Lecture 7: Clustering

Information Retrieval
Computer Science Tripos Part II

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[1] Adapted from Simone Teufel's original slides

Upcoming

- What is clustering?
- Applications of clustering in information retrieval
- K-means algorithm
- Introduction to hierarchical clustering
- Single-link and complete-link clustering

Overview

1. Clustering: Introduction
2. Non-hierarchical clustering
3. Hierarchical clustering

Clustering: Definition

- (Document) clustering is the process of grouping a set of documents into clusters of similar documents.
  - Documents within a cluster should be similar.
  - Documents from different clusters should be dissimilar.
- Clustering is the most common form of unsupervised learning.
- Unsupervised = there are no labeled or annotated data.

Difference clustering–classification

Classification	Clustering
supervised learning	unsupervised learning
classes are human-defined and part of the input to the learning algorithm	Clusters are inferred from the data without human input.
output = membership in class only	Output = membership in class + distance from centroid ("degree of cluster membership")

The cluster hypothesis

Cluster hypothesis.

Documents in the same cluster behave similarly with respect to relevance to information needs.

All applications of clustering in IR are based (directly or indirectly) on the cluster hypothesis.

Van Rijsbergen's original wording (1979): "closely associated documents tend to be relevant to the same requests".

Applications of Clustering

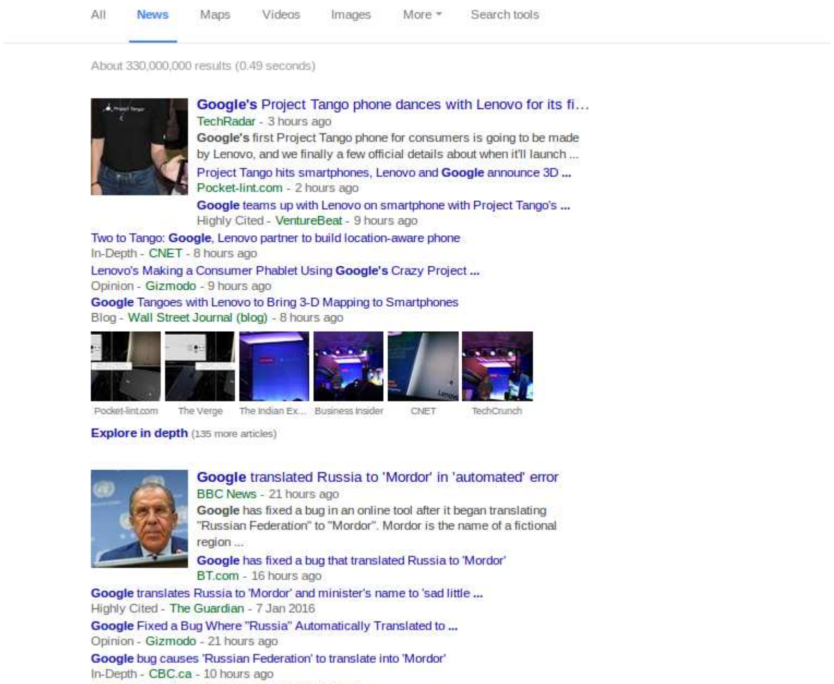
- IR: presentation of results (clustering of documents)
- Summarisation:
  - clustering of similar documents for multi-document summarisation
  - clustering of similar sentences for re-generation of sentences
- Topic Segmentation: clustering of similar paragraphs (adjacent or non-adjacent) for detection of topic structure/importance
- Lexical semantics: clustering of words by cooccurrence patterns

Clustering search results

Top **208** results of at least **20,373,974** retrieved for the query **jaguar** (Details)

1. Jag-lovers - THE source for all **Jaguar** information [new window] [frame] [cache] [preview] [clusters]
   ... Internet! Serving Enthusiasts since 1993 The Jag-lovers Web Currently with 40661 members The Premier **Jaguar** Cars web resource for all enthusiasts Lists and Forums Jag-lovers originally evolved around its ...
   www.jag-lovers.org - Open Directory 2, Wisenut 8, Ask Jeeves 8, MSN 9, Looksmart 12, MSN Search 18
2. **Jaguar** Cars [new window] [frame] [cache] [preview] [clusters]
   [...] redirected to www.**jaguar**.com
   www.jaguarcars.com - Looksmart 1, MSN 2, Lycos 3, Wisenut 6, MSN Search 9, MSN 29
3. http://www.**jaguar**.com/ [new window] [frame] [preview] [clusters]
   www.jaguar.com - MSN 1, Ask Jeeves 1, MSN Search 3, Lycos 9
4. Apple - Mac OS X [new window] [frame] [preview] [clusters]
   Learn about the new OS X Server, designed for the Internet, digital media and workgroup management. Download a technical factsheet.
   www.apple.com/macosx - Wisenut 1, MSN 3, Looksmart 26

Clustering news articles



About 330,000,000 results (0.49 seconds)

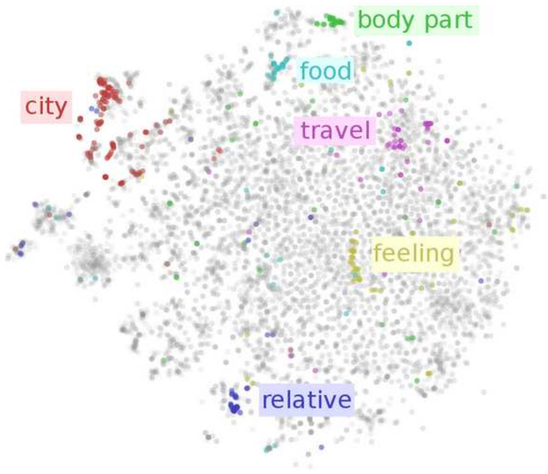
Google's Project Tango phone dances with Lenovo for its fi…
TechRadar - 3 hours ago
Google's first Project Tango phone for consumers is going to be made by Lenovo, and we finally a few official details about when it'll launch ...
Project Tango hits smartphones, Lenovo and **Google** announce 3D ...
Pocket-lint.com - 2 hours ago
Google teams up with Lenovo on smartphone with Project Tango's ...
Highly Cited - VentureBeat - 9 hours ago
Two to Tango: **Google**, Lenovo partner to build location-aware phone
In-Depth - CNET - 8 hours ago
Lenovo's Making a Consumer Phablet Using **Google's** Crazy Project ...
Opinion - Gizmodo - 9 hours ago
Google Tangoes with Lenovo to Bring 3-D Mapping to Smartphones
Blog - Wall Street Journal (blog) - 8 hours ago

Pocket-lint.com · The Verge · The Indian Ex... · Business Insider · CNET · TechCrunch

Explore in depth (135 more articles)

Google translated Russia to 'Mordor' in 'automated' error
BBC News - 21 hours ago
Google has fixed a bug in an online tool after it began translating "Russian Federation" to "Mordor". Mordor is the name of a fictional region ...
Google has fixed a bug that translated Russia to 'Mordor'
BT.com - 16 hours ago
Google translates Russia to 'Mordor' and minister's name to 'sad little ...
Highly Cited - The Guardian - 7 Jan 2016
Google Fixed a Bug Where "Russia" Automatically Translated to ...
Opinion - Gizmodo - 21 hours ago
Google bug causes 'Russian Federation' to translate into 'Mordor'
In-Depth - CBC.ca - 10 hours ago

Clustering Words



[2]

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[2] https://colah.github.io/posts/2015-01-Visualizing-Representations/

Types of Clustering

- Hard clustering v. soft clustering
  - Hard clustering: every object is member in only one cluster
  - Soft clustering: objects can be members in more than one cluster
- Hierarchical v. non-hierarchical clustering
  - Hierarchical clustering: pairs of most-similar clusters are iteratively linked until all objects are in a clustering relationship
  - Non-hierarchical clustering results in flat clusters of "similar" documents

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Desiderata for clustering

- General goal: put related docs in the same cluster, put unrelated docs in different clusters.
  - We'll see different ways of formalizing this.
- The number of clusters should be appropriate for the data set we are clustering.
  - Initially, we will assume the number of clusters K is given.
  - There also exist semiautomatic methods for determining K
- Secondary goals in clustering
  - Avoid very small and very large clusters
  - Define clusters that are easy to explain to the user
  - Many others . . .

Overview

1. Clustering: Introduction
2. Non-hierarchical clustering
3. Hierarchical clustering

Non-hierarchical (partitioning) clustering

- Partitional clustering algorithms produce a set of k non-nested partitions corresponding to k clusters of n objects.
- Advantage: not necessary to compare each object to each other object, just comparisons of objects – cluster centroids necessary
- Optimal partitioning clustering algorithms are $O(kn)$
- Main algorithm: K-means

K-means: Basic idea

- Each cluster j (with n_j elements x_i) is represented by its centroid c_j, the average vector of the cluster:

$$c_j = \frac{1}{n_j} \sum_{i=1}^{n_j} x_i$$

- Measure of cluster quality: minimise mean square distance between elements x_i and nearest centroid c_j

$$RSS = \sum_{j=1}^{k} \sum_{x_i \in j} d(\overrightarrow{x_i}, \overrightarrow{c_j})^2$$

- Distance: Euclidean; length-normalised vectors in VS
- We iterate two steps:
  - reassignment: assign each vector to its closest centroid
  - recomputation: recompute each centroid as the average of the vectors that were recently assigned to it

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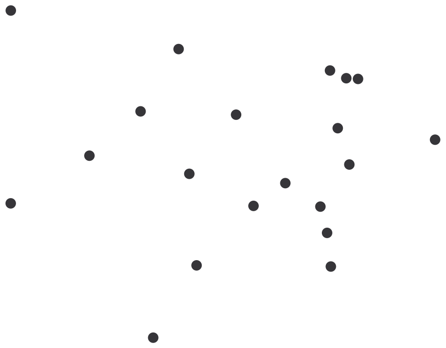
K-means algorithm

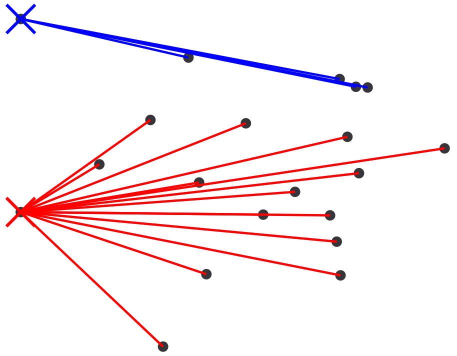
```
Given: a set $s_0 = \overrightarrow{x_1}, \ldots \overrightarrow{x_n} \subseteq \mathcal{R}^m$
Given: a distance measure $d : \mathcal{R}^m \times \mathcal{R}^m \rightarrow \mathcal{R}$
Given: a function for computing the mean $\mu : \mathcal{P}(\mathcal{R}) \rightarrow \mathcal{R}^m$

Select $k$ initial centers $\overrightarrow{c_1}, \ldots \overrightarrow{c_k}$
while stopping criterion not true:
        $\sum_{j=1}^{k} \sum_{x_i \in s_j} d(\overrightarrow{x_i}, \overrightarrow{c_j})^2 < \epsilon$ (stopping criterion)
        do
        for all clusters $s_j$ do (reassignment)
                $c_j := \{\overrightarrow{x_i} | \forall \overrightarrow{c_l} : d(\overrightarrow{x_i}, \overrightarrow{c_j}) \leq d(\overrightarrow{x_i}, \overrightarrow{c_l})\}$
        end
        for all means $\overrightarrow{c_j}$ do (centroid recomputation)
                $\overrightarrow{c_j} := \mu(s_j)$
        end
end
```

Worked Example: Set of points to be clustered



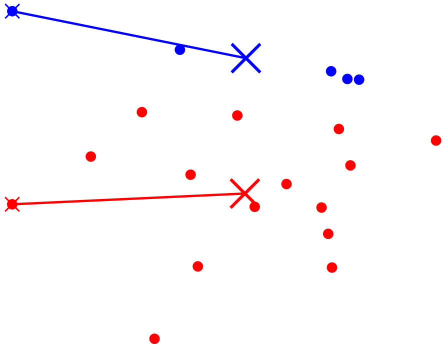
Exercise: (i) Guess what the optimal clustering into two clusters is in this case; (ii) compute the centroids of the clusters

Random seeds + Assign points to closest center



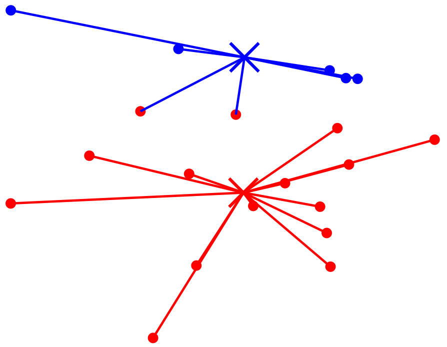
Iteration One

Worked Example: Recompute cluster centroids



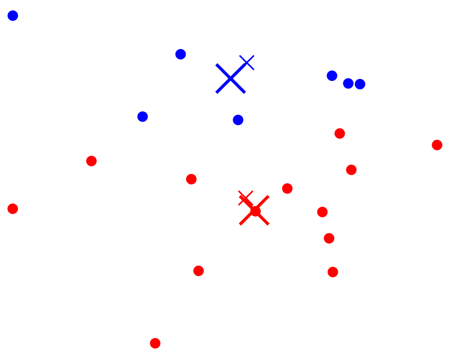
Iteration One

Worked Example: Assign points to closest centroid



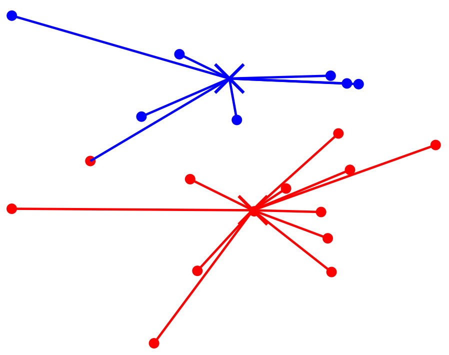
Iteration One

Worked Example: Recompute cluster centroids



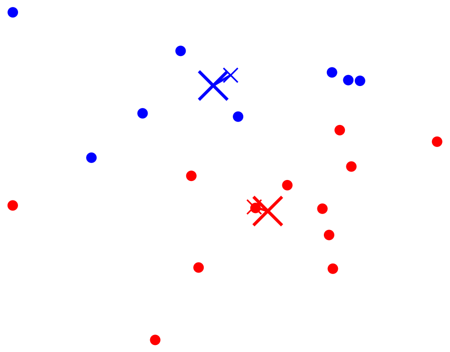
Iteration Two

Worked Example: Assign points to closest centroid



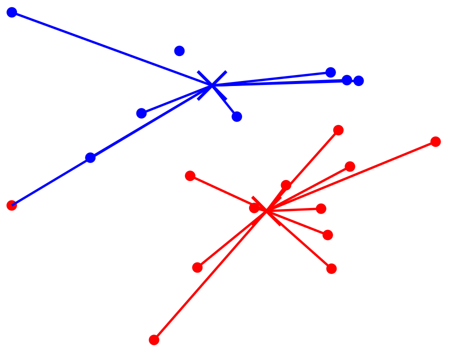
Iteration Two

Worked Example: Recompute cluster centroids



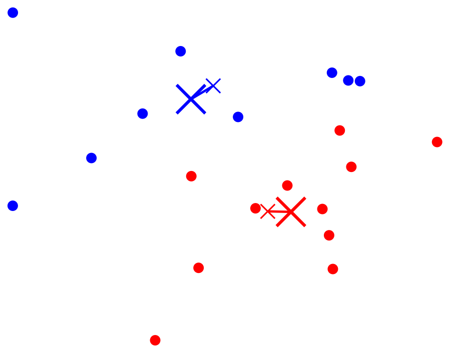
Iteration Three

Worked Example: Assign points to closest centroid



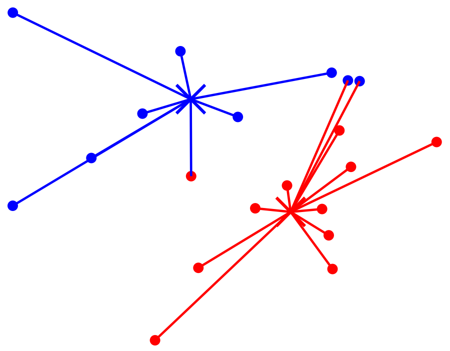
Iteration Three

Worked Example: Recompute cluster centroids



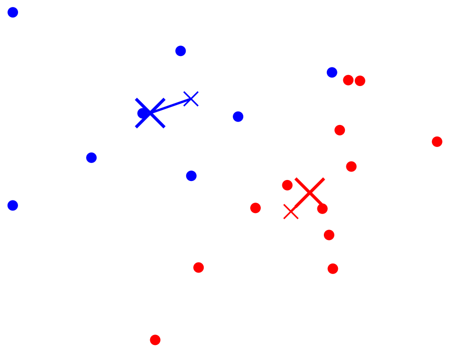
Iteration Four

Worked Example: Assign points to closest centroid



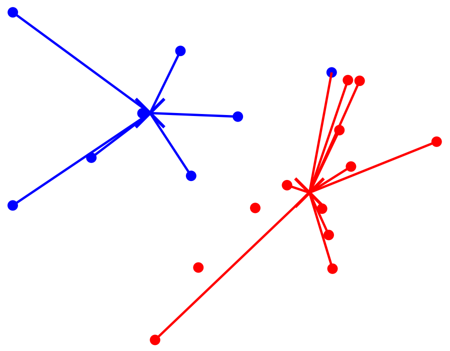
Iteration Four

Worked Example: Recompute cluster centroids



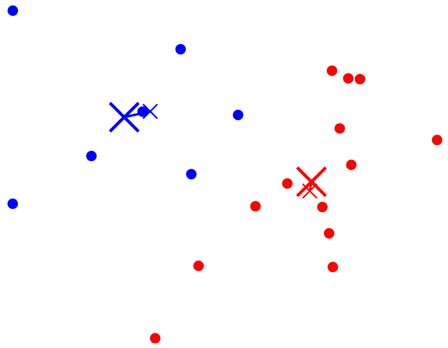
Iteration Five

Worked Example: Assign points to closest centroid



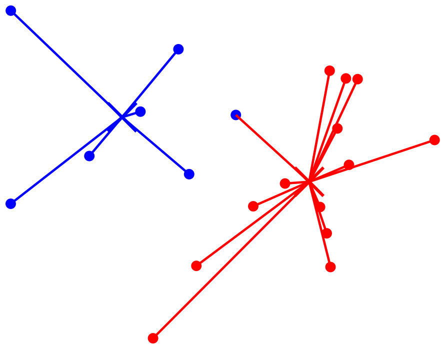
Iteration Five

Worked Example: Recompute cluster centroids



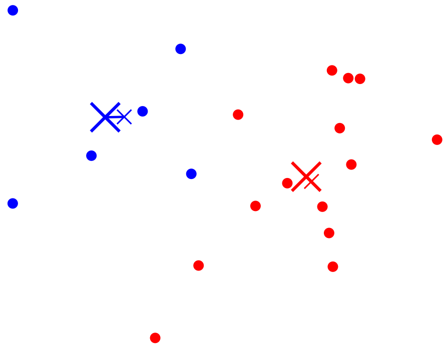
Iteration Six

Worked Example: Assign points to closest centroid



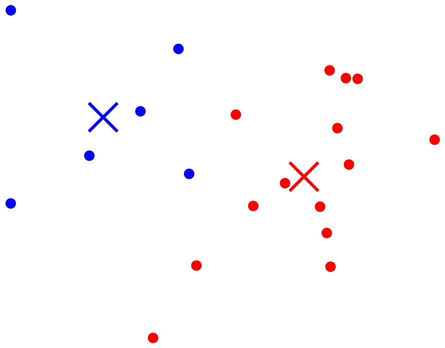
Iteration Six

Worked Example: Recompute cluster centroids



Iteration Seven

Worked Ex.: Centroids and assignments after convergence



Convergence

K-means is guaranteed to converge: Proof

- RSS decreases during each reassignment step.
  - because each vector is moved to a closer centroid
- RSS decreases during each recomputation step.
  - This follows from the definition of a centroid: the new centroid is the vector for which RSS_k reaches its minimum
- There is only a finite number of clusterings.
- Thus: We must reach a fixed point.
- Finite set & monotonically decreasing evaluation function → convergence
- Assumption: Ties are broken consistently.

Other properties of K-means

- Fast convergence
  - K-means typically converges in around 10-20 iterations (if we don't care about a few documents switching back and forth)
  - However, complete convergence can take many more iterations.
- Non-optimality
  - K-means is not guaranteed to find the optimal solution.
  - If we start with a bad set of seeds, the resulting clustering can be horrible.
- Dependence on initial centroids
  - Solution 1: Use i clusterings, choose one with lowest RSS
  - Solution 2: Use prior hierarchical clustering step to find seeds with good coverage of document space

Time complexity of K-means

- Reassignment step: $O(KNM)$ (we need to compute KN document-centroid distances, each of which costs $O(M)$)
- Recomputation step: $O(NM)$ (we need to add each of the document's $< M$ values to one of the centroids)
- Assume number of iterations bounded by I
- Overall complexity: $O(IKNM)$ – linear in all important dimensions

Overview

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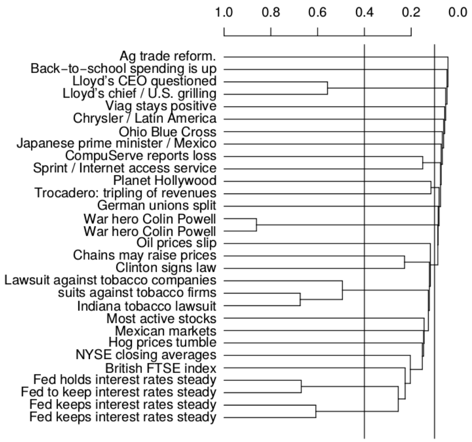
Hierarchical clustering

- Imagine we now want to create a hierachy in the form of a binary tree.
- Assumes a similarity measure for determining the similarity of two clusters.
- Up to now, our similarity measures were for documents.
- We will look at different cluster similarity measures.
- Main algorithm: HAC (hierarchical agglomerative clustering)

HAC: Basic algorithm

- Start with each document in a separate cluster
- Then repeatedly merge the two clusters that are most similar
- Until there is only one cluster.
- 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



▼ **Figure 17.1** A dendrogram of a single-link clustering of 30 documents from Reuters-RCV1. Two possible cuts of the dendrogram are shown: at 0.4 into 24 clusters and at 0.1 into 12 clusters.

Term–document matrix to document–document matrix

Log frequency weighting
and cosine normalisation

SaS	PaP	WH
0.789	0.832	0.524
0.515	0.555	0.465
0.335	0.000	0.405
0.000	0.000	0.588

SaS	P(SaS,SaS)	P(PaP,SaS)
PaP	P(SaS,PaP)	P(PaP,PaP)
WH	P(SaS,WH)	P(PaP,WH)
	SaS	PaP

SaS	1	.94	.79
PaP	.94	1	.69
WH	.79	.69	1
	SaS	PaP	WH

- Applying the proximity metric to all pairs of documents. . .
- creates the document-document matrix, which reports similarities/distances between objects (documents)
- The diagonal is trivial (identity)
- As proximity measures are symmetric, the matrix is a triangle

Hierarchical clustering: agglomerative (BottomUp, greedy)

```
Given: a set $X = x_1, ...x_n$ of objects;
Given: a function $sim : \mathcal{P}(X) \times \mathcal{P}(X) \rightarrow \mathcal{R}$

for i:= 1 to n do
        $c_i := x_i$
C :=$c_1$, ... $c_n$
j := n+1
while C > 1 do
        $(c_{n_1}, c_{n_2}) := max_{(c_u, c_v) \in C \times C} sim(c_u, c_v)$
        $c_j := c_{n_1} \cup c_{n_2}$
        C := C  $\{ c_{n_1}, c_{n_2} \} \cup c_j$
        j:=j+1
end
```

Similarity function $sim : \mathcal{P}(X) \times \mathcal{P}(X) \rightarrow \mathcal{R}$ measures similarity between clusters, not objects

Computational complexity of the basic algorithm

- First, we compute the similarity of all $N \times N$ pairs of documents.
- Then, in each of N iterations:
    - We scan the $O(N \times N)$ similarities to find the maximum similarity.
    - We merge the two clusters with maximum similarity.
    - We compute the similarity of the new cluster with all other (surviving) clusters.
- There are $O(N)$ iterations, each performing a $O(N \times N)$ "scan" operation.
- Overall complexity is $O(N^3)$.
- Depending on the similarity function, a more efficient algorithm is possible.

Hierarchical clustering: similarity functions

Similarity between two clusters c_k and c_j (with similarity measure s) can be interpreted in different ways:

- Single Link Function: Similarity of two most similar members

  $$sim(c_u, c_v) = max_{x \in c_u, y \in c_k} s(x, y)$$

- Complete Link Function: Similarity of two least similar members

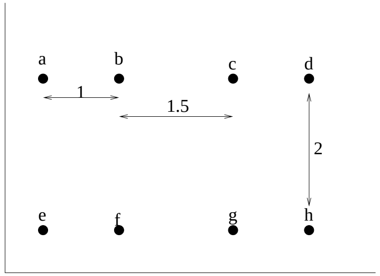
  $$sim(c_u, c_v) = min_{x \in c_u, y \in c_k} s(x, y)$$

- Group Average Function: Avg. similarity of each pair of group members

  $$sim(c_u, c_v) = avg_{x \in c_u, y \in c_k} s(x, y)$$

Example: hierarchical clustering; similarity functions

Cluster 8 objects a-h; Euclidean distances (2D) shown in diagram



b	1						
c	2.5	1.5					
d	3.5	2.5	1				
e	2	$\sqrt{5}$	$\sqrt{10.25}$	$\sqrt{16.25}$			
f	$\sqrt{5}$	2	$\sqrt{6.25}$	$\sqrt{10.25}$	1		
g	$\sqrt{10.25}$	$\sqrt{6.25}$	2	$\sqrt{5}$	2.5	1.5	
h	$\sqrt{16.25}$	$\sqrt{10.25}$	$\sqrt{5}$	2	3.5	2.5	1
	a	b	c	d	e	f	g

Single Link is O(n^2)

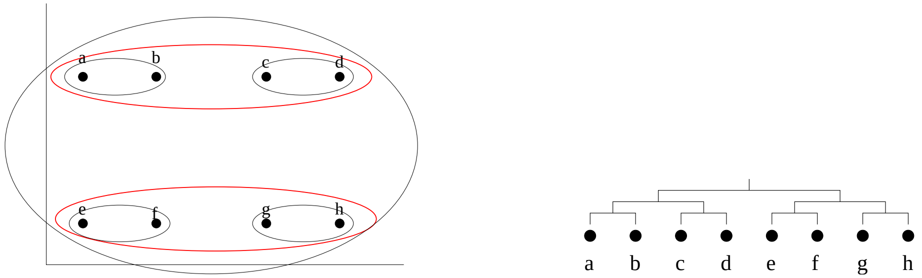
b	1						
c	2.5	1.5					
d	3.5	2.5	1				
e	2	$\sqrt{5}$	$\sqrt{10.25}$	$\sqrt{16.25}$			
f	$\sqrt{5}$	2	$\sqrt{6.25}$	$\sqrt{10.25}$	1		
g	$\sqrt{10.25}$	$\sqrt{6.25}$	2	$\sqrt{5}$	2.5	1.5	
h	$\sqrt{16.25}$	$\sqrt{10.25}$	$\sqrt{5}$	2	3.5	2.5	1
	a	b	c	d	e	f	g

After Step 4 (a–b, c–d, e–f, g–h merged):

c–d	1.5		
e–f	2	$\sqrt{6.25}$	
g–h	$\sqrt{6.25}$	2	1.5
	a–b	c–d	e–f

“min-min” at each step

Clustering Result under Single Link



Complete Link

b	1						
c	2.5	1.5					
d	3.5	2.5	1				
e	2	$\sqrt{5}$	$\sqrt{10.25}$	$\sqrt{16.25}$			
f	$\sqrt{5}$	2	$\sqrt{6.25}$	$\sqrt{10.25}$	1		
g	$\sqrt{10.25}$	$\sqrt{6.25}$	2	$\sqrt{5}$	2.5	1.5	
h	$\sqrt{16.25}$	$\sqrt{10.25}$	$\sqrt{5}$	2	3.5	2.5	1
	a	b	c	d	e	f	g

After step 4 (a–b, c–d, e–f, g–h merged):

c–d	2.5 1.5 $\boxed{3.5}$ 2.5		
e–f	2 $\sqrt{5}$ $\boxed{\sqrt{5}}$ 2	$\sqrt{10.25}$ $\boxed{\sqrt{16.25}}$ $\sqrt{6.25}$ $\sqrt{10.25}$	
g–h	$\sqrt{10.25}$ $\sqrt{6.25}$ $\boxed{\sqrt{16.25}}$ $\sqrt{10.25}$	2 $\boxed{\sqrt{5}}$ $\sqrt{5}$ 2	2.5 1.5 $\boxed{3.5}$ 2.5
	a–b	c–d	e–f

“max-min” at each step

Complete Link

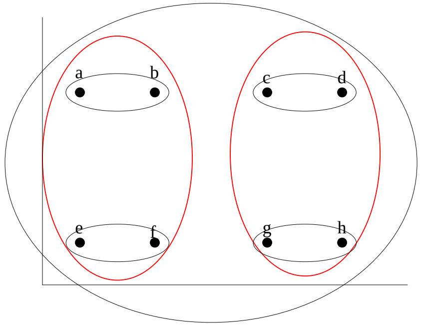
b	1						
c	2.5	1.5					
d	3.5	2.5	1				
e	2	$\sqrt{5}$	$\sqrt{10.25}$	$\sqrt{16.25}$			
f	$\sqrt{5}$	2	$\sqrt{6.25}$	$\sqrt{10.25}$	1		
g	$\sqrt{10.25}$	$\sqrt{6.25}$	2	$\sqrt{5}$	2.5	1.5	
h	$\sqrt{16.25}$	$\sqrt{10.25}$	$\sqrt{5}$	2	3.5	2.5	1
	a	b	c	d	e	f	g

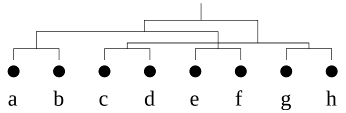
After step 4 (a–b, c–d, e–f, g–h merged):

c–d	2.5 1.5 $\boxed{3.5}$ 2.5		
e–f	2 $\sqrt{5}$ $\boxed{\sqrt{5}}$ 2	$\sqrt{10.25}$ $\boxed{\sqrt{16.25}}$ $\sqrt{6.25}$ $\sqrt{10.25}$	
g–h	$\sqrt{10.25}$ $\sqrt{6.25}$ $\boxed{\sqrt{16.25}}$ $\sqrt{10.25}$	2 $\boxed{\sqrt{5}}$ $\sqrt{5}$ 2	2.5 1.5 $\boxed{3.5}$ 2.5
	a–b	c–d	e–f

“max-min” at each step → ab/ef and cd/gh merges next

Clustering result under complete link





Complete Link is O(n^3)

Example: gene expression data

- An example from biology: cluster genes by function
- Survey 112 rat genes which are suspected to participate in development of CNS
- Take 9 data points: 5 embryonic (E11, E13, E15, E18, E21), 3 postnatal (P0, P7, P14) and one adult
- Measure expression of gene (how much mRNA in cell?)
- These measures are normalised logs; for our purposes, we can consider them as weights
- Cluster analysis determines which genes operate at the same time

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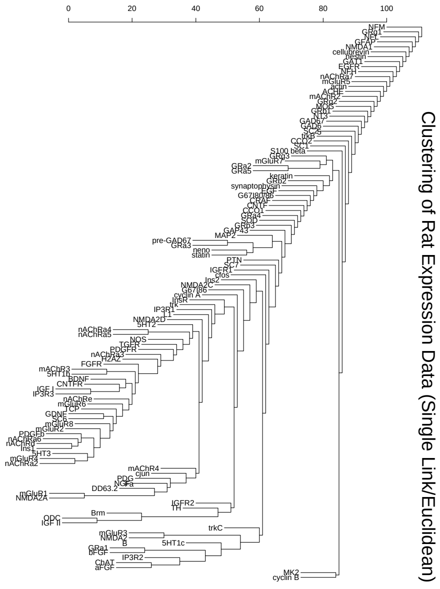
Rat CNS gene expression data (excerpt)

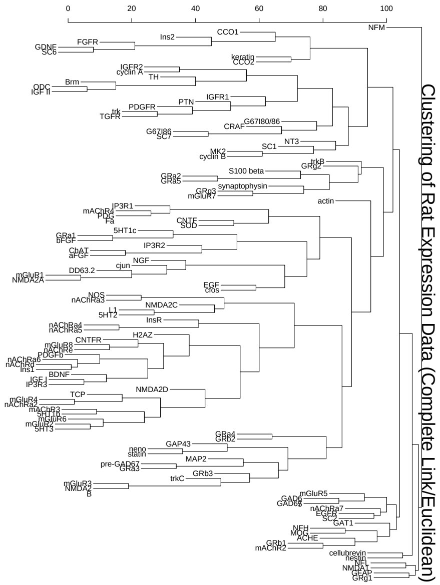
gene	genbank locus	E11	E13	E15	E18	E21	P0	P7	P14	A
keratin	RNKER19	1.703	0.349	0.523	0.408	0.683	0.461	0.32	0.081	0
cellubrevin	s63830	5.759	4.41	1.195	2.134	2.306	2.539	3.892	3.953	2.72
nestin	RATNESTIN	2.537	3.279	5.202	2.807	1.5	1.12	0.532	0.514	0.443
MAP2	RATMAP2	0.04	0.514	1.553	1.654	1.66	1.491	1.436	1.585	1.894
GAP43	RATGAP43	0.874	1.494	1.677	1.937	2.322	2.296	1.86	1.873	2.396
L1	S55536	0.062	0.162	0.51	0.929	0.966	0.867	0.493	0.401	0.384
NFL	RATNFL	0.485	5.598	6.717	9.843	9.78	13.466	14.921	7.862	4.484
NFM	RATNFM	0.571	3.373	5.155	4.092	4.542	7.03	6.682	13.591	27.692
NFH	RATNFHPEP	0.166	0.141	0.545	1.141	1.553	1.667	1.929	4.058	3.859
synaptophysin	RNSYN	0.205	0.636	1.571	1.476	1.948	2.005	2.381	2.191	1.757
neno	RATENONS	0.27	0.704	1.419	1.469	1.861	1.556	1.639	1.586	1.512
S100 beta	RATS100B	0.052	0.011	0.491	1.303	1.487	1.357	1.438	2.275	2.169
GFAP	RNU03700	0	0	0	0.292	2.705	3.731	8.705	7.453	6.547
MOG	RATMOG	0	0	0	0	0.012	0.385	1.462	2.08	1.816
GAD65	RATGAD65	0.353	1.117	2.539	3.808	3.212	2.792	2.671	2.327	2.351
pre-GAD67	RATGAD67	0.073	0.18	1.171	1.436	1.443	1.383	1.164	1.003	0.985
GAD67	RATGAD67	0.297	0.307	1.066	2.796	3.572	3.182	2.604	2.307	2.079
G67I80/86	RATGAD67	0.767	1.38	2.35	1.88	1.332	1.002	0.668	0.567	0.304
G67I86	RATGAD67	0.071	0.204	0.641	0.764	0.406	0.202	0.052	0.022	0
GAT1	RATGABAT	0.839	1.071	5.687	3.864	4.786	4.701	4.879	4.601	4.679
ChAT	(*)	0	0.022	0.369	0.322	0.663	0.597	0.795	1.015	1.424
ACHE	S50879	0.174	0.425	1.63	2.724	3.279	3.519	4.21	3.885	3.95
ODC	RATODC	1.843	2.003	1.803	1.618	1.569	1.565	1.394	1.314	1.11
TH	RATTOHA	0.633	1.225	1.007	0.801	0.654	0.691	0.23	0.287	0
NOS	RRBNOS	0.051	0.141	0.675	0.63	0.86	0.926	0.792	0.646	0.448
GRa1	(#)	0.454	0.626	0.802	0.972	1.021	1.182	1.297	1.469	1.511

. . .

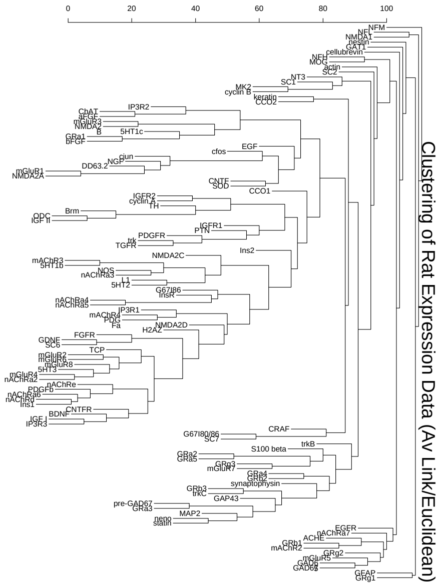
Rat CNS gene clustering – single link



Rat CNS gene clustering – complete link



Rat CNS gene clustering – group average link



Flat or hierarchical clustering?

- When a hierarchical structure is desired: hierarchical algorithm
- Humans are bad at interpreting hiearchical clusterings (unless cleverly visualised)
- For high efficiency, use flat clustering
- For deterministic results, use HAC
- HAC also can be applied if K cannot be predetermined (can start without knowing K)

Take-away

- Partitional clustering
  - Provides less information but is more efficient (best: $O(kn)$)
  - K-means
- Hierarchical clustering
  - Best algorithms $O(n^2)$ complexity
  - Single-link vs. complete-link (vs. group-average)
- Hierarchical and non-hierarchical clustering fulfills different needs

Reading

- MRS Chapters 16.1-16.4
- MRS Chapters 17.1-17.2