Introduction to Information Retrieval

http://informationretrieval.org

IIR 17: Hierarchical Clustering

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Overview

1. Recap
2. Introduction
3. Single-link/Complete-link
4. Centroid/GAAC
5. Labeling clusters
6. Variants

Outline

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Applications of clustering in IR

Application	What is clustered?	Benefit	Example
Search result clustering	search results	more effective information presentation to user	
Scatter-Gather	(subsets of) collection	alternative user interface: "search without typing"	
Collection clustering	collection	effective information presentation for exploratory browsing	McKeown et al. 2002, news.google.com
Cluster-based retrieval	collection	higher efficiency: faster search	Salton 1971

K-means algorithm

K-MEANS$(\{\vec{x}_1, \ldots, \vec{x}_N\}, K)$

$(\vec{s}_1, \vec{s}_2, \ldots, \vec{s}_K) \leftarrow$ SELECTRANDOMSEEDS$(\{\vec{x}_1, \ldots, \vec{x}_N\}, K)$

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

do $\vec{\mu}_k \leftarrow \vec{s}_k$

while stopping criterion has not been met

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

    do $\omega_k \leftarrow \{\}$

    for $n \leftarrow 1$ **to** N

    do $j \leftarrow \arg\min_{j'} |\vec{\mu}_{j'} - \vec{x}_n|$

        $\omega_j \leftarrow \omega_j \cup \{\vec{x}_n\}$ *(reassignment of vectors)*

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

    do $\vec{\mu}_k \leftarrow \frac{1}{|\omega_k|} \sum_{\vec{x} \in \omega_k} \vec{x}$ *(recomputation of centroids)*

return $\{\vec{\mu}_1, \ldots, \vec{\mu}_K\}$

Initialization of K-means

- Random seed selection is just one of many ways K-means can be initialized.
- Random seed selection is not very robust: It's easy to get a suboptimal clustering.
- Better heuristics:
  - Select seeds not randomly, but using some heuristic (e.g., filter out outliers or find a set of seeds that has "good coverage" of the document space)
  - Use hierarchical clustering to find good seeds (next class)
  - Select i (e.g., $i = 10$) different sets of seeds, do a K-means clustering for each, select the clustering with lowest RSS

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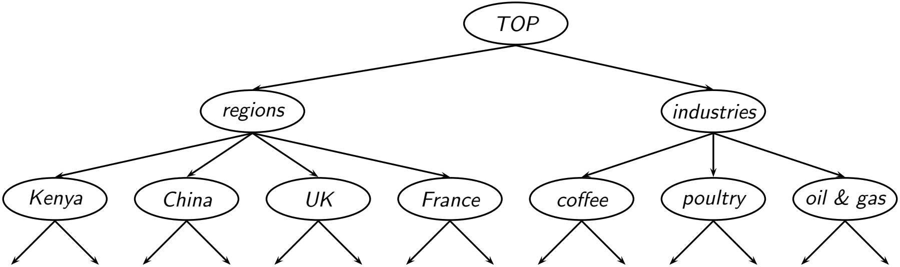

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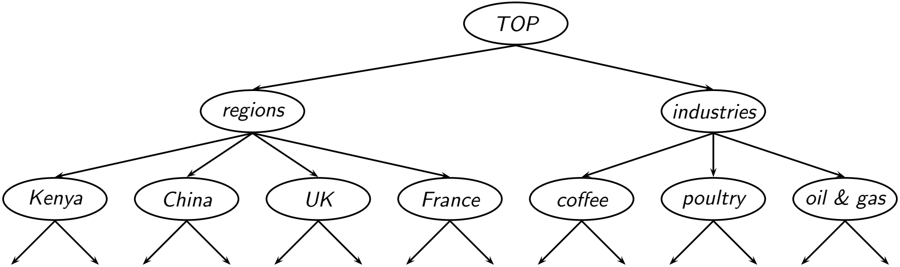

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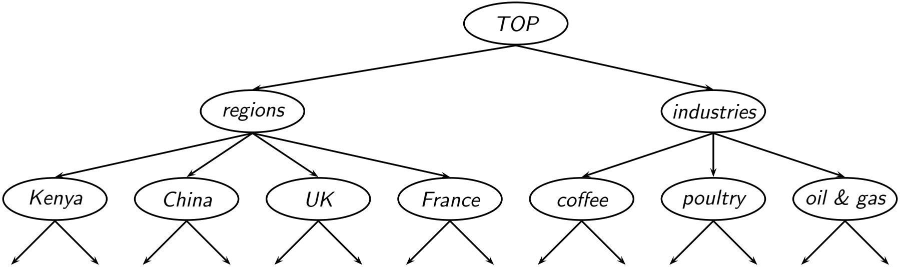

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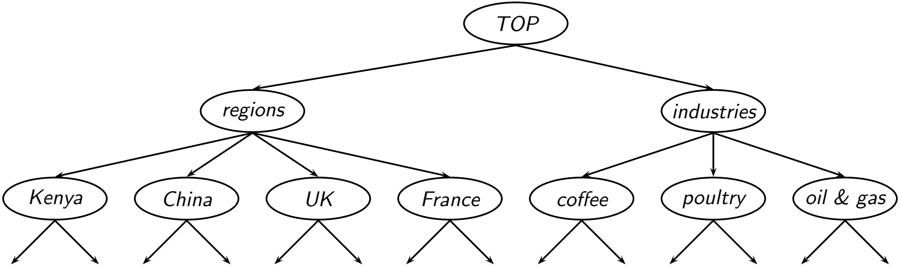

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The best known bottom-up method is hierarchical agglomerative clustering.

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- We will look at four different cluster similarity measures.

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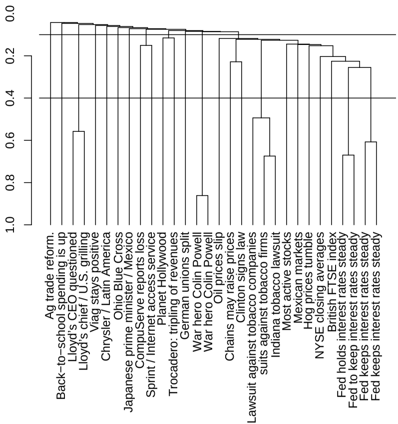
- The history of merging is a hierarchy in the form of a binary tree.
- The standard way of depicting this history is a dendrogram.

A dendrogram



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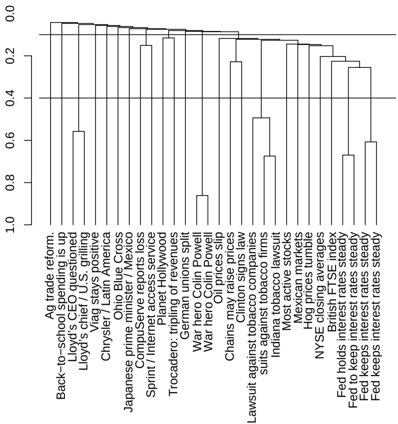

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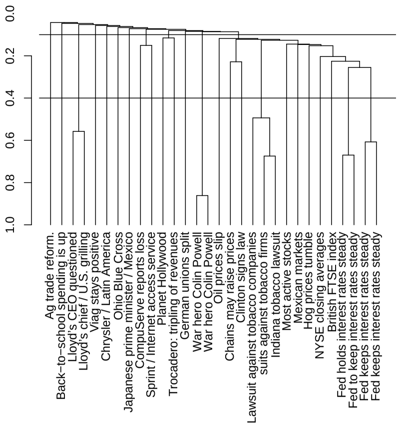

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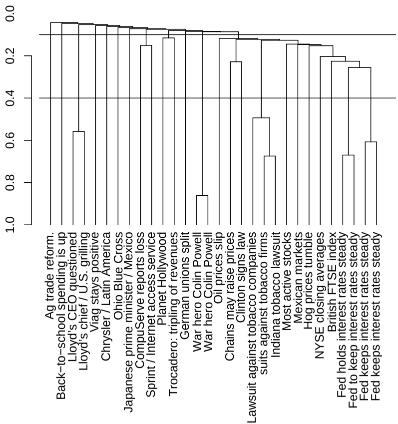

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- The horizontal line of each merger tells us what the similarity of the merger was.
- We can cut the dendrogram at a particular point (e.g., at 0.1 or 0.4) to get a flat clustering.

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- For now: HAC (= bottom-up)

Naive HAC algorithm

```
SimpleHAC(d_1, ..., d_N)
for n ← 1 to N
do for i ← 1 to N
    do C[n][i] ← Sim(d_n, d_i)
    I[n] ← 1  (keeps track of active clusters)
A ← []  (collects clustering as a sequence of merges)
for k ← 1 to N − 1
do ⟨i, m⟩ ← arg max_{⟨i,m⟩: i≠m ∧ I[i]=1 ∧ I[m]=1} C[i][m]
    A.Append(⟨i, m⟩)  (store merge)
    for j ← 1 to N
    do  (use i as representative for < i, m >)
        C[i][j] ← Sim(< i, m >, j)
        C[j][i] ← Sim(< i, m >, j)
    I[m] ← 0  (deactivate cluster)
return A
```

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- There are $O(N)$ iterations, each performing a $O(N \times N)$ "scan" operation.
- Overall complexity is $O(N^3)$.
- We'll look at more efficient algorithms later.

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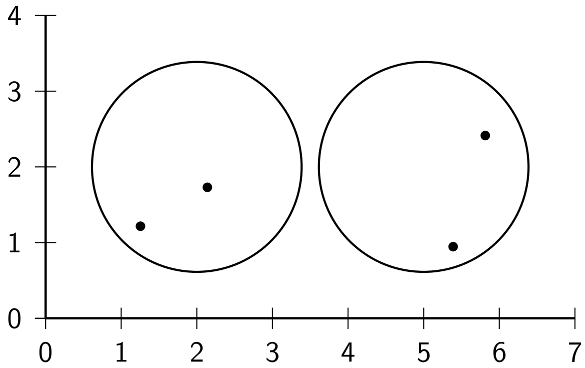
Cluster similarity: Example



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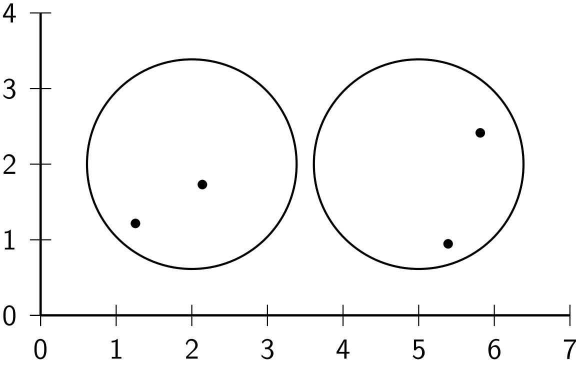

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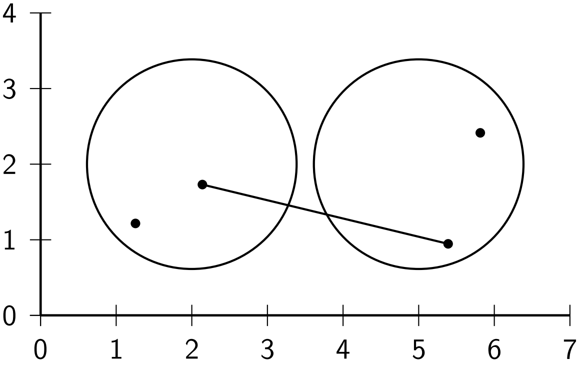

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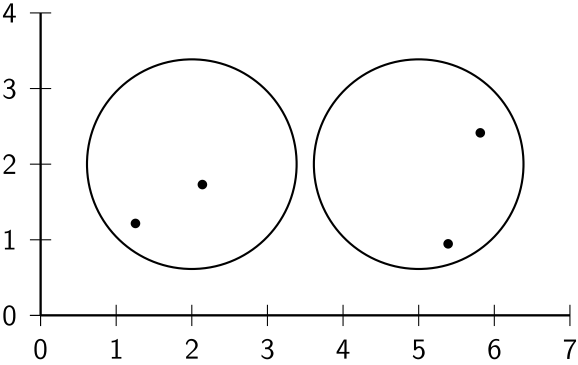

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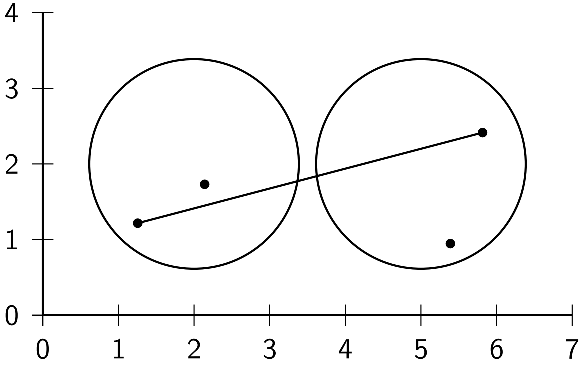

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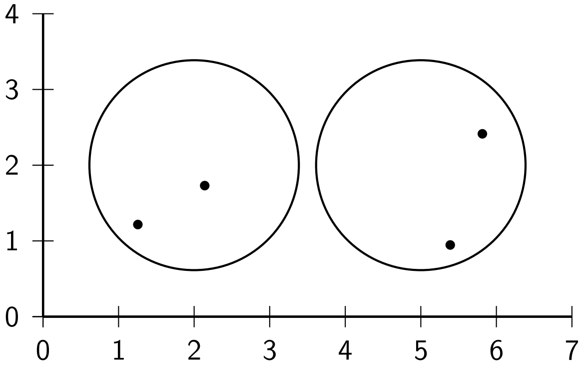

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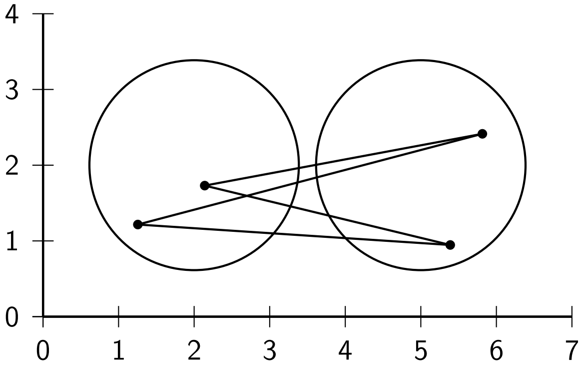

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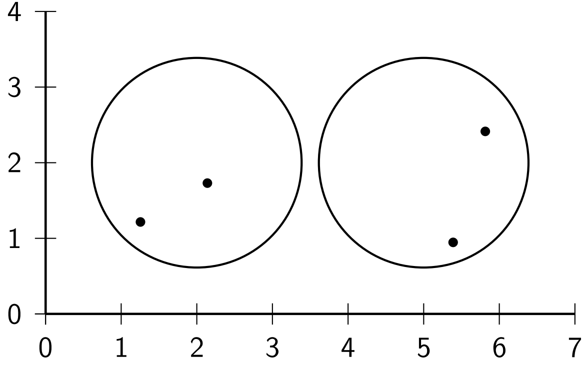

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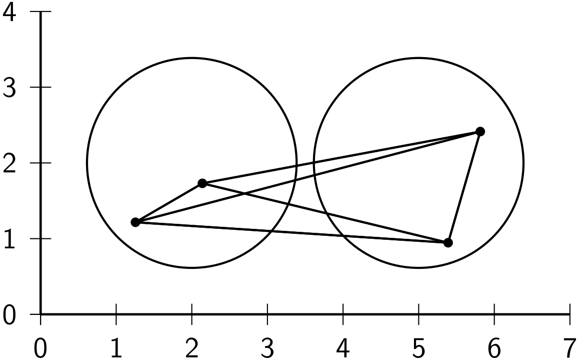
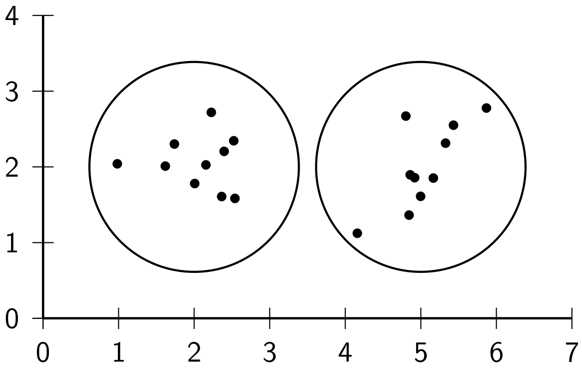


Cluster similarity: Larger Example



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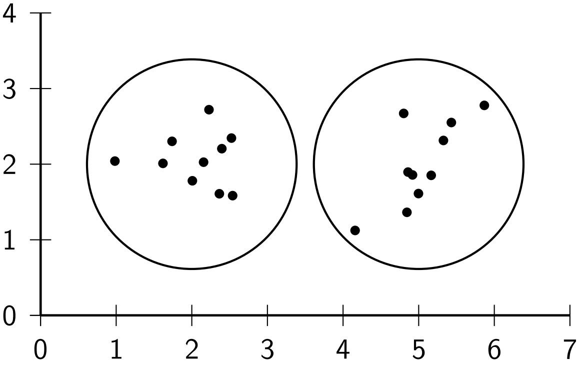

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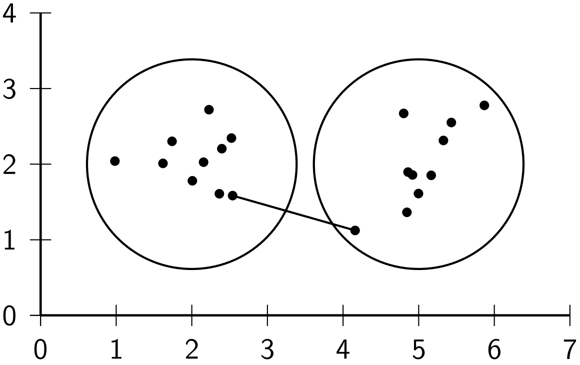

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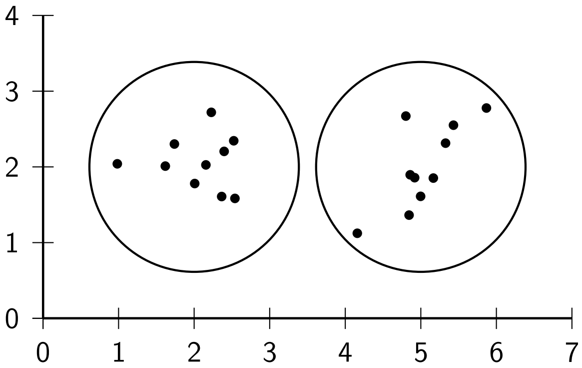

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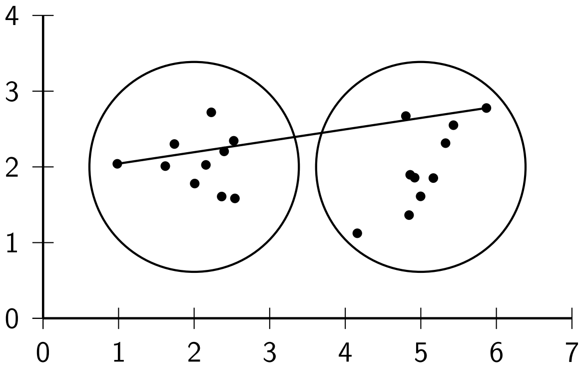

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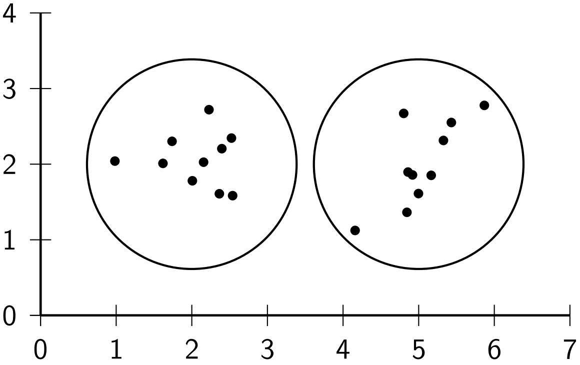

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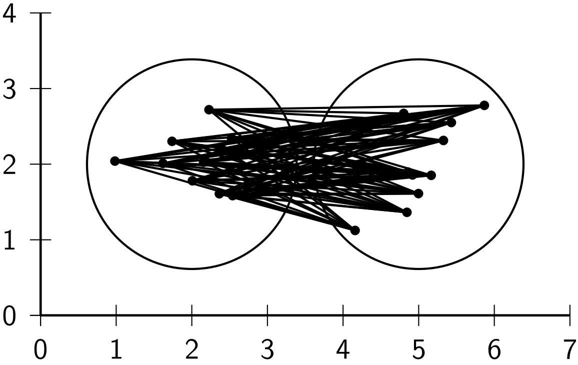

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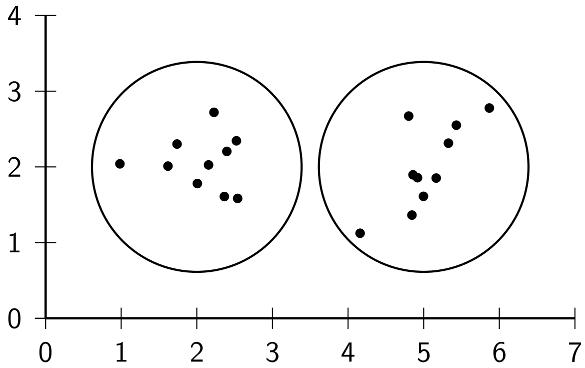

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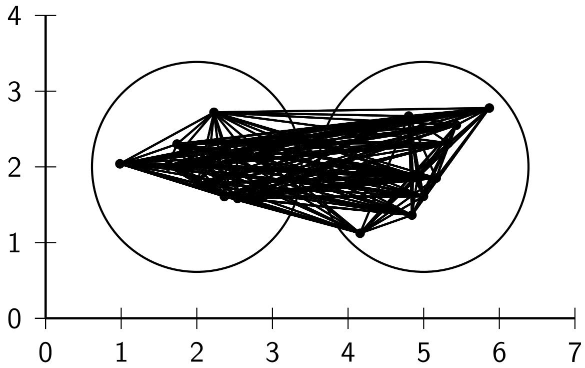

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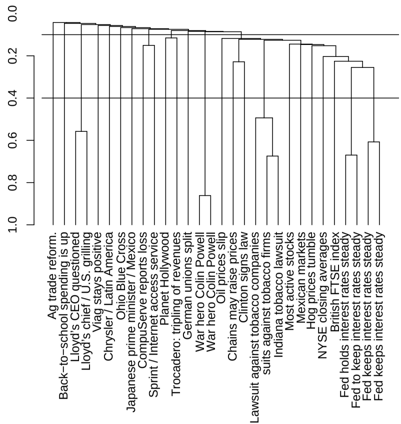
- Once we have merged two clusters, how do we update the similarity matrix?
- This is simple for single link:

$$\text{SIM}(\omega_i, (\omega_{k_1} \cup \omega_{k_2})) = \max(\text{SIM}(\omega_i, \omega_{k_1}), \text{SIM}(\omega_i, \omega_{k_2}))$$

□

This dendrogram was produced by single-link



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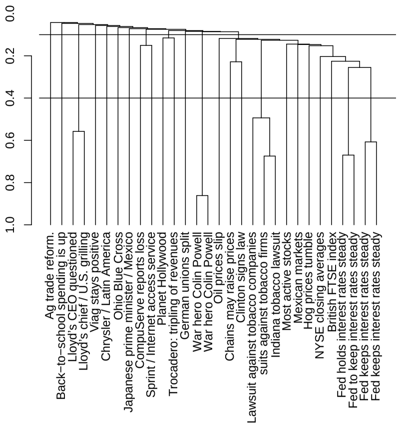

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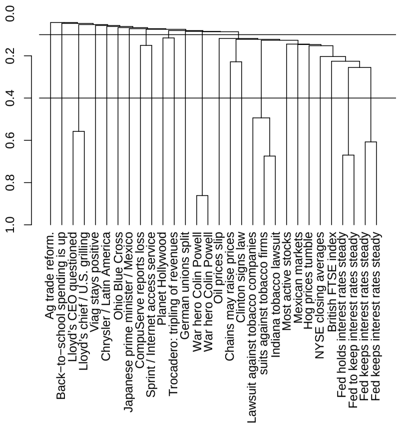

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- There is no balanced 2-cluster or 3-cluster clustering that can be derived by cutting the dendrogram.

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

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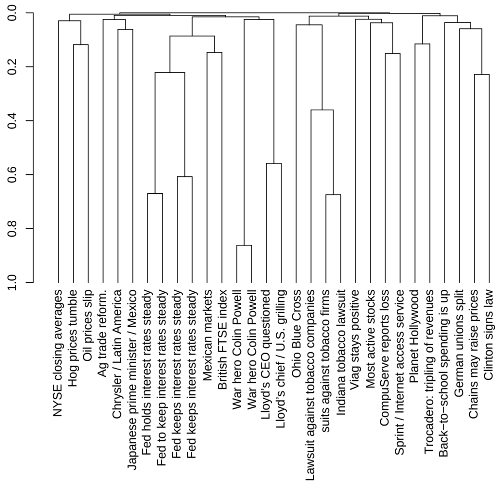

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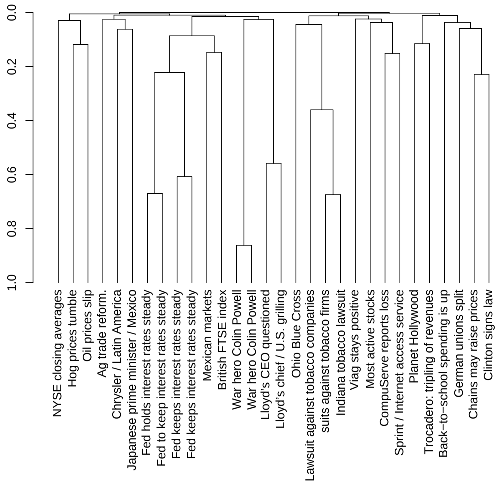

- Notice that this dendrogram is much more balanced than the single-link one.

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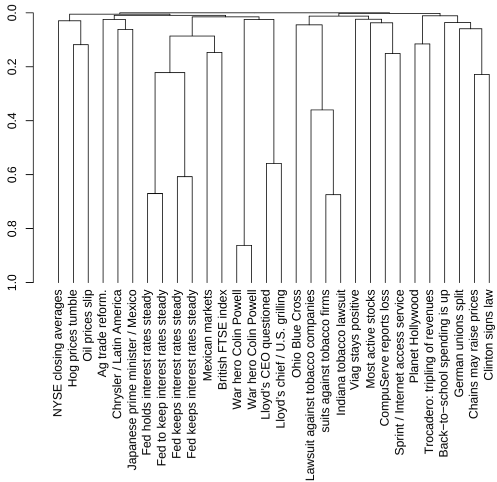
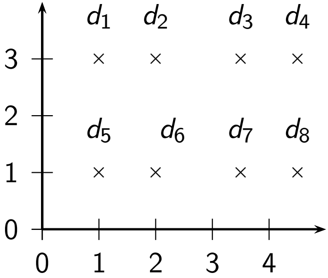
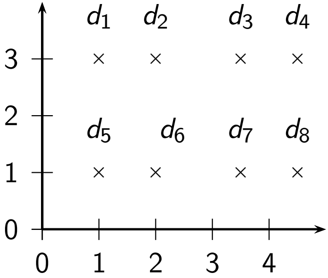


- Notice that this dendrogram is much more balanced than the single-link one.
- We can create a 2-cluster clustering with two clusters of about the same size.

Exercise: Compute single and complete link clusterings



Single-link clustering



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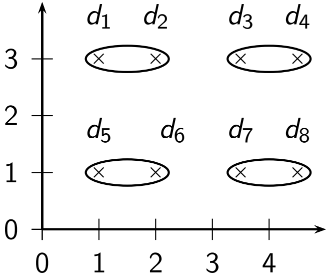

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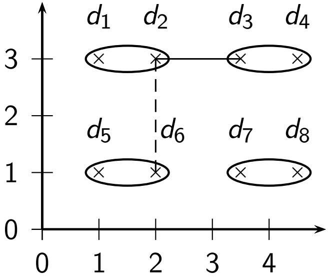

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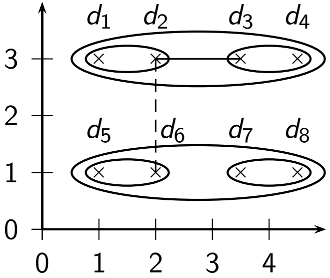

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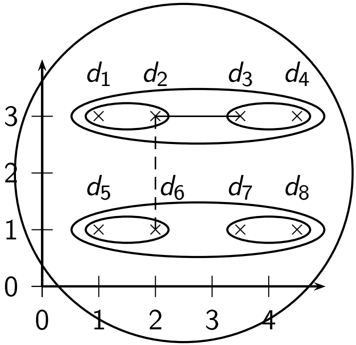

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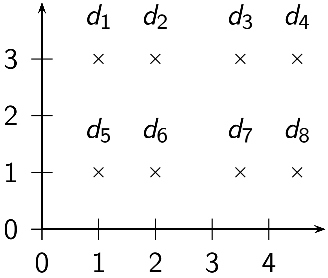

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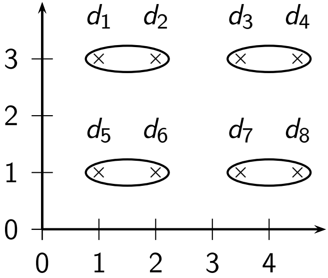

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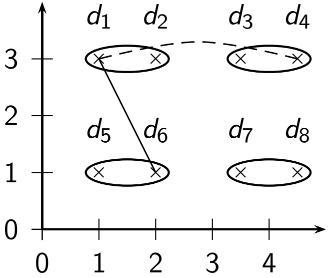

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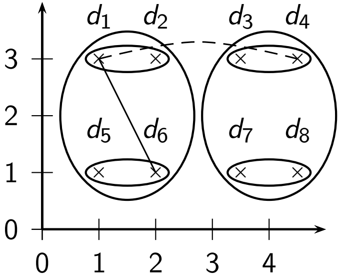

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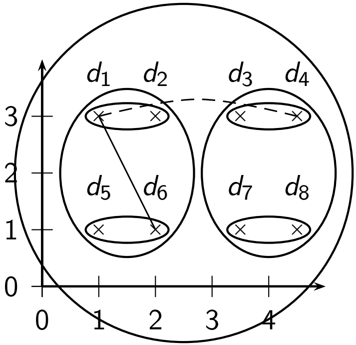
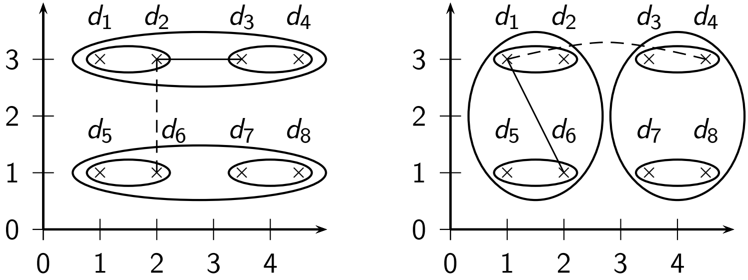
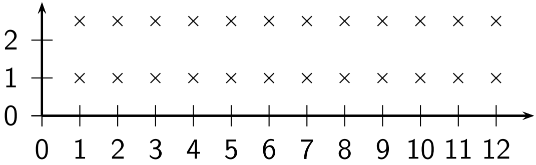


Single-link vs. Complete link clustering



Single-link: Chaining



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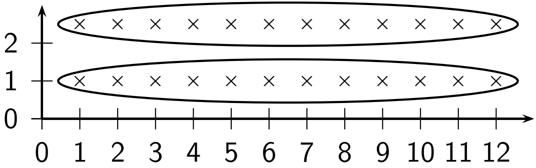

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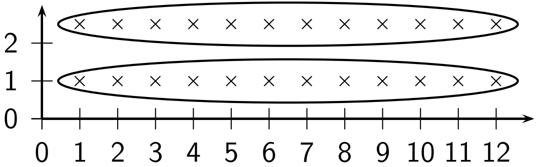
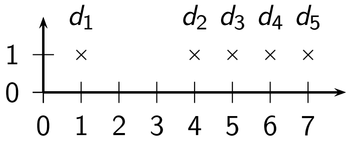


Single-link clustering often produces long, straggly clusters. For most applications, these are undesirable.

What 2-cluster clustering will complete-link produce?



Coordinates: $1 + 2 \times \epsilon, 4, 5 + 2 \times \epsilon, 6, 7 - \epsilon$.

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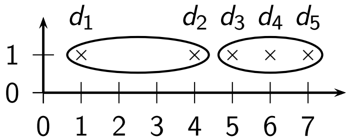

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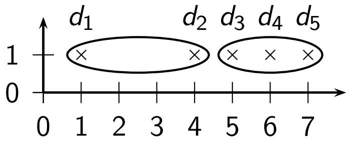
Complete-link: Sensitivity to outliers



- The complete-link clustering of this set splits d_2 from its right neighbors – clearly undesirable.

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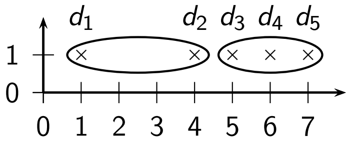

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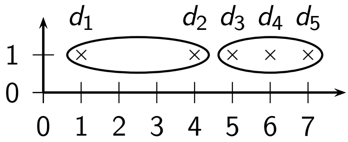

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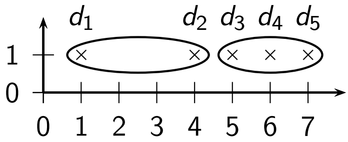

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- This shows that a single outlier can negatively affect the outcome of complete-link clustering.
- Single-link clustering does better in this case.

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1. Recap
2. Introduction
3. Single-link/Complete-link
4. Centroid/GAAC
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- The similarity of two clusters is the average intersimilarity – the average similarity of documents from the first cluster with documents from the second cluster.

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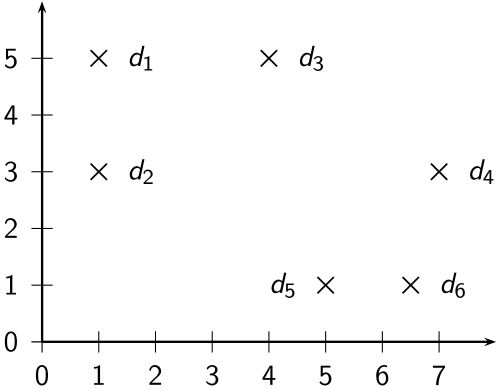
- Note: this is the dot product, not cosine similarity!

Exercise: Compute centroid clustering



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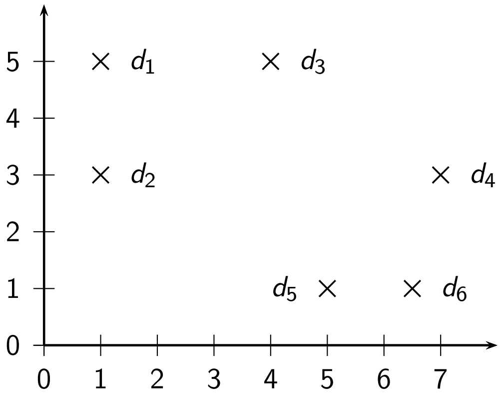

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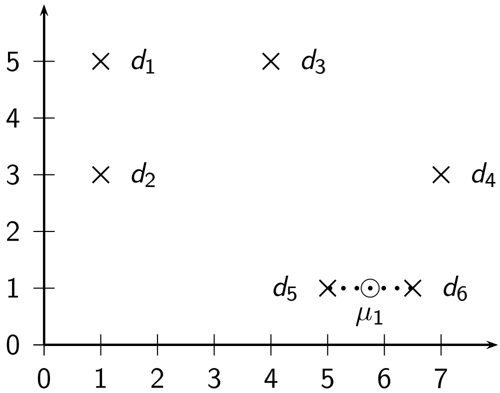

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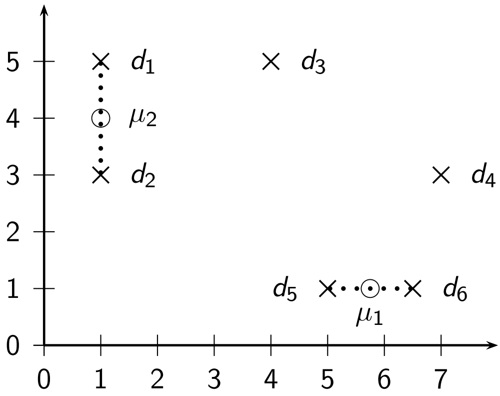

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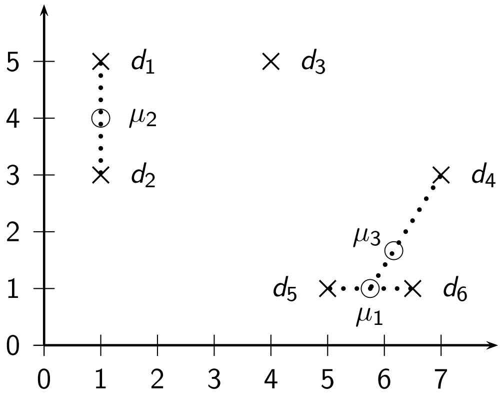
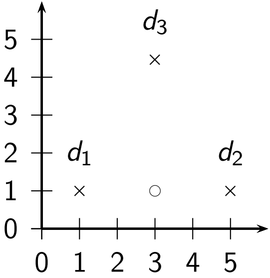
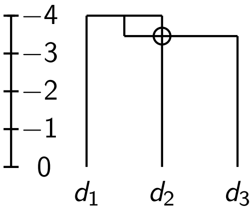


Inversion in centroid clustering

- In an inversion, the similarity increases during a merge sequence. Results in an "inverted" dendrogram.





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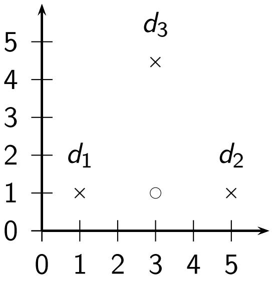
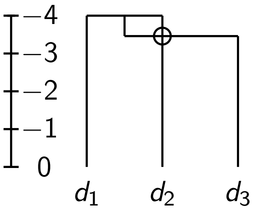
- Below: Similarity of the first merger ($d_1 \cup d_2$) is -4.0, similarity of second merger ($(d_1 \cup d_2) \cup d_3$) is ≈ -3.5.





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- An inversion contradicts this intuition: we have a large cluster that is more coherent than one of its subclusters.
- The fact that inversions can occur in centroid clustering is a reason not to use it. □

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- But we exclude self-similarities. □

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

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

$$\frac{1}{(N_i + N_j)(N_i + N_j - 1)}[(\sum_{d_m \in \omega_i \cup \omega_j} \vec{d}_m)^2 - (N_i + N_j)]$$

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- 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) □

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- We need a pithy label for each cluster.
- For example, in search result clustering for "jaguar", The labels of the three clusters could be "animal", "car", and "operating system".
- Topic of this section: How can we automatically find good labels for clusters?

Exercise

- Come up with an algorithm for labeling clusters
- Input: a set of documents, partitioned into K clusters (flat clustering)
- Output: A label for each cluster
- Part of the exercise: What types of labels should we consider? Words?

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- (but the latter is actually not discriminative) □

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  - E.g., select terms with high weights in the centroid (if we are using a vector space model)
- Non-discriminative methods sometimes select frequent terms that do not distinguish clusters.
- 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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- Split the cluster into 2 using K-means
- Of the clusters produced so far, select one to split (e.g. select the largest one)
- 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 $\omega_k \leftarrow \textsc{PickClusterFrom}(\textit{leaves})$

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

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

return *leaves*

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- But bisecting K-means is not deterministic.
- There are deterministic versions of bisecting K-means (see resources at the end), but they are much less efficient.

Efficient single link clustering

```
SingleLinkClustering(d_1, ..., d_N, K)
for n ← 1 to N
do for i ← 1 to N
     do C[n][i].sim ← SIM(d_n, d_i)
          C[n][i].index ← i
     I[n] ← n
     NBM[n] ← arg max_{X∈{C[n][i]:n≠i}} X.sim
A ← []
for n ← 1 to N − 1
do i_1 ← arg max_{{i:I[i]=i}} NBM[i].sim
     i_2 ← I[NBM[i_1].index]
     A.Append(⟨i_1, i_2⟩)
     for i ← 1 to N
     do if I[i] = i ∧ i ≠ i_1 ∧ i ≠ i_2
             then C[i_1][i].sim ← C[i][i_1].sim ← max(C[i_1][i].sim, C[i_2][i].sim)
          if I[i] = i_2
             then I[i] ← i_1
     NBM[i_1] ← arg max_{X∈{C[i_1][i]:I[i]=i∧i≠i_1}} X.sim
return A
```

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- The single-link algorithm we just saw is $O(N^2)$.
- Much more efficient than the $O(N^3)$ algorithm we looked at earlier!
- There are also $O(N^2)$ algorithms for complete-link, centroid and GAAC. □

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

What to do with the hierarchy?

- Use as is (e.g., for browsing as in Yahoo hierarchy)

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- Use as is (e.g., for browsing as in Yahoo hierarchy)
- Cut at a predetermined threshold
- Cut to get a predetermined number of clusters K
  - Ignores hierarchy below and above cutting line.

Take-away today

- Introduction to hierarchical clustering
- Single-link and complete-link clustering
- Centroid and group-average agglomerative clustering (GAAC)
- Bisecting K-means
- How to label clusters automatically

Resources

- Chapter 17 of IIR
- Resources at `http://cislmu.org`
  - Columbia Newsblaster (a precursor of Google News): McKeown et al. (2002)

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  - Columbia Newsblaster (a precursor of Google News): McKeown et al. (2002)
  - Bisecting K-means clustering: Steinbach et al. (2000)
  - PDDP (similar to bisecting K-means; deterministic, but also less efficient): Saravesi and Boley (2004)