Hierarchical Clustering

- Build a tree-like hierarchical taxonomy (dendrogram) from a set of unlabeled documents.
Dendrogram – Example

http://dir.yahoo.com/science
Clustering of News Stories: Reuters RCV1
Dendrogram ➔ Clusters

- Clustering can be obtained by cutting the dendrogram at a desired level: each *connected* component forms a cluster.

- The number of clusters is not required in advance.
Divisive vs. Agglomerative

- **Divisive (Top-Down)**
  - Start with all documents belong to the same cluster. Eventually each node forms a cluster on its own.
  - Recursive application of a (flat) partitional clustering algorithm
    - e.g., $k$-means ($k=2$) $\rightarrow$ bi-secting $k$-means.

- **Agglomerative (Bottom-Up)**
  - Start with each document being a single cluster. Eventually all documents belong to the same cluster.
Hierarchical Agglomerative Clustering

- Starts with each doc in a separate cluster.
- Repeat until there is only one cluster:
  - Among the current clusters, determine the pair of closest pair of clusters, $c_i$ and $c_j$
  - Then merges $c_i$ and $c_j$ to a single cluster.
- The history of merging forms a binary tree or hierarchy (dendrogram).
**HAC Alg.**

**EfficientHAC**($\bar{d}_1, \ldots, \bar{d}_N$)

1. for $n \leftarrow 1$ to $N$
2. do for $i \leftarrow 1$ to $N$
3. do $C[n][i].\text{sim} \leftarrow \bar{d}_n \cdot \bar{d}_i$
4. $C[n][i].\text{index} \leftarrow i$
5. $I[n] \leftarrow 1$
6. $P[n] \leftarrow$ priority queue for $C[n]$ sorted on sim
7. $P[n].\text{DELETE}(C[n][n])$ (don’t want self-similarities)
8. $A \leftarrow []$
9. for $k \leftarrow 1$ to $N - 1$
10. do $k_1 \leftarrow \text{arg max}_{k : I[k] = 1} P[k].\text{Max().sim}$
11. $k_2 \leftarrow P[k_1].\text{Max().index}$
12. $A.\text{APPEND}((k_1, k_2))$
13. $I[k_2] \leftarrow 0$
14. $P[k_1] \leftarrow []$
15. for each $i$ with $I[i] = 1 \land i \neq k_1$
16. do $P[i].\text{DELETE}(C[i][k_1])$
17. $P[i].\text{DELETE}(C[i][k_2])$
18. $C[i][k_1].\text{sim} \leftarrow \text{SIM}(i, k_1, k_2)$
19. $P[i].\text{INSERT}(C[i][k_1])$
20. $C[k_1][i].\text{sim} \leftarrow \text{SIM}(i, k_1, k_2)$
21. $P[k_1].\text{INSERT}(C[k_1][i])$
22. return $A$
Time Complexity

- In the initialization step, compute similarity of all pairs of \( n \) documents which is \( O(n^2) \).
- In each of the subsequent \( n-2 \) merging iterations, compute the distance between the most recently created cluster and all other existing clusters.
- The overall time complexity is often \( O(n^3) \) if done naively or \( O(n^2 \log n) \) if done more cleverly using a priority-queue.
HAC Variants

- How to define the closest pair of clusters
  - Single-Link
    - maximum similarity between pairs of docs
  - Complete-Link
    - minimum similarity between pairs of docs
  - Average-Link
    - average similarity between pairs of docs
  - Centroid
    - maximum similarity between cluster centroids
(a) single link: maximum similarity

(b) complete link: minimum similarity

(c) centroid: average inter-similarity

(d) group-average: average of all similarities
The similarity between a pair of clusters is defined by the single strongest link (i.e., maximum cosine-similarity) between their members:

\[ \text{sim} \left( c_i, c_j \right) = \max_{x \in c_i, \; y \in c_j} \text{sim} \left( x, y \right) \]

After merging \( c_i \) and \( c_j \), the similarity of the resulting cluster to another cluster, \( c_k \), is:

\[ \text{sim} \left( (c_i \cup c_j), c_k \right) = \max \left( \text{sim} \left( c_i, c_k \right), \text{sim} \left( c_j, c_k \right) \right) \]
HAC – Example

- As clusters *agglomerate*, documents fall into a dendrogram.
HAC – Example

Single-Link
## HAC – Exercise

<table>
<thead>
<tr>
<th>Digital Camera</th>
<th>Megapixel</th>
<th>Zoom</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>1</td>
<td>8</td>
</tr>
<tr>
<td>B</td>
<td>3</td>
<td>8</td>
</tr>
<tr>
<td>C</td>
<td>2</td>
<td>6</td>
</tr>
<tr>
<td>D</td>
<td>1.5</td>
<td>1</td>
</tr>
<tr>
<td>E</td>
<td>4</td>
<td>2</td>
</tr>
</tbody>
</table>
HAC – Exercise
Chaining Effect

- Single-Link HAC can result in “straggly” (long and thin) clusters due to the chaining effect.