Introduction to Information Retrieval

http://informationretrieval.org

IIR 17: Hierarchical Clustering

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Overview

Outline

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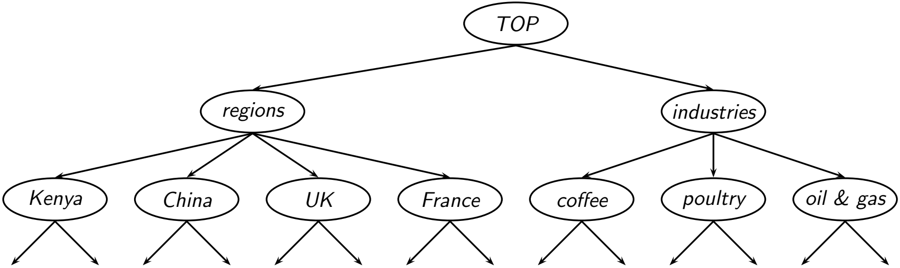
Hierarchical clustering

Our goal in hierarchical clustering is to create a hierarchy like the one we saw earlier in Reuters:



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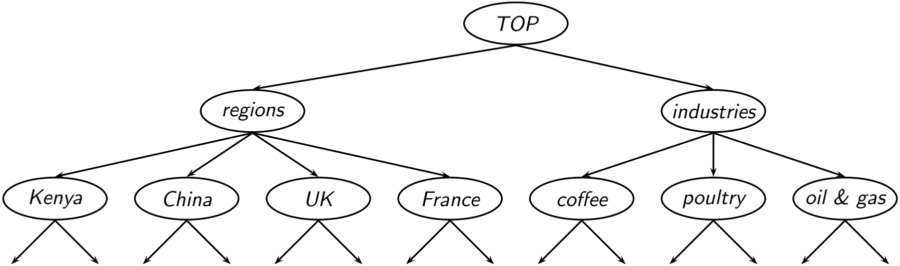

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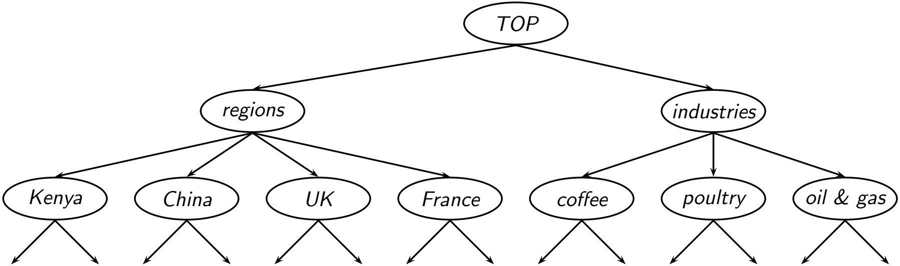

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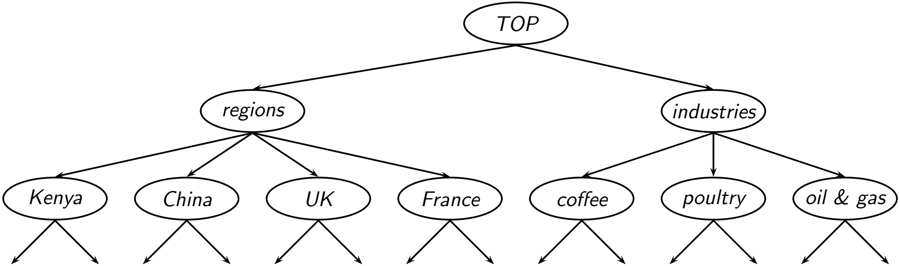

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The best known bottom-up method is hierarchical agglomerative clustering.

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- Assumes a similarity measure for determining the similarity of two clusters (up to now: similarity of documents).

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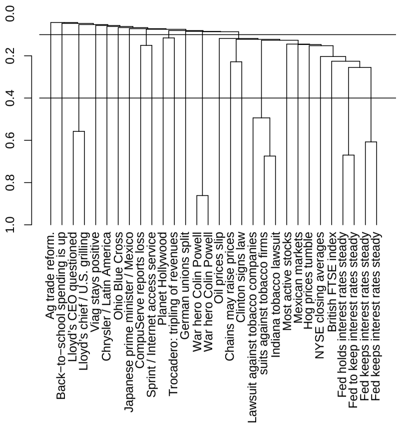
- The standard way of depicting this history is a dendrogram.

A dendrogram



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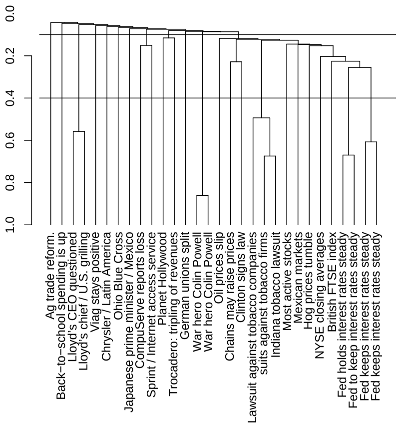

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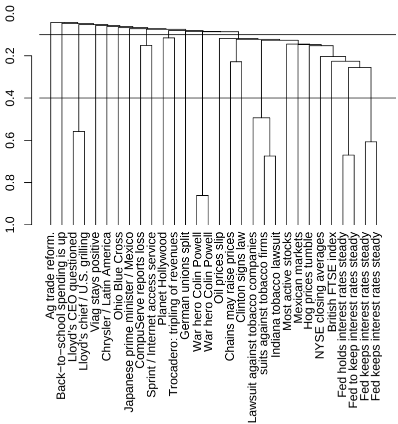

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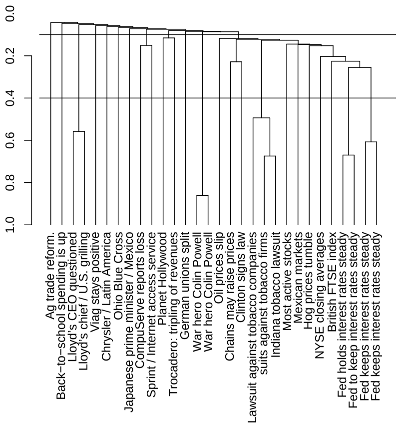

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- The horizontal line of each merger tells us what the similarity of the merger was.
- We can cut the dendrogram at a particular point (e.g., at 0.1 or 0.4) to get a flat clustering.

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- → Bisecting K-means at the end
- For now: HAC

Naive HAC algorithm

$\text{SIMPLEHAC}(d_1, \ldots, d_N)$

for $n \leftarrow 1$ **to** N
do for $i \leftarrow 1$ **to** N
  do $C[n][i] \leftarrow \text{SIM}(d_n, d_i)$
  $I[n] \leftarrow 1$ *(keeps track of active clusters)*
$A \leftarrow []$ *(collects clustering as a sequence of merges)*
for $k \leftarrow 1$ **to** $N - 1$
do $\langle i, m \rangle \leftarrow \arg\max_{\{\langle i,m \rangle : i \neq m \wedge I[i]=1 \wedge I[m]=1\}} C[i][m]$
  $A.\text{APPEND}(\langle i, m \rangle)$ *(store merge)*
  for $j \leftarrow 1$ **to** N
  do $C[i][j] \leftarrow \text{SIM}(i, m, j)$
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  $I[m] \leftarrow 0$ *(deactivate cluster)*
return A

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- Overall complexity is $O(N^3)$.
- We'll look at more efficient algorithms later.

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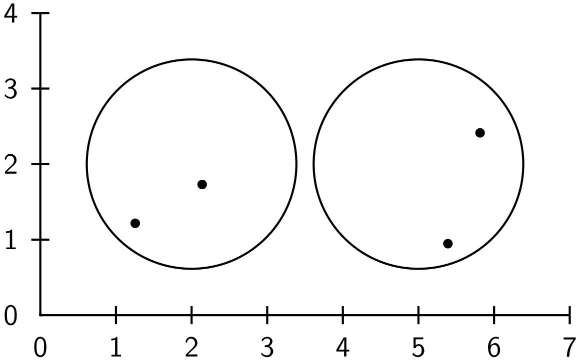
- Group-average: Average "intrasimilarity"
  - Average over all document pairs, including pairs of docs in the same cluster

Cluster similarity: Example



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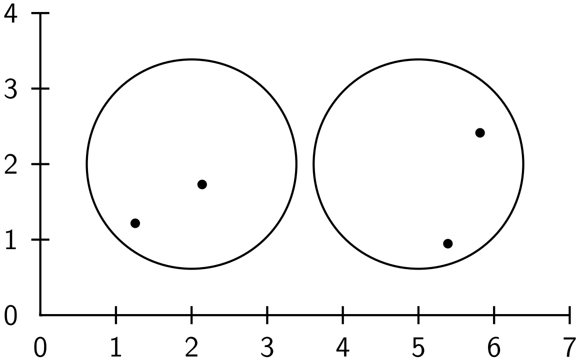

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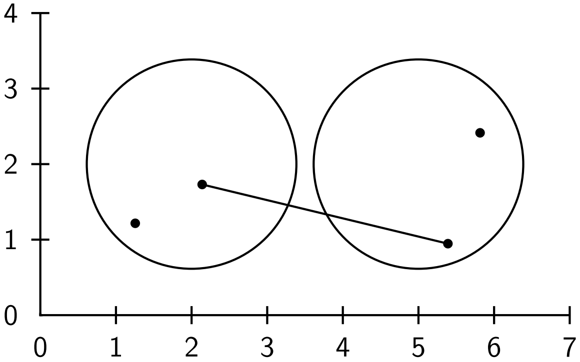

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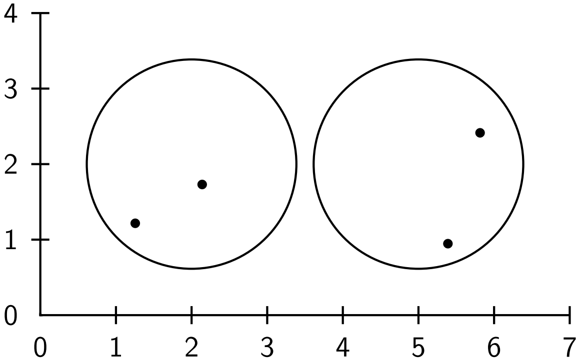

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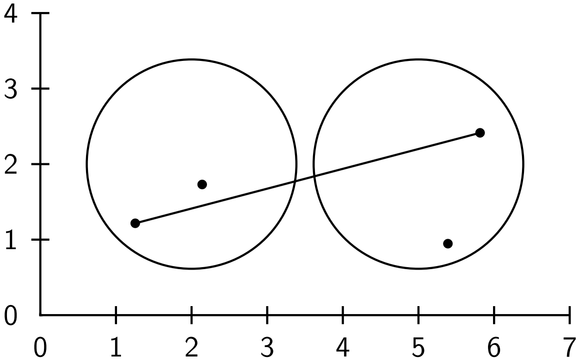

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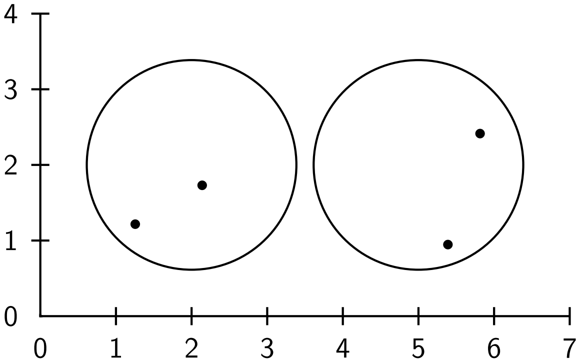
intersimilarity = similarity of two documents in different clusters



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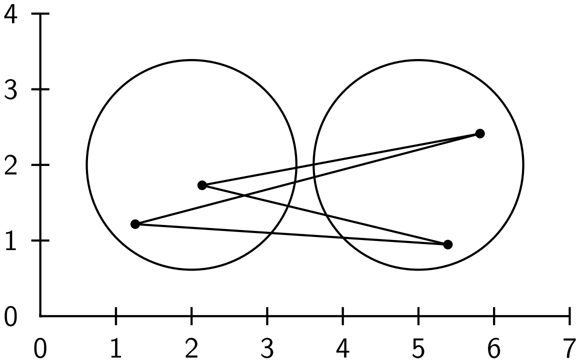

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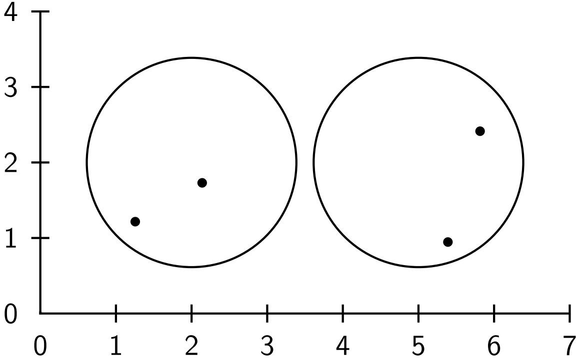

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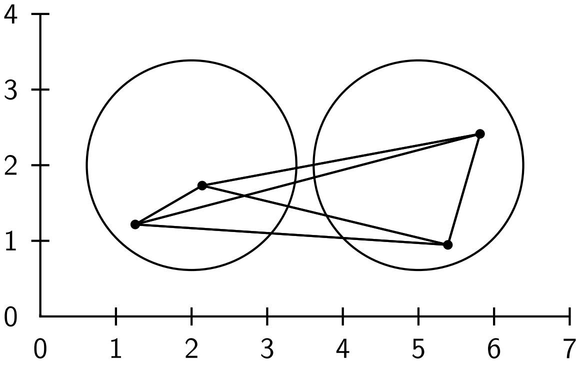
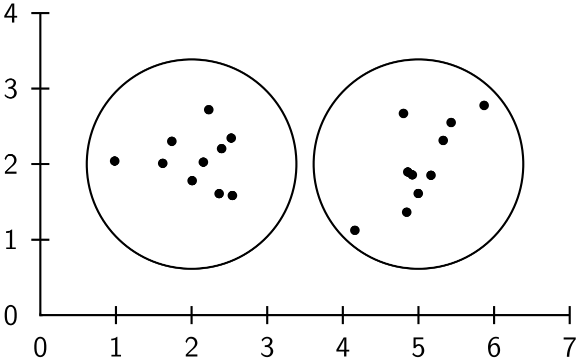


Cluster similarity: Larger example



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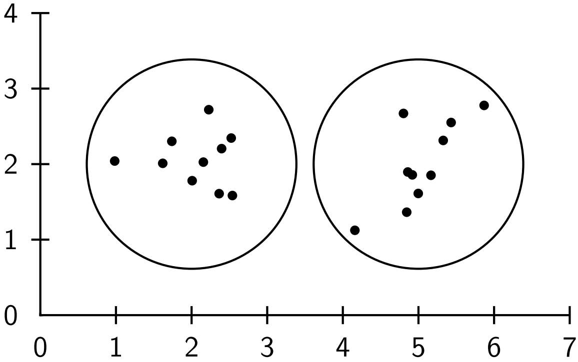

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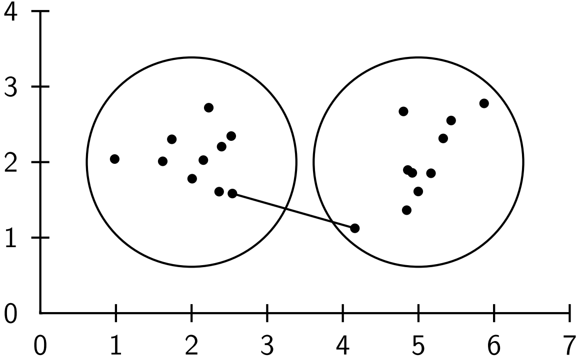

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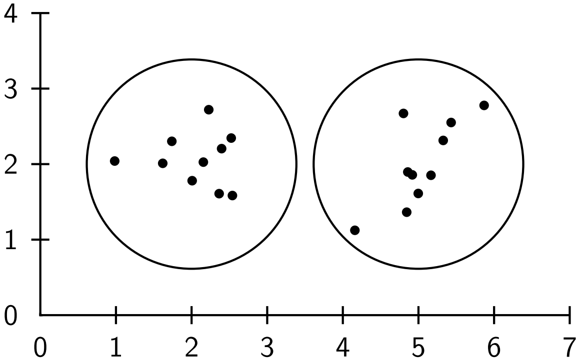

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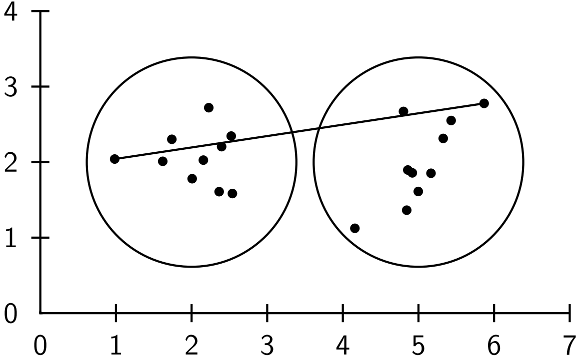

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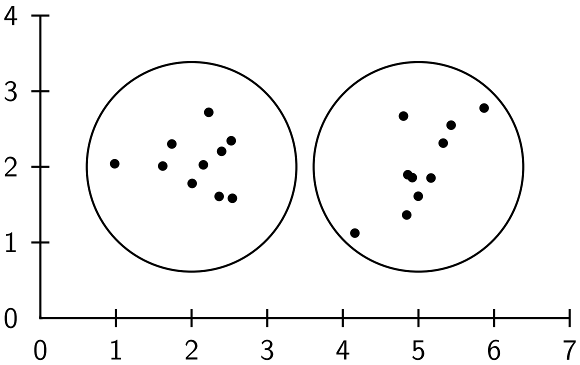

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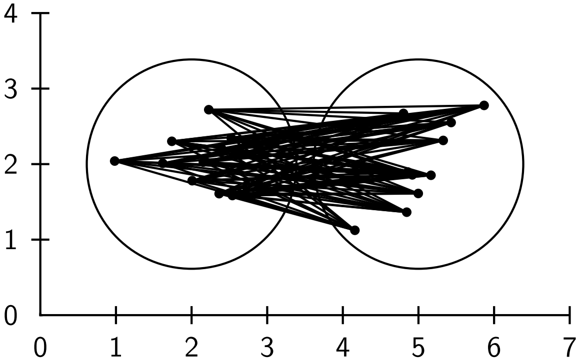

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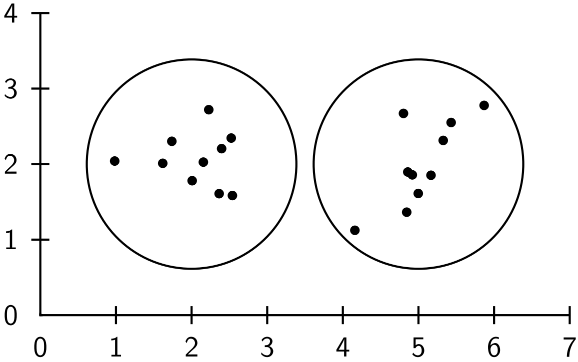

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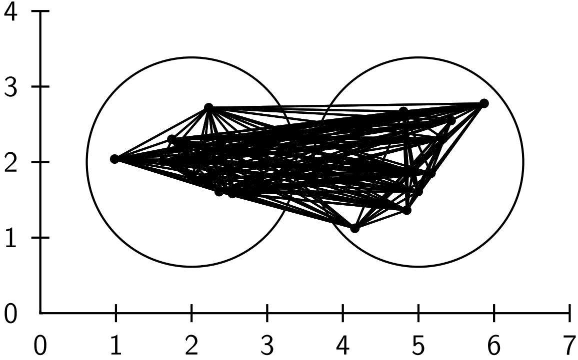

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- Once we have merged two clusters, how do we update the similarity matrix?
- This is simple for single link:

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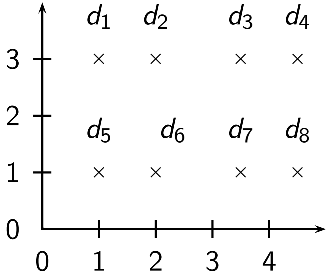

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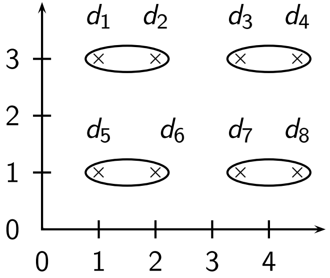

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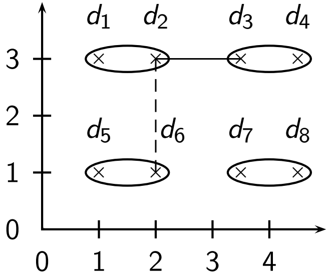

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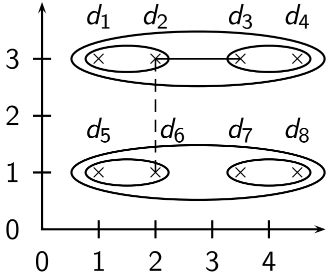

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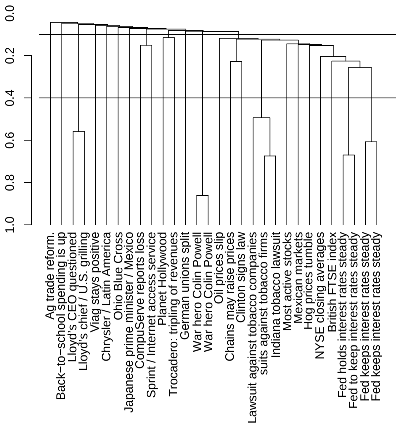

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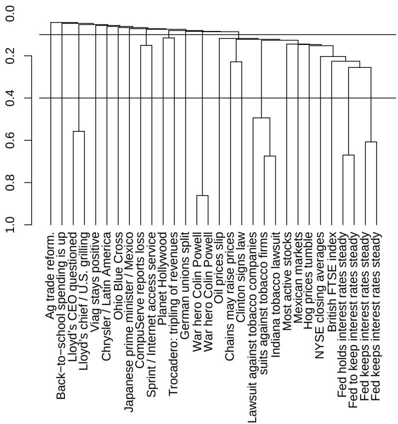

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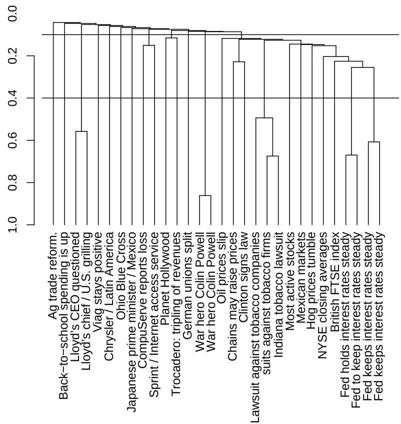
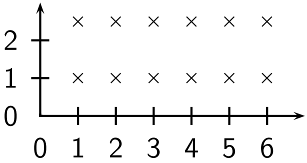
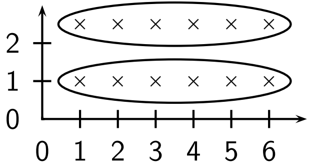


- Notice: many small clusters (1 or 2 members) being added to the main cluster
- There is no balanced 2-cluster or 3-cluster clustering that can be derived by cutting the dendrogram.

What cluster structure after 10 mergers?



Single-link: Chaining



Single-link clustering often produces long, straggly clusters. For most applications, these are undesirable.

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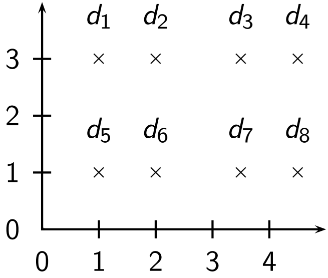
- We measure the similarity of two clusters by computing the radius of the cluster that we would get if we merged them.

Complete link clustering: Example



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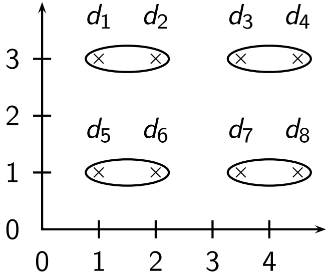

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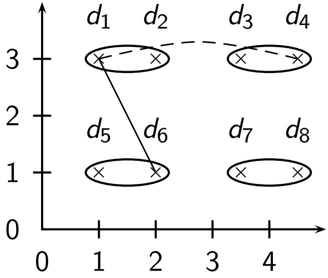

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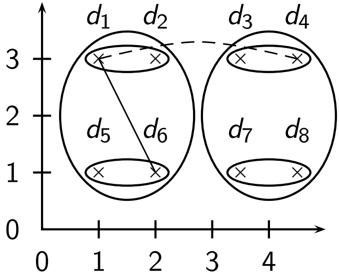
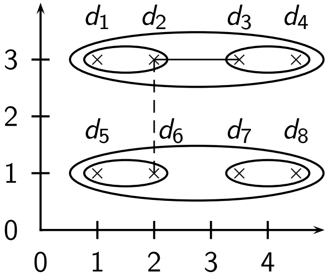
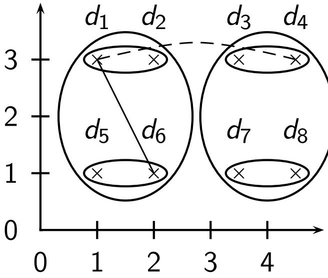
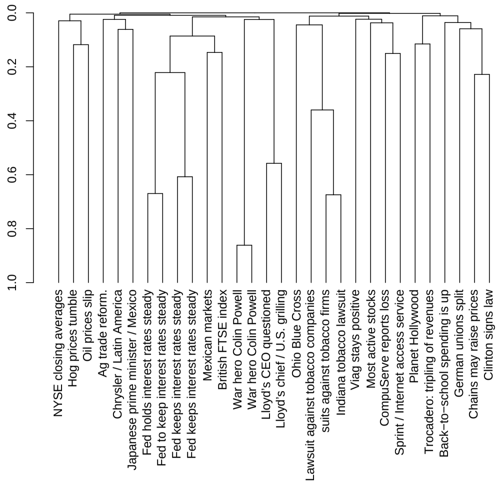


Single-link vs. Complete link clustering





Complete-link dendrogram



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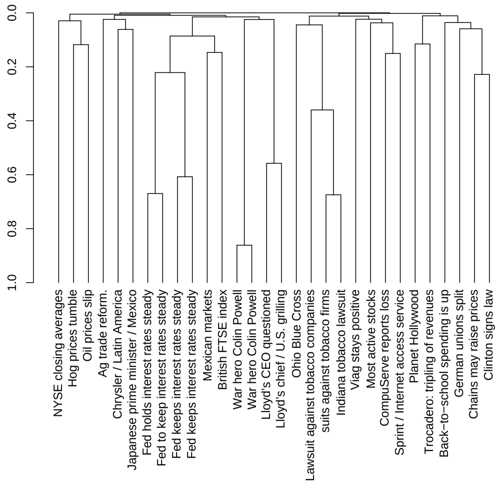

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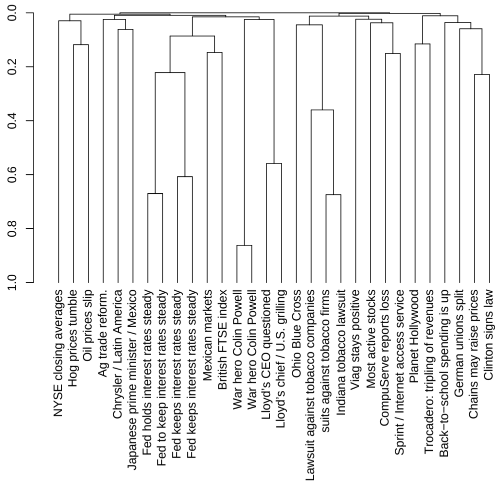
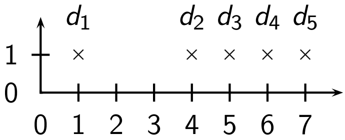


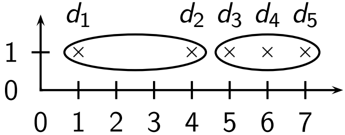
- Notice that this dendrogram is much more balanced than the single-link one.
- We can create a 2-cluster clustering with two clusters of about the same size.

Complete-link: Sensitivity to outliers



What is the intuitively best 2-cluster clustering here?

Complete-link: Sensitivity to outliers



The complete-link clustering of this set. It's not intuitive.

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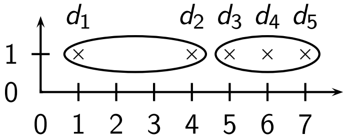

The complete-link clustering of this set. It's not intuitive. This shows that a single outlier can have a large effect on the final outcome of complete-link clustering. Coordinates: $1 + 2 \times \epsilon, 4, 5 + 2 \times \epsilon, 6, 7 - \epsilon$.

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Centroid HAC

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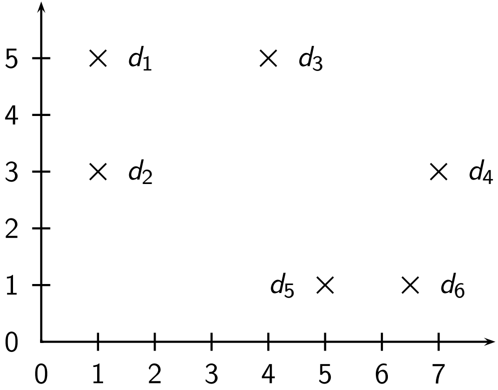
- Note: this is the dot product, not cosine similarity!

Centroid clustering: Example



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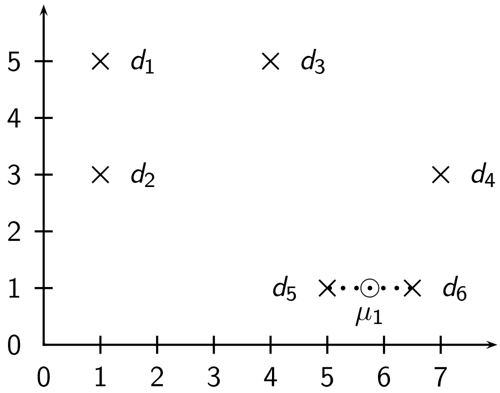

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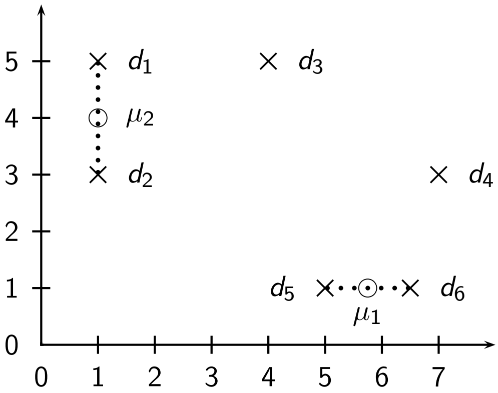

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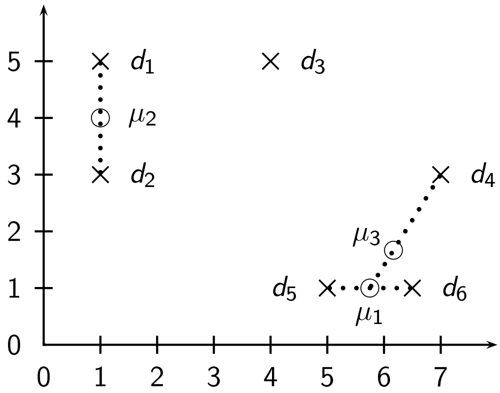

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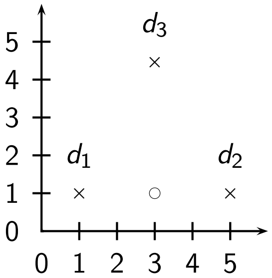

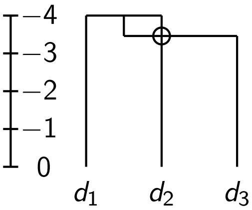

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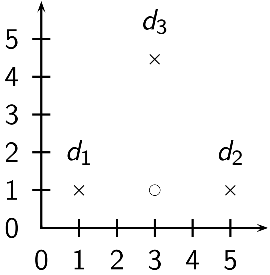
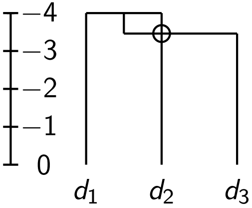
- Below: Similarity of the first merger ($d_1 \cup d_2$) is -4.0, similarity of second merger ($(d_1 \cup d_2) \cup d_3$) is ≈ -3.5.





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- An inversion contradicts this intuition: we have a large cluster that is more coherent than one of its subclusters.

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- But we exclude self-similarities.

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- Again, the above definition is inefficient ($O(N^2)$) and there is an equivalent, more efficient, centroid-based definition:

$$\text{SIM-GA}(\omega_i, \omega_j) =$$

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- For other types of document representations (or if only pairwise similarities for document are available): use complete-link.
- There are also some applications for single-link (e.g., duplicate detection in web search).

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- When a hierarchical structure is desired: hierarchical algorithm
- HAC also can be applied if K cannot be predetermined (can start without knowing K)

Outline

Efficient single link clustering

$\textsc{SingleLinkClustering}(d_1, \ldots, d_N)$

for $n \leftarrow 1$ **to** N
do for $i \leftarrow 1$ **to** N
    do $C[n][i].\text{sim} \leftarrow \text{SIM}(d_n, d_i)$
        $C[n][i].\text{index} \leftarrow i$
    $I[n] \leftarrow n$
    $NBM[n] \leftarrow \arg\max_{X \in \{C[n][i]:n \neq i\}} X.\text{sim}$
$A \leftarrow []$
for $n \leftarrow 1$ **to** $N - 1$
do $i_1 \leftarrow \arg\max_{\{i:I[i]=i\}} NBM[i].\text{sim}$
    $i_2 \leftarrow I[NBM[i_1].\text{index}]$
    $A.\textsc{Append}(\langle i_1, i_2 \rangle)$
    for $i \leftarrow 1$ **to** N
    do if $I[i] = i \wedge i \neq i_1 \wedge i \neq i_2$
            then $C[i_1][i].\text{sim} \leftarrow C[i][i_1].\text{sim} \leftarrow \max(C[i_1][i].\text{sim}, C[i_2][i].\text{sim})$
        if $I[i] = i_2$
            then $I[i] \leftarrow i_1$
    $NBM[i_1] \leftarrow \arg\max_{X \in \{C[i_1][i]:I[i]=i \wedge i \neq i_1\}} X.\text{sim}$
return A

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- Best time complexity for these three is $O(N^2 \log N)$: See book.
- In practice: little difference between $O(N^2 \log N)$ and $O(N^2)$.

Combination similarities of the four algorithms

clustering algorithm	$\text{sim}(\ell, k_1, k_2)$
single-link	$\max(\text{sim}(\ell, k_1), \text{sim}(\ell, k_2))$
complete-link	$\min(\text{sim}(\ell, k_1), \text{sim}(\ell, k_2))$
centroid	$(\frac{1}{N_m}\vec{v}_m) \cdot (\frac{1}{N_\ell}\vec{v}_\ell)$
group-average	$\frac{1}{(N_m+N_\ell)(N_m+N_\ell-1)}[(\vec{v}_m + \vec{v}_\ell)^2 - (N_m + N_\ell)]$

Comparison of HAC algorithms

method	combination similarity	time compl.	optimal?	comment
single-link	max intersimilarity of any 2 docs	$\Theta(N^2)$	yes	chaining effect
complete-link	min intersimilarity of any 2 docs	$\Theta(N^2 \log N)$	no	sensitive to outliers
group-average	average of all sims	$\Theta(N^2 \log N)$	no	best choice for most applications
centroid	average intersimilarity	$\Theta(N^2 \log N)$	no	inversions can occur

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What to do with the hierarchy?

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- Hierarchical clustering is often used to get K flat clusters. The hierarchy is then ignored.

K-means vs. HAC

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- Is HAC likely to produce results different from the above?

Bisecting K-means: A top-down algorithm

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- Repeat until we have produced the desired number of clusters

Bisecting K-means

$\textsc{BisectingKMeans}(d_1, \ldots, d_N)$

$\omega_0 \leftarrow \{\vec{d}_1, \ldots, \vec{d}_N\}$

leaves $\leftarrow \{\omega_0\}$

for $k \leftarrow 1$ **to** $K - 1$

do $\omega_k \leftarrow \textsc{PickClusterFrom}(\mathit{leaves})$

$\quad \{\omega_i, \omega_j\} \leftarrow \textsc{KMeans}(\omega_k, 2)$

$\quad \mathit{leaves} \leftarrow \mathit{leaves} \setminus \{\omega_k\} \cup \{\omega_i, \omega_j\}$

return *leaves*

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Bisecting K-means

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- But bisecting K-means is not deterministic.
- Why?
- There are deterministic versions, see below – but they are much less efficient.

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- Find terms or phrases that distinguish ω from the other clusters
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- (but the latter is actually not discriminative)

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- For example, MONDAY, TUESDAY, . . . in newspaper text

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- Alternative: titles
- For example, the titles of two or three documents that are closest to the centroid.
- Titles are easier to scan than a list of phrases.

Cluster labeling: Example

		labeling method		
	# docs	centroid	mutual information	title
4	622	oil plant mexico production crude **power 000 refinery gas** bpd	plant oil production **barrels** crude bpd mexico **dolly capacity petroleum**	MEXICO: Hurricane Dolly heads for Mexico coast
9	1017	police security **russian** people military peace killed told **grozny court**	police killed military security peace told **troops forces rebels** people	RUSSIA: Russia's Lebed meets rebel chief in Chechnya
10	1259	00 000 tonnes traders futures wheat prices **cents september** tonne	**delivery** traders futures tonne tonnes **desk** wheat prices 000 00	USA: Export Business - Grain/oilseeds complex

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- Three methods: most prominent terms in centroid, differential labeling using MI, title of doc closest to centroid
- All three methods do a pretty good job.

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- PDDP (similar to bisecting K-means; deterministic, but also less efficient): Saravesi and Boley (2004)