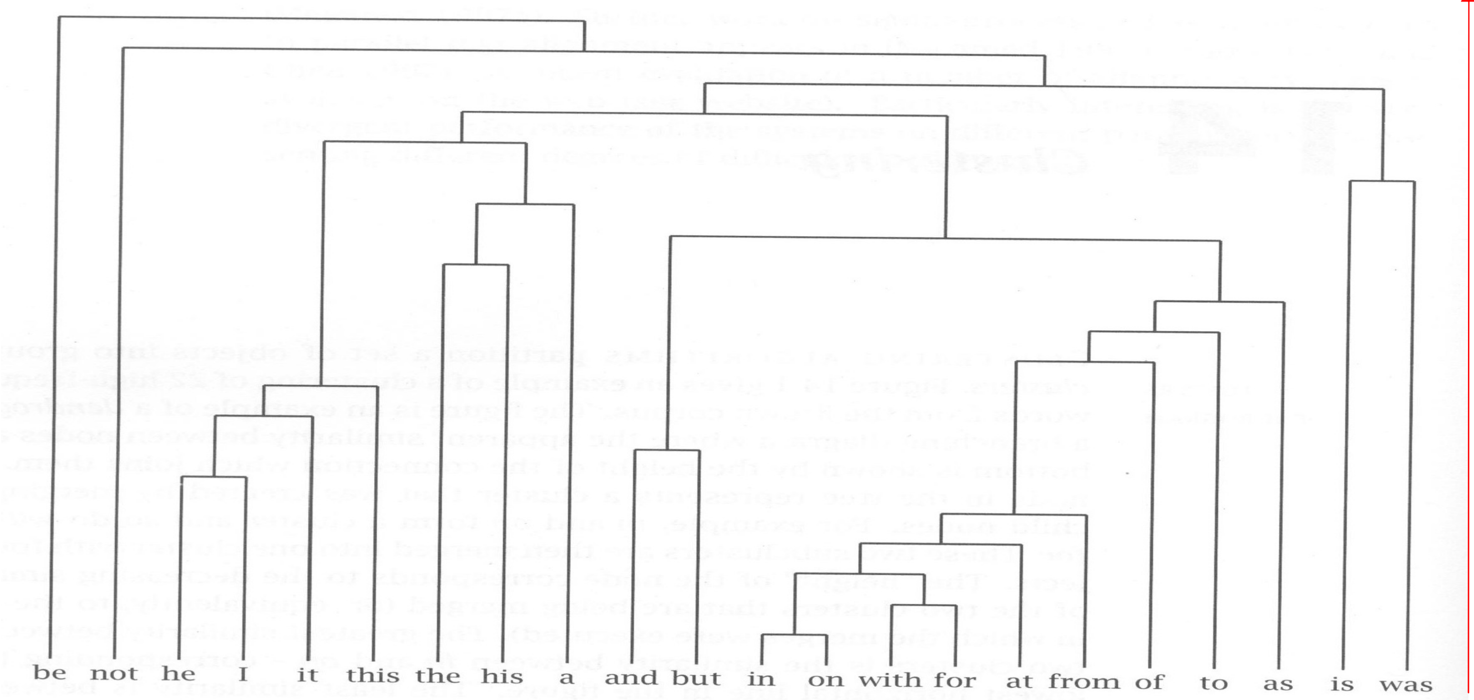
– The average similarity for their union will be

$$SIM(c_i \cup c_j) = \frac{\left(\vec{s}(c_i) + \vec{s}(c_j)\right)\cdot\left(\vec{s}(c_i) + \vec{s}(c_j)\right) - \left(|c_i| + |c_j|\right)}{\left(|c_i| + |c_j|\right)\left(|c_i| + |c_j| - 1\right)}$$



Example: Word Clustering

- Words (objects) are described and clustered using a set of features and values
  - E.g., the left and right neighbors of tokens of words



higher nodes: decreasing of similarity

Figure 14.1 A single-link clustering of 22 frequent English words represented as a dendrogram.

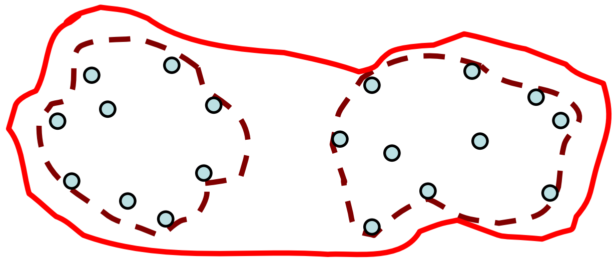
"be" has least similarity with the other 21 words !

Divisive Clustering (1/2)

- A top-down approach
- Start with all objects in a single cluster
- At each iteration, select the least **coherent** cluster and **split** it
- Continue the iterations until a predefined criterion (e.g., the cluster number) is achieved
- The history of clustering forms a binary tree or hierarchy

Divisive Clustering (2/2)

- To select the least coherent cluster, the measures used in bottom-up clustering (e.g. HAC) can be used again here
  - Single link measure
  - Complete-link measure
  - Group-average measure



- How to split a cluster
  - Also is a clustering task (finding two sub-clusters)
  - Any clustering algorithm can be used for the splitting operation, e.g.,
    - Bottom-up (agglomerative) algorithms
    - Non-hierarchical clustering algorithms (e.g., *K*-means)

Divisive Clustering: Algorithm

Given: a set $\mathcal{X} = \{x_1, \ldots x_n\}$ of objects
    a function coh: $\mathcal{P}(\mathcal{X}) \to \mathbb{R}$
    a function split: $\mathcal{P}(\mathcal{X}) \to \mathcal{P}(\mathcal{X}) \times \mathcal{P}(\mathcal{X})$
$C := \{\mathcal{X}\} \quad (= \{c_1\})$
$j := 1$
while $\exists c_i \in C$ s.t. $|c_i| > 1$
    $c_u := \arg\min_{c_v \in C} \mathrm{coh}(c_v)$
    $(c_{j+1}, c_{j+2}) := \mathrm{split}(c_u)$
    $C := C \backslash \{c_u\} \cup \{c_{j+1}, c_{j+2}\}$
    $j := j + 2$

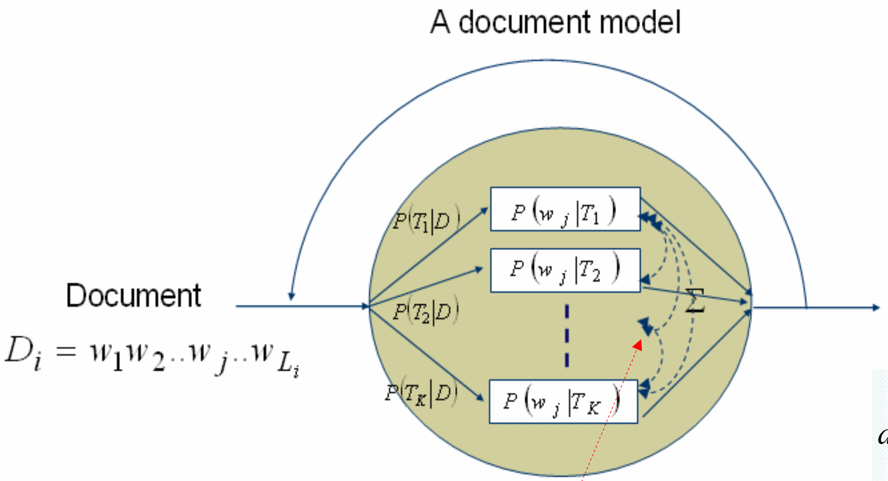
split the least coherent cluster

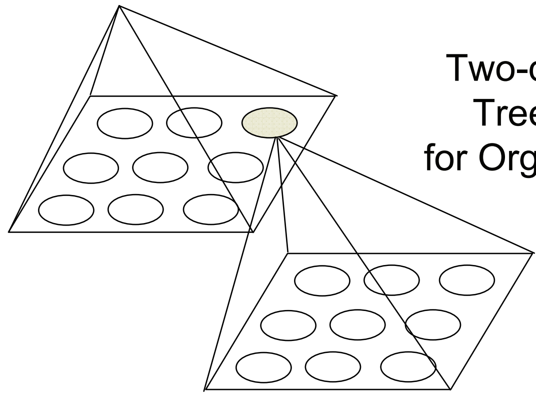
Generate two new clusters and remove the original one

Figure 14.3 Top-down hierarchical clustering.

Hierarchical Document Organization (1/7)

- Explore the Probabilistic Latent Topical Information
  - TMM/PLSA approach





Two-dimensional
Tree Structure
for Organized Topics

$$P(w_j|D_i) = \sum_{k=1}^{K} P(T_k|D_i)\left[\sum_{l=1}^{K} \boxed{P(T_l|Y_k)} P(w_j|T_l)\right]$$

$$dist(T_i,T_j) = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2} \qquad E(T_l,T_k) = \frac{1}{\sqrt{2\pi}\,\sigma}\exp\left[-\frac{dist(T_k,T_l)^2}{2\sigma^2}\right]$$

$$P(T_l|Y_k) = \frac{E(T_l,T_k)}{\sum_{s=1}^{K} E(T_s,T_k)}$$

- Documents are clustered by the latent topics and organized in a two-dimensional tree structure, or a two-layer map
- Those related documents are in the same cluster and the relationships among the clusters have to do with the distance on the map
- When a cluster has many documents, we can further analyze it into an other map on the next layer

Hierarchical Document Organization (2/7)

- The model can be trained by maximizing the total log-likelihood of all terms observed in the document collection

$$L_T = \sum_{i=1}^{N} \sum_{n=1}^{J} c\left(w_j, D_i\right) \log P\left(w_j \middle| D_i\right)$$

$$= \sum_{i=1}^{N} \sum_{n=1}^{J} c\left(w_j, D_i\right) \log \left\{ \sum_{k=1}^{K} P\left(T_k \middle| D_i\right) \left[\sum_{l=1}^{K} P\left(T_l \middle| Y_k\right) P\left(w_j \middle| T_l\right) \right] \right\}$$

  - EM training can be performed

$$\hat{P}\left(w_j \mid T_k\right) = \frac{\sum_{i=1}^{N} c\left(w_j, D_i\right) P\left(T_k \mid w_j, D_i\right)}{\sum_{j'=1}^{J} \sum_{i'=1}^{N} c\left(w_{j'}, D_{i'}\right) P\left(T_k \mid w_{j'}, D_{i'}\right)}$$

$$\hat{P}\left(T_k \mid D_i\right) = \frac{\sum_{j=1}^{J} c\left(w_j, D_i\right) P\left(T_k \mid w_j, D_i\right)}{c\left(D_i\right)}$$

where

$$P'\left(T_k \mid w_j, D_i\right) = \frac{\left[\sum_{l=1}^{K} P\left(w_j \mid T_l\right) P\left(T_l \mid T_k\right)\right] \cdot P\left(T_k \mid D_i\right)}{\sum_{k'=1}^{K} \left\{ \left[\sum_{l'=1}^{K} P\left(w_j \mid T_{l'}\right) P\left(T_{l'} \mid T_{k'}\right) \right] \cdot P\left(T_{k'} \mid D_i\right) \right\}}$$

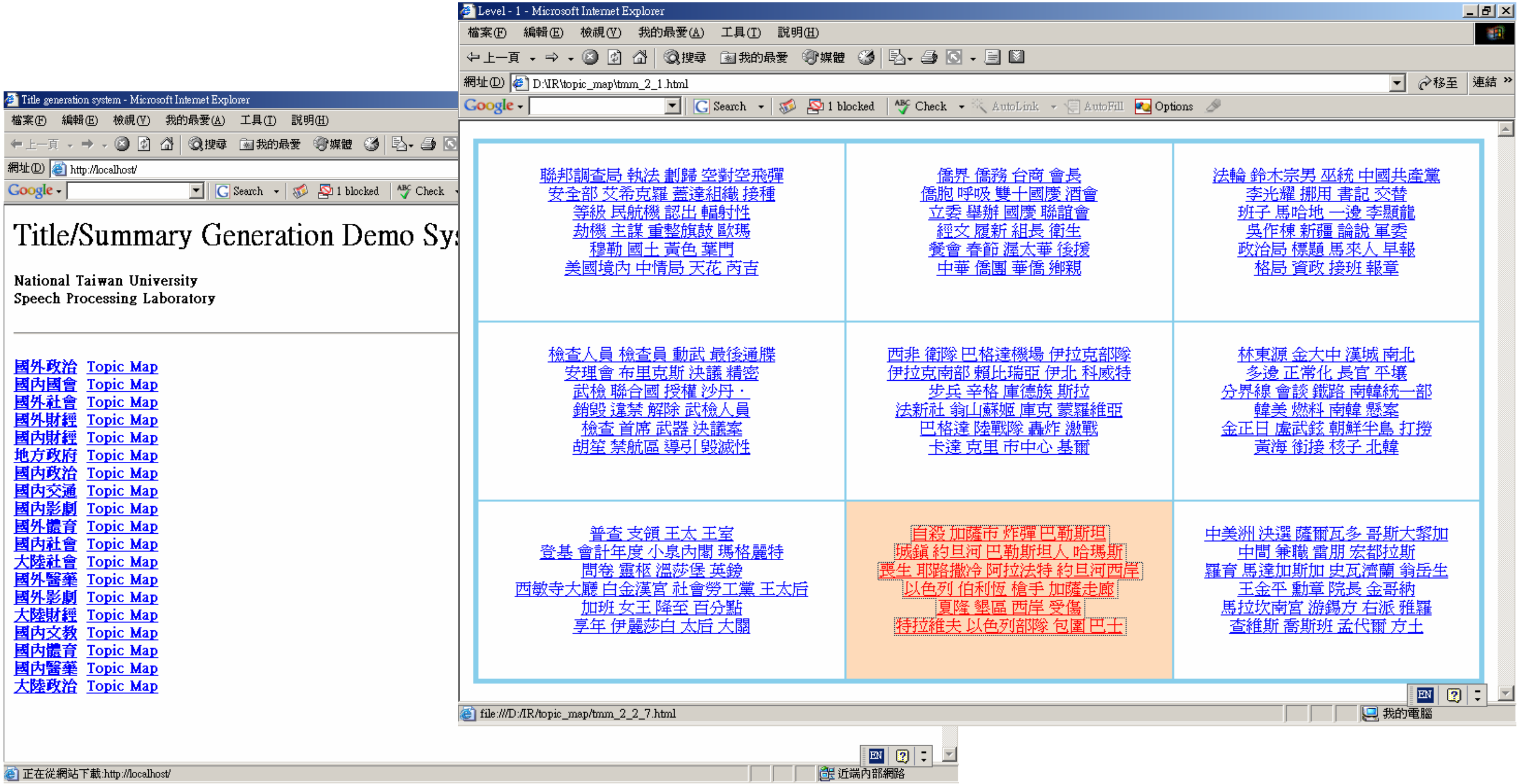
Hierarchical Document Organization (3/7)

- Criterion for Topic Word Selecting

$$S\left(w_j, T_k\right) = \frac{\sum_{i=1}^{N} c\left(w_j, D_i\right) P\left(T_k \mid D_i\right)}{\sum_{i'=1}^{N} c\left(w_j, D_{i'}\right)\left[1 - P\left(T_k \mid D_{i'}\right)\right]}$$

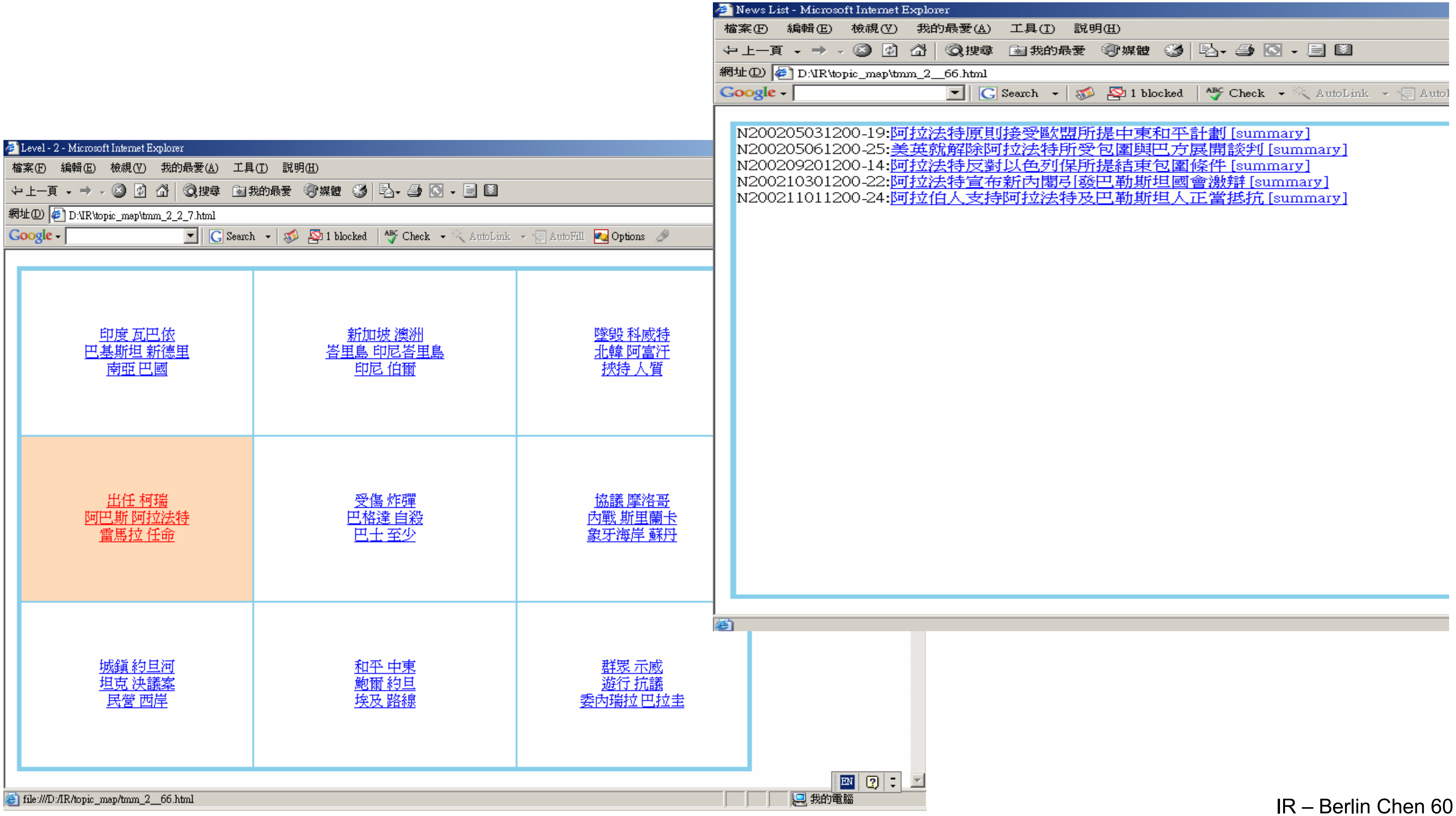
Hierarchical Document Organization (4/7)

- Example



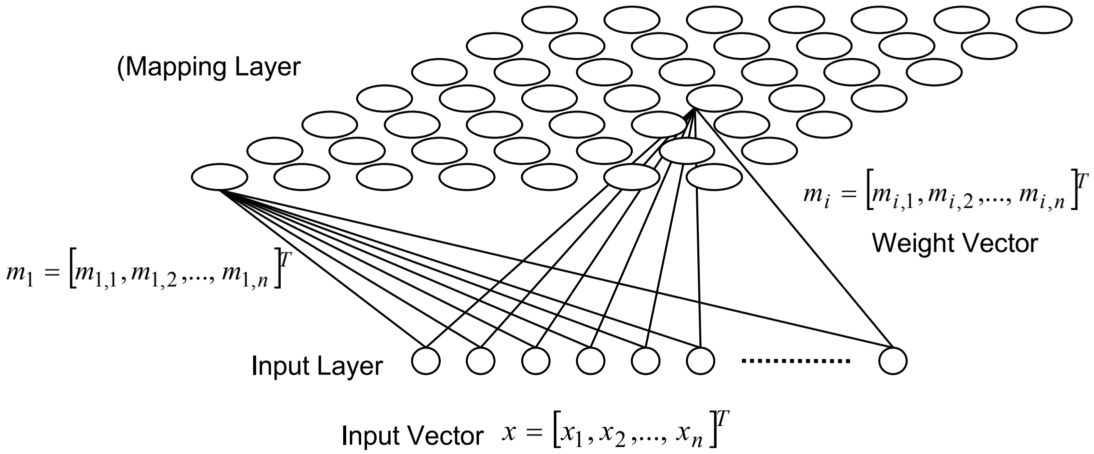
Hierarchical Document Organization (5/7)

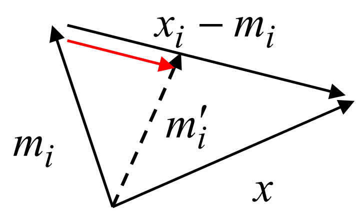
- Example (cont.)



Hierarchical Document Organization (6/7)

- Self-Organization Map (SOM)
  - A recursive regression process





$$m_i(t+1) = m_i(t) + h_{c(x),i}(t)[x(t) - m_i(t)]$$

$$c(x) = \arg \min_{i'} \left\| x - m_{i'} \right\|$$

where

$$\left\| x - m_{i'} \right\| = \sqrt{\sum_n \left(x_n - m_{i',n} \right)^2}$$

$$h_{c(x),i}(t) = \alpha(t) \exp\left(- \frac{\left\| r_i - r_{c(x)} \right\|^2}{2\sigma^2(t)} \right)$$

Hierarchical Document Organization (7/7)

- Results

Model	Iterations	$dist_{Between}/dist_{Within}$
TMM	10	1.9165
	20	2.0650
	30	1.9477
	40	1.9175
SOM	100	2.0604

$$R_{Dist} = \frac{dist_{Between}}{dist_{Within}}$$

where

$$dist_{Between} = \frac{\sum_{i=1}^{|D|}\sum_{j=i+1}^{|D|} f_{Between}(i,j)}{\sum_{i=1}^{|D|}\sum_{j=i+1}^{|D|} C_{Between}(i,j)}$$

$$f_{Between}(i,j) = \begin{cases} dist_{Map}(i,j) & T_{r,i} \neq T_{r,j} \\ 0 & otherwise \end{cases}$$

$$dist_{Map}(i,j) = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}$$

$$C_{Between}(i,j) = \begin{cases} 1 & T_{r,i} \neq T_{r,j} \\ 0 & otherwise \end{cases}$$

$$dist_{Within} = \frac{\sum_{i=1}^{|D|}\sum_{j=i+1}^{|D|} f_{Within}(i,j)}{\sum_{i=1}^{|D|}\sum_{j=i+1}^{|D|} C_{Within}(i,j)}$$

$$f_{Within}(i,j) = \begin{cases} dist_{Map}(i,j) & T_{r,i} = T_{r,j} \\ 0 & otherwise \end{cases}$$

$$C_{Within}(i,j) = \begin{cases} 1 & T_{r,i} = T_{r,j} \\ 0 & otherwise \end{cases}$$