Clustering Techniques for Information Retrieval

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References:
2. Modern Information Retrieval, Chapters 5 & 7
Clustering

• Place **similar objects** in the same group and assign **dissimilar objects** to different groups (typically using a distance measure, such as Euclidean distance)
  – 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

• Nevertheless, 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
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 sub-cluster 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 is seemingly only applicable/optimal for some applications)
  – Less efficient than flat clustering (minimally have to compute $n \times n$ 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)
Some Applications of Clustering in IR (1/5)

- **Cluster Hypothesis** (for IR): Documents in the same cluster behave similarly with respect to relevance to information needs

- Possible applications of Clustering in IR

<table>
<thead>
<tr>
<th>Application</th>
<th>What is clustered?</th>
<th>Benefit</th>
<th>Example</th>
</tr>
</thead>
<tbody>
<tr>
<td>Result set clustering</td>
<td>result set</td>
<td>more effective information presentation to user</td>
<td>Figure 16.2</td>
</tr>
<tr>
<td>Scatter-Gather</td>
<td>(subsets of)</td>
<td>alternative user interface: “search without typing”</td>
<td>Figure 16.3</td>
</tr>
<tr>
<td>Collection clustering</td>
<td>collection</td>
<td>effective information presentation for exploratory browsing</td>
<td>McKeown et al. (2002), <a href="http://news.google.com">http://news.google.com</a></td>
</tr>
<tr>
<td>Language modeling</td>
<td>collection</td>
<td>increased precision and/or recall</td>
<td>Liu and Croft (2004)</td>
</tr>
<tr>
<td>Cluster-based retrieval</td>
<td>collection</td>
<td>higher efficiency: faster search</td>
<td>Salton (1971a)</td>
</tr>
</tbody>
</table>

- These possible applications differ in
  - The collection of documents to be clustered
  - The aspect of the IR system to be improved
Some Applications of Clustering in IR (2/5)

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 (for a collection of New York Times)

Users often prefer browsing over searching, because they are unsure about which search terms to use.

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).
Some Applications of Clustering in IR (3/5)

2. Improve recall in search applications
   - Achieve better search results by
     • Alleviating the term-mismatch (synonym) problem facing the vector space model
       - First, identify an initial set of documents that match the query (i.e., contain some of the query words)
       - Then, add other documents from the same clusters even if they have low similarity to the query
     • 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

\[
\hat{P}(Q|M_D) = \prod_{i=1}^{N} \left[ \lambda \cdot P(w_i|M_D) + (1 - \lambda) \cdot P(w_i|M_{\text{Cluster}(D)}) \right]
\]
Some Applications of Clustering in IR (4/5)

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

Top 235 results of at least 55,449,081 retrieved for the query jaguar (definition) (details)

1. **Jaguar**
   - The jaguar (*Panthera onca*) is a large member of the cat family native to warm regions of the Americas. It is closely related to the lion, tiger, and leopard of the Old World, and is the largest species of the cat family found in the Americas.

2. **Jaguar**
   - Official worldwide web site of Jaguar Cars. Directs users to pages tailored to country-specific markets.
   - [www.jaguar.com](http://www.jaguar.com) - [cache] - Live, Open Directory, Ask

3. **Jag-lovers**
   - All Jaguar's Cars. We support our users by hosting multiple Web Sites and Web-based Forums for the various Jaguar models. Registered trademarks and are the property of Jaguar Cars, England. Some images may also be ©Jaguar Cars. Mirroring...

4. **Jacksonville Jaguars**
   - The official team site with scores, news items, game schedule, and roster.

5. **www.jaguarusa.com**
   - Build Your Jaguar, Request Brochure, Get Email Updates, Locate a Dealer, Search, Your Profile, Site Map. Contact Us. ... - XK, XJ, S-TYPE, X-TYPE, PRE-OWNED, LATEST, OWNERSHIP, Highlights.

http://clusty.com
4. Speed 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 closest to the query and then only consider documents from these clusters
       - Within this much smaller set, we can compute similarities exhaustively and rank documents in the usual way
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 (documents 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 effectiveness 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

\[
Purity(\Omega, \Gamma) = \frac{1}{N} \sum_{k} \max_{j} |\omega_j \cap c_k|
\]

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

\[
Purity(\Omega, \Gamma) = \frac{1}{17} (5 + 4 + 3) = 0.71
\]
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 $N(N-1)/2$ pairs of $N$ distinct documents in the cluster and the true class

<table>
<thead>
<tr>
<th>Number of document pairs</th>
<th>Same cluster in clustering</th>
<th>Different clusters in clustering</th>
</tr>
</thead>
<tbody>
<tr>
<td>Same class in ground truth</td>
<td>TP (True Positive)</td>
<td>FN (False Negative)</td>
</tr>
<tr>
<td>Different classes in ground truth</td>
<td>FP (False Positive)</td>
<td>TN (True Negative)</td>
</tr>
</tbody>
</table>

$$RI = \frac{TP + TN}{TP + FP + FN + TN}$$
Rand Index (2/3)

\[ \text{TP} = \binom{5}{2} + \binom{4}{2} + \binom{3}{2} + \binom{2}{2} = 20 \]
\[ \text{FP} = \binom{5}{1} + \binom{4}{1} + \binom{3}{1} + \binom{2}{1} + \binom{1}{1} + \binom{3}{2} = 20 \]
\[ \left( \binom{6}{2} + \binom{6}{2} + \binom{5}{2} \right) - \text{TP} \]

<table>
<thead>
<tr>
<th>Same cluster</th>
<th>Different clusters</th>
</tr>
</thead>
<tbody>
<tr>
<td>TP=20</td>
<td>FN=24</td>
</tr>
<tr>
<td>FN=24</td>
<td>TN=72</td>
</tr>
</tbody>
</table>

\[ \text{RI} = \frac{20 + 72}{20 + 20 + 24 + 72} = 0.68 \]

all positive pairs

all negative 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 (documents)
  – 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)

\[ P = \frac{TP}{TP + FP}, \quad R = \frac{TP}{TP + FN} \]

\[ F_b = \frac{b^2 + 1}{b^2 \left( \frac{1}{R} + \frac{P}{P} \right)} = \frac{b^2 + 1}{b^2 P + R} \]

- If we want to penalize false negatives (FN) more strongly than false positives (FP), then we can set \( b > 1 \) (separating similar documents is sometimes worse than putting dissimilar documents in the same cluster)
- That is, giving more weight to recall (R)

<table>
<thead>
<tr>
<th></th>
<th>Same cluster</th>
<th>Different clusters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Same class</td>
<td>TP</td>
<td>FN</td>
</tr>
<tr>
<td>Different classes</td>
<td>FP</td>
<td>TN</td>
</tr>
</tbody>
</table>
Normalized Mutual Information (NMI)

• NMI is an information-theoretical measure

\[ \text{NMI}(\Omega, C) = \frac{I(\Omega; C)}{(H(\Omega) + H(C))/2} \]

\[ I(\Omega; C) = \sum_k \sum_j p(\omega_k \cap c_j) \log \frac{p(\omega_k \cap c_j)}{p(\omega_k)p(c_j)} \]

\[ = \sum_k \sum_j \frac{|\omega_k \cap c_j|}{N} \log \frac{N|\omega_k \cap c_j|}{|\omega_k||c_j|} \quad (\text{ML estimate}) \]

\[ H(\Omega) = -\sum_k p(\omega_k) \log p(\omega_k) \]

\[ = -\sum_k \frac{|\omega_k|}{N} \log \frac{|\omega_k|}{N} \quad (\text{ML estimate}) \]

– NMI will have a value between 0 and 1

• NMI has the same problem as purity

– NMI does not penalize large cardinalities and thus does not formalize our bias, other thing being equal, fewer clusters are better
Summary of External Evaluation Measures

Table 16.2 The four external evaluation measures applied to the clustering in Figure 16.4.

<table>
<thead>
<tr>
<th></th>
<th>purity</th>
<th>NMI</th>
<th>RI</th>
<th>$F_5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>lower bound</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>maximum</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>value for Figure</td>
<td>0.71</td>
<td>0.36</td>
<td>0.68</td>
<td>0.46</td>
</tr>
</tbody>
</table>
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) ?  $k-1 \rightarrow k \rightarrow k+1$

• **Algorithms** introduced here
  – The $K$-means algorithm
  – The EM algorithm

Hierarchical clustering is also faced with 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
  - Objects (e.g., documents) should be represented in **vector form**
- 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) → 8 bits/pixel (256 colors)
    - A compression rate of 3

\[
X = \{x^t\}_{t=1}^n \quad \text{index } j \rightarrow \quad F = \{m_j\}_{j=1}^k \quad \text{Dim}(x^t)=24 \rightarrow |F|=2^8
\]

\[m_j: \text{cluster centroid or reference vector, code word, code vector}\]
The $K$-means Algorithm (2/10)

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

**Total reconstruction error (RSS : residual sum of squares)**

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

where $b_i^t = \begin{cases} 1 & \text{if } \|x^t - m_i\| = \min_j \|x^t - m_j\| \\ 0 & \text{otherwise} \end{cases}$

- $b_i^t$ and $m_i$ are unknown in advance
- $b_i^t$ depends on $m_i$ and this optimization problem cannot be solved analytically
The $K$-means Algorithm (3/10)

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

- **Recursion**
  - Assign each object $x^t$ to the cluster whose center is closest
    
    $$b_i^t = \begin{cases} 1 & \text{if } \|x^t - m_i\| = \min_j \|x^t - m_j\| \\ 0 & \text{otherwise} \end{cases}$$

  - Then, re-compute the center of each cluster as the centroid or mean (average) of its members
    
    $$m_i = \frac{\sum_{t=1}^N b_i^t \cdot x^t}{\sum_{t=1}^N b_i^t}$$

  - These two steps are repeated until $m_i$ stabilizes (a stopping criterion)

- Or, we can instead use the medoid as the cluster center?
  - (a medoid is one of the objects in the cluster that is closest to the centroid)
The \( K \)-means Algorithm (4/10)

- Algorithm

\[
\text{Initialize } m_i, i = 1, \ldots, k, \text{ for example, to } k \text{ random } x_t \\
\text{Repeat} \\
\text{For all } x_t \in \mathcal{X} \\
\quad b^t_i \left\{ \begin{array}{ll} 
1 & \text{if } \|x_t - m_i\| = \min_j \|x_t - m_j\| \\
0 & \text{otherwise} 
\end{array} \right. \\
\text{For all } m_i, i = 1, \ldots, k \\
\quad m_i \leftarrow \sum_t b^t_i x_t / \sum_t b^t_i \\
\text{Until } m_i \text{ converge}
\]
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

<table>
<thead>
<tr>
<th>Cluster</th>
<th>Members</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>ballot (0.28), polls (0.28), Gov (0.30), seats (0.32)</td>
</tr>
<tr>
<td>2</td>
<td>profit (0.21), finance (0.21), payments (0.22)</td>
</tr>
<tr>
<td>3</td>
<td>NFL (0.36), Reds (0.28), Sox (0.31), inning (0.33), quarterback (0.30), scored (0.30), score (0.33)</td>
</tr>
<tr>
<td>4</td>
<td>researchers (0.23), science (0.23)</td>
</tr>
<tr>
<td>5</td>
<td>Scott (0.28), Mary (0.27), Barbara (0.27), Edward (0.29)</td>
</tr>
</tbody>
</table>

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.

\[
s_{u,v} = \frac{\vec{s}_u \cdot \vec{s}_v}{|\vec{s}_u| \times |\vec{s}_v|}
\]
The $K$-means Algorithm (7/10)

- Complexity: $O(\text{IKNM})$
  - $I$: 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 $m$ of all data and generate $k$ initial centers $m_i$ by adding small random vector to the mean $m \pm \delta$
  - 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 $m_i$
  - 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

• Possible 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-mean Algorithm (10/10)

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

\[
\{ \mu_1, \Sigma_1, \omega_1 \} \quad \rightarrow \quad \{ \mu_2, \Sigma_2, \omega_2 \} \quad \rightarrow \quad \{ \mu_3, \Sigma_3, \omega_3 \} \quad \rightarrow \quad \{ \mu_4, \Sigma_4, \omega_4 \}
\]

Total reconstruction error (residual sum of squares)

\[
E\left( \{ m_i \}_{i=1}^k \mid X \right) = \sum_{t=1}^N \sum_{i=1}^k b_i^t \left\| x' - m_i \right\|^2
\]
The EM Algorithm (1/3)

- EM (Expectation-Maximization) algorithm
  - A kind of model-based clustering
  - Also can be viewed as a generalization of $K$-means
  - Each cluster is a “model” for generating the data
    - The centroid is good representative for each model
    - Generate an object (e.g., document) consists of first picking a centroid at random and then adding some noise
      - If the noise is normally distributed, the procedure will result in clusters of spherical shape

- Physical Models for EM
  - Discrete: Mixture of multinomial distributions
  - Continuous: Mixture of Gaussian distributions
The EM Algorithm (2/3)

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

\[
P(\bar{x}_i|\Theta) = \sum_{k=1}^{K} P(\bar{x}_i|\omega_k;\Theta)P(\omega_k|\Theta)
\]

**Continuous case:**
\[
P(\bar{x}_i|\omega_k;\Theta) = \frac{1}{\sqrt{(2\pi)^m |\Sigma_k|}} \exp\left(-\frac{1}{2} (\bar{x}_i - \bar{\mu}_k)^T \Sigma_k^{-1} (\bar{x}_i - \bar{\mu}_k) \right)
\]

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

\[X = \{\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_n\}\]
The EM Algorithm (2/3)

Figure 14.10 An example of using the EM algorithm for soft clustering.
Maximum Likelihood Estimation (MLE) (1/2)

- Hard Assignment

Cluster $\omega_1$

- $P(B | \omega_1) = 2/4 = 0.5$
- $P(W | \omega_1) = 2/4 = 0.5$
Maximum Likelihood Estimation (2/2)

- Soft Assignment

\[
P(\omega_1) = \frac{(0.7 + 0.4 + 0.9 + 0.5)}{(0.7 + 0.4 + 0.9 + 0.5 + 0.3 + 0.6 + 0.1 + 0.5)} = \frac{2.5}{4} = 0.625
\]

\[
P(\omega_2) = 1 - P(\omega_1) = 0.375
\]

\[
P(B|\omega_1) = \frac{(0.7 + 0.9)}{(0.7 + 0.4 + 0.9 + 0.5)} = \frac{1.6}{2.5} = 0.64
\]

\[
P(B|\omega_2) = \frac{(0.4 + 0.5)}{(0.7 + 0.4 + 0.9 + 0.5)} = \frac{0.9}{2.5} = 0.36
\]

\[
P(B|\omega_1) = \frac{(0.4 + 0.9 + 0.5)}{(0.7 + 0.4 + 0.9 + 0.5)} = \frac{0.9}{2.5} = 0.36
\]

\[
P(B|\omega_2) = \frac{(0.3 + 0.1 + 0.5)}{(0.3 + 0.6 + 0.1 + 0.5)} = \frac{0.4}{1.5} = 0.27
\]

\[
P(B|\omega_2) = \frac{(0.6 + 0.5)}{(0.3 + 0.6 + 0.1 + 0.5)} = \frac{0.11}{1.5} = 0.73
\]
Expectation-Maximization Updating Formulas (1/3)

• Expectation

\[ \gamma_{ik} = \frac{P(\vec{x}_i | \omega_k, \Theta)P(\omega_k | \Theta)}{\sum_{l=1}^{K} P(\vec{x}_i | \omega_l, \Theta)P(\omega_l | \Theta)} \]

– Compute the likelihood that each cluster \( \omega_k \) generates a document vector \( \vec{x}_i \)
Expectation-Maximization Updating Formulas (2/3)

- **Maximization**
  - **Mixture Weight**
    \[
    P(\omega_k | \hat{\Theta}) = \frac{\sum_{i=1}^{n} \gamma_{ik}}{\sum_{k'=1}^{K} \sum_{i=1}^{n} \gamma_{ik'}} = \frac{\sum_{i=1}^{n} \gamma_{ik}}{n}
    \]
  - **Mean of Gaussian**
    \[
    \hat{\mu}_k = \frac{\sum_{i=1}^{n} \gamma_{ik} \cdot \vec{x}_i}{\sum_{i'=1}^{n} \gamma_{i'k}}
    \]
Expectation-Maximization Updating Formulas (3/3)

- Covariance Matrix of Gaussian

\[
\hat{\Sigma}_k = \frac{\sum_{i=1}^{n} \gamma_{i,k} \cdot (\bar{x}_i - \hat{\mu}_k)(\bar{x}_i - \hat{\mu}_k)^T}{\sum_{i' = 1}^{n} \gamma_{i',k}}
\]

\[
= \frac{\sum_{i=1}^{n} \gamma_{i,k} \cdot (\bar{x}_i - \hat{\mu}_k)(\bar{x}_i - \hat{\mu}_k)^T}{\sum_{i' = 1}^{n} \gamma_{i',k}}
\]
More facts about The EM Algorithm

- The initial cluster distributions can be estimated using the $K$-means algorithm, which EM can then “soften up”

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

• Can be in either bottom-up or top-down manners
  – **Bottom-up** (*agglomerative*)
    • Start with individual objects and try to group the most similar ones
      – E.g., with the minimum distance apart
    • The procedure terminates when one cluster containing all objects has been formed
  – **Top-down** (*divisive*)
    • Start with all objects in a group and divide them into groups so as to maximize **within-group** similarity

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

distance measures will be discussed later on
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 only one cluster survived

• The history of merging/clustering forms a binary tree or hierarchy
HAC: Algorithm

1. Given: a set $X = \{x_1, \ldots, x_n\}$ of objects
2. a function $\text{sim}: \mathcal{P}(X) \times \mathcal{P}(X) \to \mathbb{R}$
3. for $i := 1$ to $n$ do
   4. $c_i := \{x_i\}$ end
5. $C := \{c_1, \ldots, c_n\}$
6. $j := n + 1$
7. while $|C| > 1$ do
8.   $(c_{n_1}, c_{n_2}) := \arg \max_{(c_u, c_v) \in C \times C} \text{sim}(c_u, c_v)$
9.   $c_j := c_{n_1} \cup c_{n_2}$
10. $C := C \setminus \{c_{n_1}, c_{n_2}\} \cup \{c_j\}$
11. $j := j + 1$

Figure 14.2 Bottom-up hierarchical clustering.

- $c_i$ denotes a specific cluster here
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)

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

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

\[ 1 - \frac{\vec{x} \cdot \vec{y}}{||\vec{x}|| \cdot ||\vec{y}||} \]

ranged between 0 and 1
Measures of Cluster Similarity (1/9)

• Especially for the bottom-up approaches

1. **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

\[
sim(\omega_i, \omega_j) = \max_{\bar{x} \in \omega_i, \bar{y} \in \omega_j} \sim(\bar{x}, \bar{y})
\]

cf. the minimal spanning tree
2. **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.

\[
sim(\omega_i, \omega_j) = \min_{\bar{x} \in \omega_i, \bar{y} \in \omega_j} \sim(\bar{x}, \bar{y})
\]

- More sensitive to outliers.

**Figure 17.6** Outliers in complete-link clustering. The four points have the coordinates $-3 + 2 \times \epsilon, 01 + 2 \times \epsilon, 2$ 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 (3/9)

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 (4/9)

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 \( \approx 0.56 \). 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 (5/9)

3. **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

\[
sim(\bar{x}, \bar{y}) = \cos(\bar{x}, \bar{y}) = \frac{\bar{x} \cdot \bar{y}}{\|\bar{x}\| \|\bar{y}\|} = \bar{x} \cdot \bar{y}
\]
Measures of Cluster Similarity (6/9)

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

- The average similarity $SIM$ between vectors in a cluster $\omega_j$ is defined as

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

- The sum of members in a cluster $\omega_j$: $\bar{s}(\omega_j) = \sum_{\bar{x} \in \omega_j} \bar{x}$

- Express $SIM(\omega_j)$ in terms of $\bar{s}(\omega_j)$

$$\bar{s}(\omega_j) \cdot \bar{s}(\omega_j) = \sum_{\bar{x} \in \omega_j} \bar{x} \cdot \bar{s}(\omega_j) = \sum_{\bar{x} \in \omega_j} \sum_{\bar{y} \in \omega_j} \bar{x} \cdot \bar{y}$$

$$= |\omega_j|(|\omega_j| - 1)SIM(\omega_j) + \sum_{\bar{x} \in \omega_j} \bar{x} \cdot \bar{x}$$

$$= |\omega_j|(|\omega_j| - 1)SIM(\omega_j) + |\omega_j|$$

$$\therefore SIM(c_j) = \frac{\bar{s}(\omega_j) \cdot \bar{s}(\omega_j) - |\omega_j|}{|\omega_j|(|\omega_j| - 1)}$$
Measures of Cluster Similarity (7/9)

3. Group-average agglomerative clustering (cont.)

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

$$\vec{s}(\omega_{New}) = \vec{s}(\omega_i) + \vec{s}(\omega_j), \quad |\omega_{New}| = |\omega_i| + |\omega_j|$$

- The average similarity for their union will be

$$SIM(\omega_i \cup \omega_j) = \frac{(\vec{s}(\omega_i) + \vec{s}(\omega_j)) \cdot (\vec{s}(\omega_i) + \vec{s}(\omega_j)) - (|\omega_i| + |\omega_j|)}{(\omega_i + |\omega_j|)(\omega_i + |\omega_j|) - 1}$$

$$\vec{s}(\omega_i) \bullet \omega_i \quad \vec{s}(\omega_j) \bullet \omega_j$$
Measures of Cluster Similarity (8/9)

4. **Centroid clustering**
   - The similarity of two clusters is defined as the similarity of their centroids

\[
sim(\omega_i, \omega_j) = \bar{\mu}(\omega_i) \cdot \bar{\mu}(\omega_j)
\]

\[
= \left( \frac{1}{N_i} \sum_{\bar{x}_s \in \omega_i} \bar{x}_s \right) \cdot \left( \frac{1}{N_j} \sum_{\bar{x}_t \in \omega_j} \bar{x}_t \right)
\]

\[
= \frac{1}{N_i N_j} \sum_{\bar{x}_s \in \omega_i} \sum_{\bar{x}_t \in \omega_j} \bar{x}_s \cdot \bar{x}_t
\]
Measures of Cluster Similarity (9/9)

- Graphical summary of four cluster similarity measures

![Graphical summary of four cluster similarity measures](image)

Figure 17.3 The different notions of cluster similarity used by the four HAC algorithms. An inter-similarity is a similarity between two documents from different clusters.

<table>
<thead>
<tr>
<th>Clustering Algorithm</th>
<th>( \text{SIM}(i, k_1, k_2) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>single-link</td>
<td>max(( \text{SIM}(i, k_1), \text{SIM}(i, k_2) ))</td>
</tr>
<tr>
<td>complete-link</td>
<td>min(( \text{SIM}(i, k_1), \text{SIM}(i, k_2) ))</td>
</tr>
<tr>
<td>centroid</td>
<td>( (\frac{1}{N_m} \overrightarrow{v}_m) \cdot (\frac{1}{N_i} \overrightarrow{v}_i) )</td>
</tr>
<tr>
<td>group-average</td>
<td>( \frac{1}{(N_m+N_i)(N_m+N_i-1)} [(\overrightarrow{v}_m + \overrightarrow{v}_i)^2 - (N_m + N_i)] )</td>
</tr>
</tbody>
</table>
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

"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

1. Given: a set $\mathcal{X} = \{x_1, \ldots, x_n\}$ of objects
2. a function $\text{coh}: \mathcal{P}(\mathcal{X}) \rightarrow \mathbb{R}$
3. a function $\text{split}: \mathcal{P}(\mathcal{X}) \rightarrow \mathcal{P}(\mathcal{X}) \times \mathcal{P}(\mathcal{X})$
4. $C := \{\mathcal{X}\} \; (= \{c_1\})$
5. $j := 1$

6. while $\exists c_i \in C \; \text{s.t.} \; |c_i| > 1$
7. \hspace{1em} $c_u := \arg \min_{c_v \in C} \text{coh}(c_v)$
8. \hspace{1em} $(c_{j+1}, c_{j+2}) := \text{split}(c_u)$
9. \hspace{1em} $C := C \setminus \{c_u\} \cup \{c_{j+1}, c_{j+2}\}$
10. $j := j + 2$

Figure 14.3  Top-down hierarchical clustering.

- $c_u$ denotes a specific cluster here
Hierarchical Document Organization (1/7)

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

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 another map on the next layer.

Mathematical expressions:

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

\[
dist(T_i, T_j) = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}
\]

\[
E(T_i, T_k) = \frac{1}{\sqrt{2\pi\sigma}} \exp \left[ -\frac{dist(T_k, T_i)^2}{2\sigma^2} \right]
\]

\[
P(T_l | Y_k) = \frac{E(T_l, T_k)}{\sum_{s=1}^{K} E(T_s, T_k)}
\]
Hierarchical Document Organization (2/7)

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

\[
L_T = \sum_{i=1}^{N} \sum_{n=1}^{J} c(w_j, D_i) \log P(w_j | D_i)
\]

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

- EM training can be performed

\[
\hat{P}(w_j | T_k) = \frac{\sum_{i=1}^{N} c(w_j, D_i) P(T_k | w_j, D_i)}{\sum_{j'=1}^{J} \sum_{i'=1}^{N} c(w_{j'}, D_{i'}) P(T_k | w_{j'}, D_{i'})}
\]

\[
\hat{P}(T_k | D_i) = \frac{\sum_{j=1}^{J} c(w_j, D_i) P(T_k | w_j, D_i)}{c(D_i)}
\]

where

\[
P(T_k | w_j, D_i) = \frac{\left[ \sum_{l=1}^{K} P(w_j | T_l) P(T_l | T_k) \right] \cdot P(T_k | D_i)}{\sum_{k'=1}^{K} \left[ \sum_{l'=1}^{K} P(w_j | T_{l'}) P(T_{l'} | T_{k'}) \right] \cdot P(T_{k'} | D_i)}
\]
Hierarchical Document Organization (3/7)

- Criterion for Topic Word Selecting
  - Topic Ratio

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

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

\[ c(x) = \arg \min_{i'} \| x - m_{i'} \| \]

where

\[ \| x - m_i \| = \sqrt{\sum_n (x_n - m_{i',n})^2} \]

\[ h_{c(x),i}(t) = \alpha(t) \exp \left( -\frac{\| r_i - r_{c(x)} \|^2}{2\sigma^2(t)} \right) \]
Hierarchical Document Organization (7/7)

- Results

<table>
<thead>
<tr>
<th>Model</th>
<th>Iterations</th>
<th>( \text{dist}<em>{\text{Between}} / \text{dist}</em>{\text{Within}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>TMM</td>
<td>10</td>
<td>1.9165</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>2.0650</td>
</tr>
<tr>
<td></td>
<td>30</td>
<td>1.9477</td>
</tr>
<tr>
<td></td>
<td>40</td>
<td>1.9175</td>
</tr>
<tr>
<td>SOM</td>
<td>100</td>
<td>2.0604</td>
</tr>
</tbody>
</table>

\[
R_{\text{Dist}} = \frac{\text{dist}_{\text{Between}}}{\text{dist}_{\text{Within}}}
\]

\[
dist_{\text{Between}}(i, j) = \frac{\sum_{i=1}^{D} \sum_{j=i+1}^{D} f_{\text{Map}}(i, j) \cdot T_{r,i} \neq T_{r,j}}{\sum_{i=1}^{D} \sum_{j=i+1}^{D} C_{\text{Between}}(i, j)}
\]

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

\[
f_{\text{Between}}(i, j) = \begin{cases} 
\text{dist}_{\text{Map}}(i, j) & T_{r,i} \neq T_{r,j} \\
0 & \text{otherwise}
\end{cases}
\]

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

\[
dist_{\text{Within}}(i, j) = \frac{\sum_{i=1}^{D} \sum_{j=i+1}^{D} f_{\text{Map}}(i, j) \cdot T_{r,i} = T_{r,j}}{\sum_{i=1}^{D} \sum_{j=i+1}^{D} C_{\text{Within}}(i, j)}
\]

\[
f_{\text{Within}}(i, j) = \begin{cases} 
\text{dist}_{\text{Map}}(i, j) & T_{r,i} = T_{r,j} \\
0 & \text{otherwise}
\end{cases}
\]

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