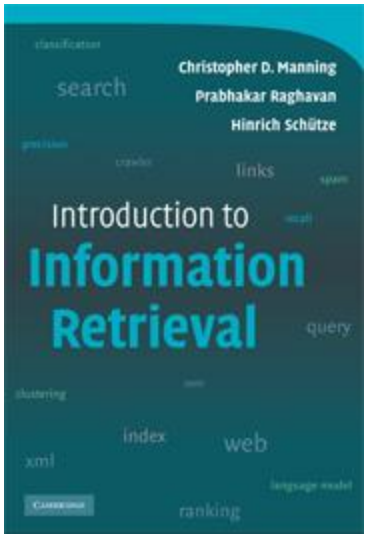
Information Retrieval and Organisation



Chapter 17

Hierarchical Clustering

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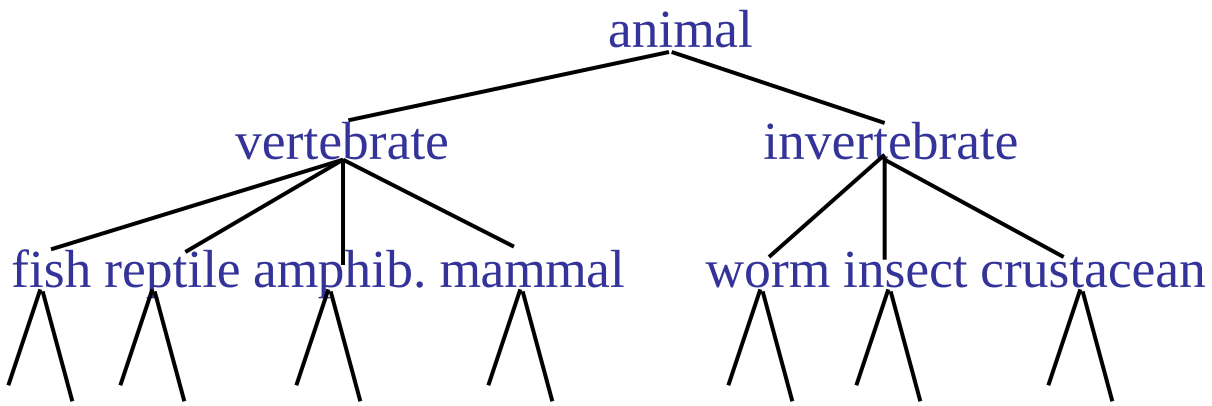
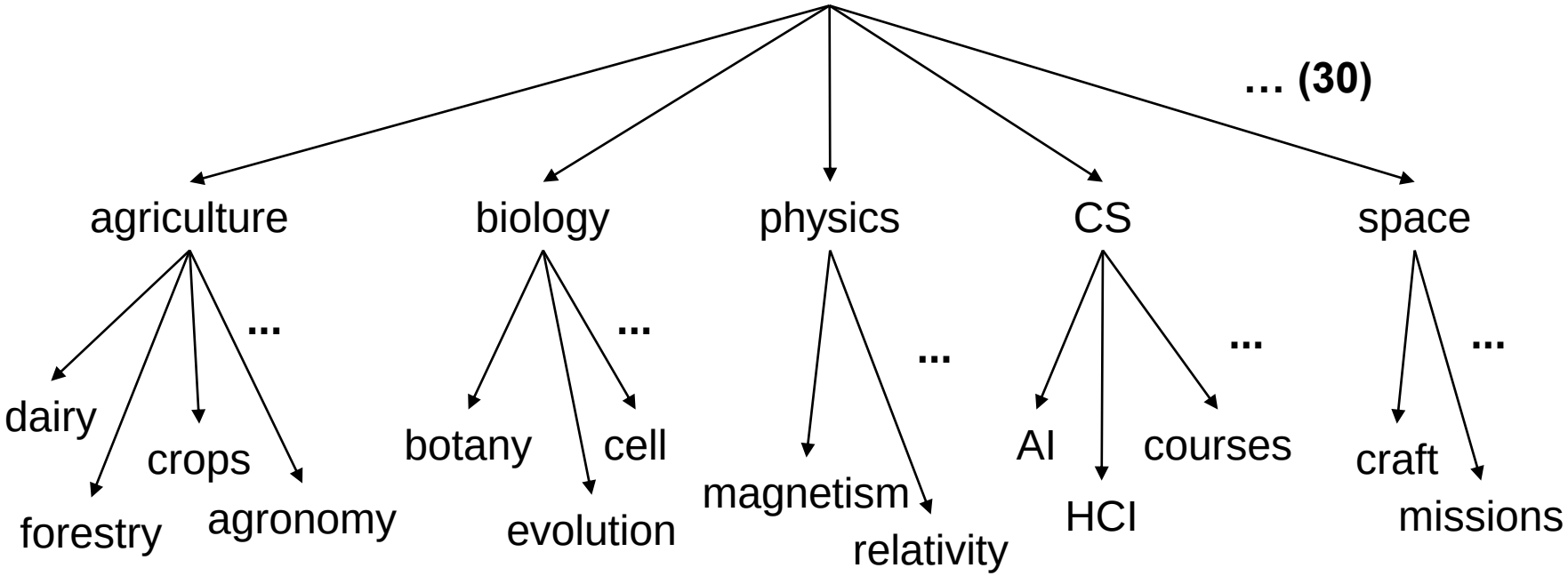
Hierarchical Clustering

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



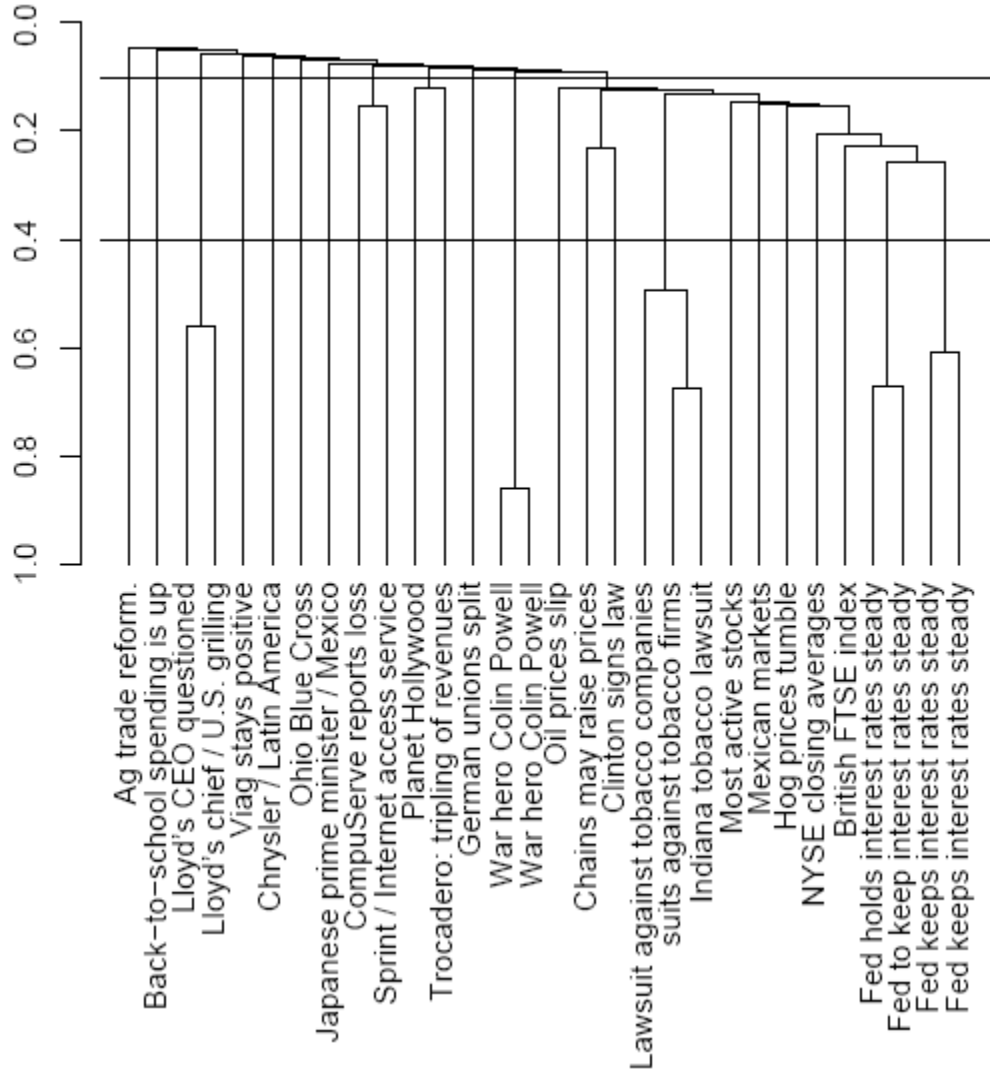
Dendrogram – Example

http://dir.yahoo.com/science



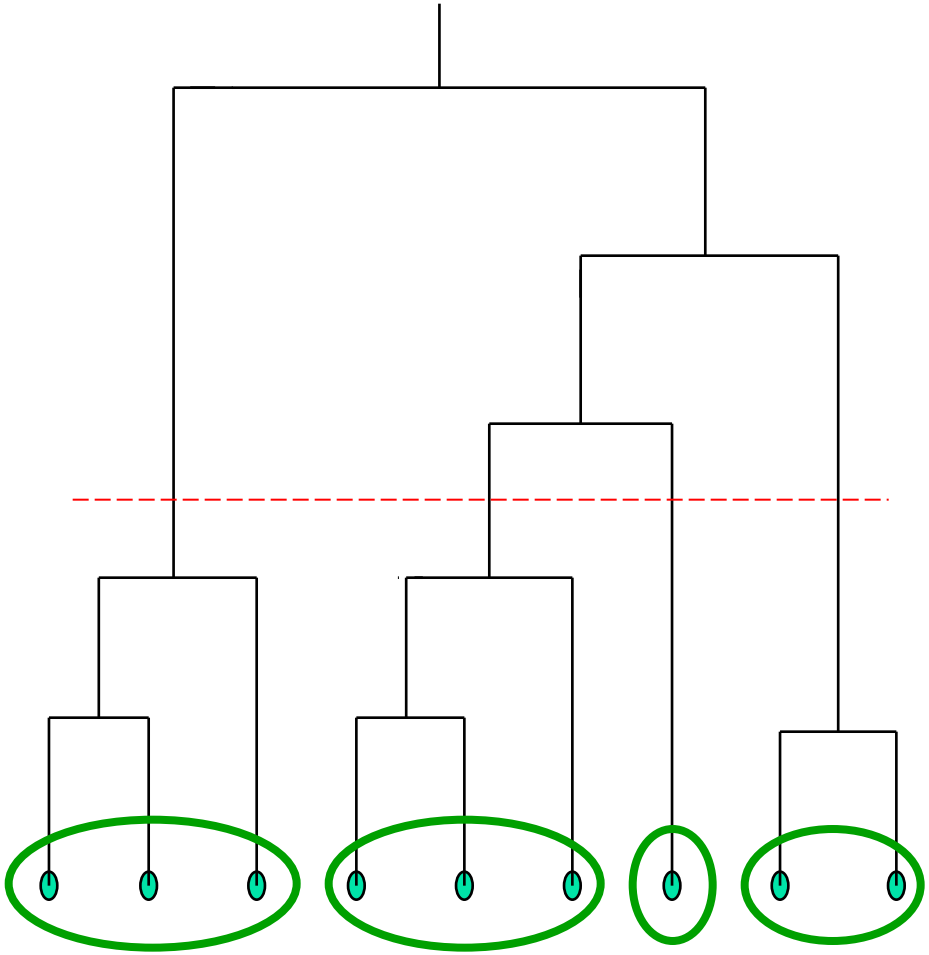
Dendrogram – Example

Clusters 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) ➔ bi-secting *k*-means.
- Agglomerative (Bottom-Up)
  - Start with each document being a single cluster. Eventually all documents belong to the same cluster.

HAC Algorithm

- **H**ierarchical **A**gglomerative **C**lustering
  - 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($\vec{d}_1, \ldots, \vec{d}_N$)

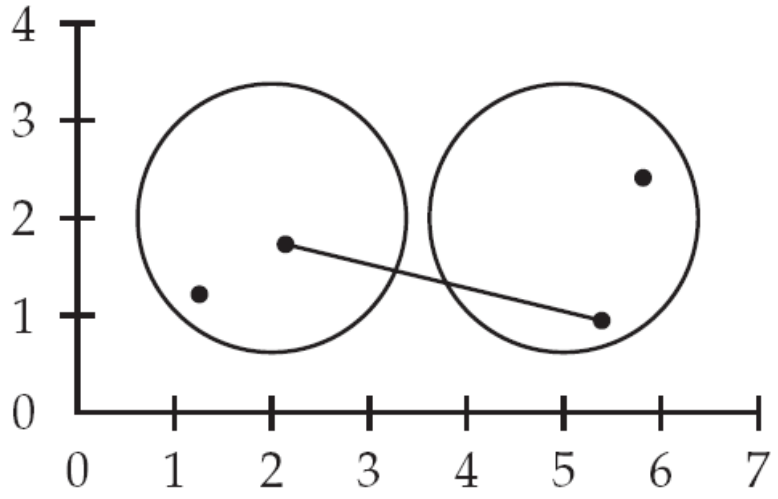
```
1  for n ← 1 to N
2  do for i ← 1 to N
3      do C[n][i].sim ← d_n · d_i
4          C[n][i].index ← i
5      I[n] ← 1
6      P[n] ← priority queue for C[n] sorted on sim
7      P[n].DELETE(C[n][n])  (don't want self-similarities)
8  A ← []
9  for k ← 1 to N − 1
10 do k_1 ← arg max_{k:I[k]=1} P[k].MAX().sim
11     k_2 ← P[k_1].MAX().index
12     A.APPEND(⟨k_1, k_2⟩)
13     I[k_2] ← 0
14     P[k_1] ← [ ]
15     for each i with I[i] = 1 ∧ i ≠ k_1
16     do P[i].DELETE(C[i][k_1])
17         P[i].DELETE(C[i][k_2])
18         C[i][k_1].sim ← SIM(i, k_1, k_2)
19         P[i].INSERT(C[i][k_1])
20         C[k_1][i].sim ← SIM(i, k_1, k_2)
21         P[k_1].INSERT(C[k_1][i])
22 return A
```

Time Complexity

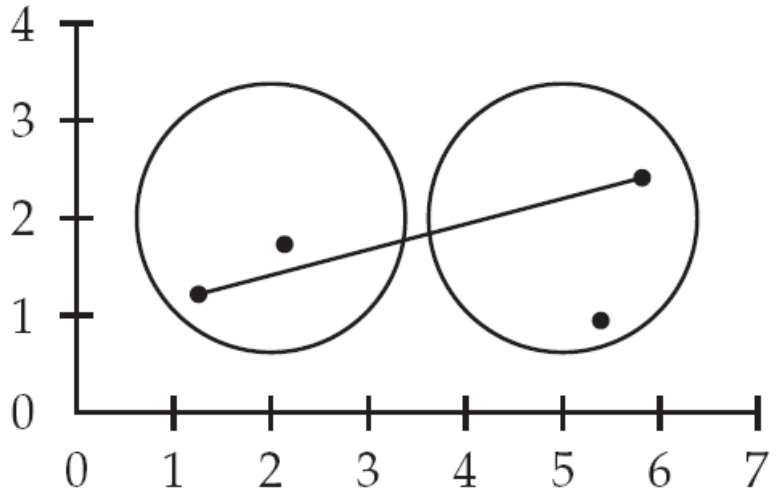
- In the initialization step, compute similarity of all pairs of n documents which is $O(n^2)$.
- In each of the subsequent $n-2$ merging iterations, compute the distance between the most recently created cluster and all other existing clusters.
- The overall time complexity is often $O(n^3)$ if done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

HAC Variants

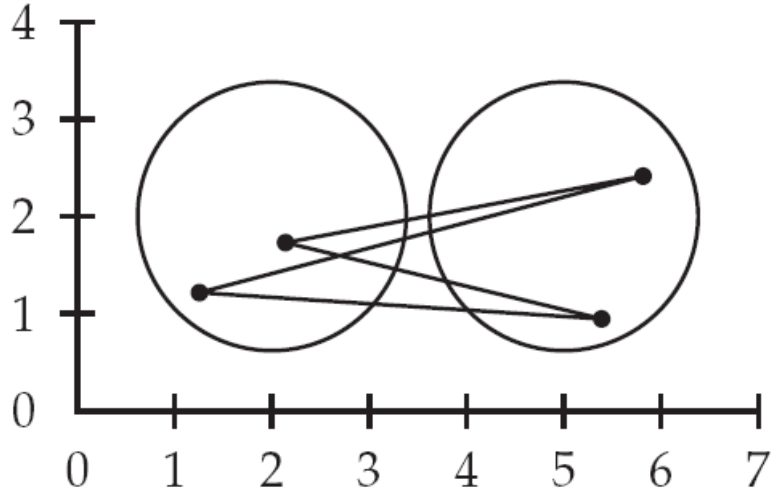
- How to define the closest pair of clusters
  - Single-Link
    - maximum similarity between pairs of docs
  - Complete-Link
    - minimum similarity between pairs of docs
  - Average-Link
    - average similarity between pairs of docs
  - Centroid
    - maximum similarity between cluster centroids



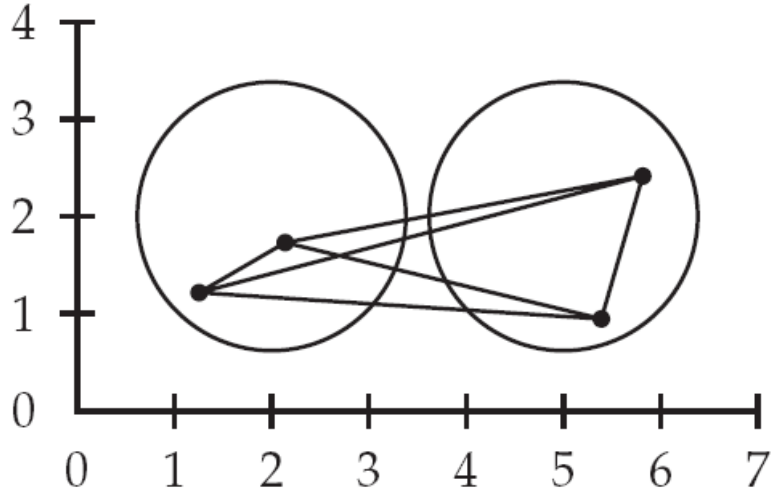
(a) single link: maximum similarity



(b) complete link: minimum similarity



(c) centroid: average inter-similarity



(d) group-average: average of all similarities

Single-Link

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

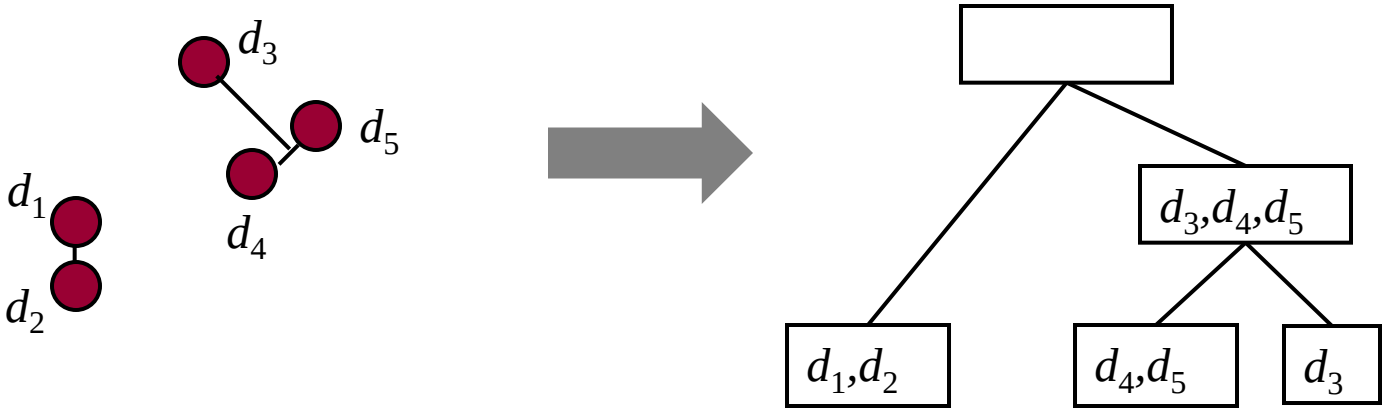
$$sim\ (c_i, c_j) = \max_{x \in c_i, y \in c_j} sim\ (x, y)$$

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

$$sim\ ((c_i \cup c_j), c_k) = \max\left(sim\ (c_i, c_k), sim\ (c_j, c_k)\right)$$

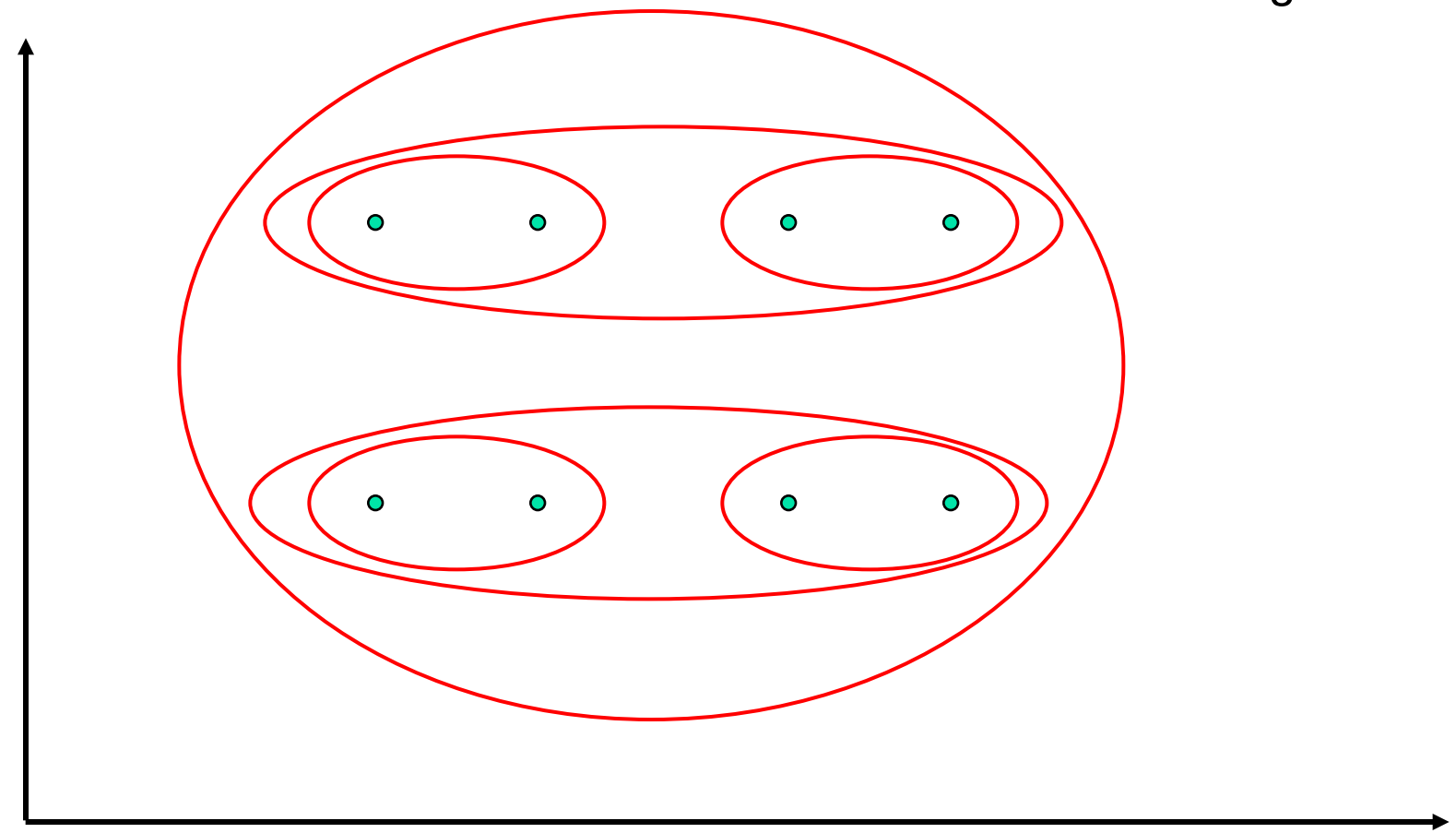
HAC – Example

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



HAC – Example

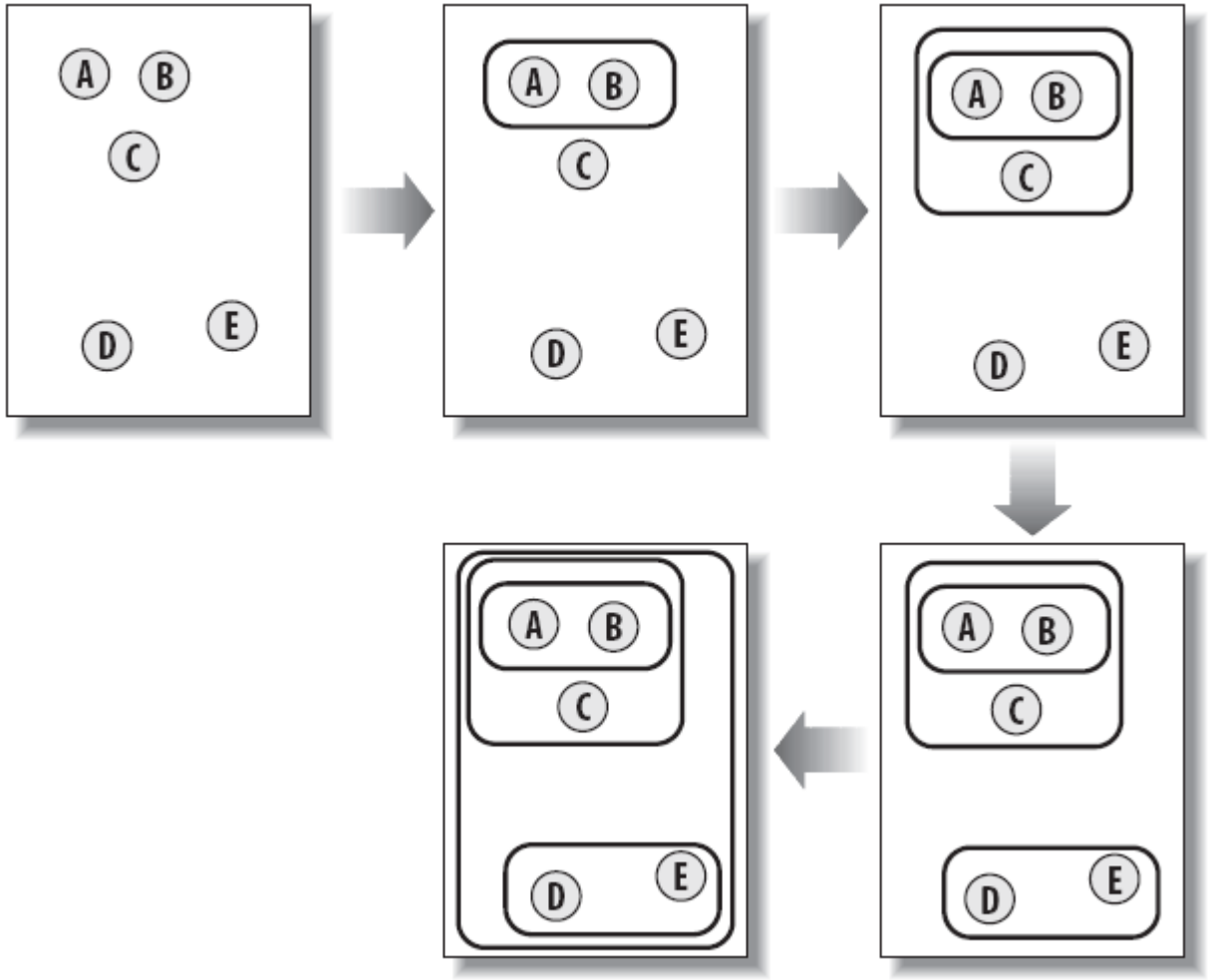
Single-Link



HAC – Exercise

Digital Camera	Megapixel	Zoom
A	1	8
B	3	8
C	2	6
D	1.5	1
E	4	2

HAC – Exercise



Chaining Effect

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