Agglomerative Clustering

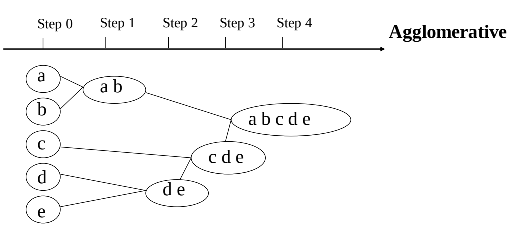
HAC

Introduction

- Hierarchical Clustering Approach
  - A typical clustering analysis approach by partitioning data set sequentially
  - Construct nested partitions layer by layer by grouping objects into a tree of clusters (without the need to know the number of clusters in advance)
  - Use (generalised) distance matrix as clustering criteria

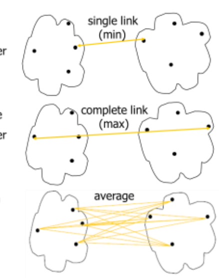
Introduction

- Example



Cluster Distance Measures

- Single link: smallest distance between an element in one cluster and an element in the other, i.e., $d(C_i, C_j) = \min\{d(x_{ip}, x_{jq})\}$
- Complete link: largest distance between an element in one cluster and an element in the other, i.e., $d(C_i, C_j) = \max\{d(x_{ip}, x_{jq})\}$
- Average: avg distance between elements in one cluster and elements in the other, i.e., $d(C_i, C_j) = \text{avg}\{d(x_{ip}, x_{jq})\}$



Cluster Distance Measures

Example: Given a data set of five objects characterised by a single continuous feature, assume that there are two clusters: C_1: {a, b} and C_2: {c, d, e}.

	a	b	c	d	e
Feature	1	2	4	5	6

1. Calculate the distance matrix

	a	b	c	d	e
a	0				
b	1	0			
c	3	2	0		
d	4	3	1	0	
e	5	4	2	1	0

2. Calculate three cluster distances between C_1 and C_2.

$$\text{dist}(C_1, C_2) = \min\{d(a,c), d(a,d), d(a,e), d(b,c), d(b,d), d(b,e)\} = \min\{3, 4, 5, 2, 3, 4\} = 2$$

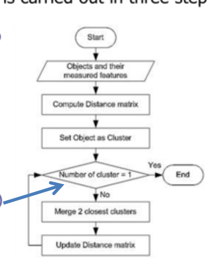
$$\text{dist}(C_1, C_2) = \max\{d(a,c), d(a,d), d(a,e), d(b,c), d(b,d), d(b,e)\} = \max\{3, 4, 5, 2, 3, 4\} = 5$$

$$\text{dist}(C_1, C_2) = \frac{d(a,c) + d(a,d) + d(a,e) + d(b,c) + d(b,d) + d(b,e)}{6} = \frac{3+4+5+2+3+4}{6} = \frac{21}{6} = 3.5$$

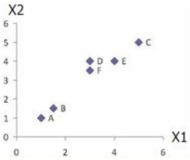
HAC-Algorithm

- The *Agglomerative* algorithm is carried out in three steps:

1) Convert all object features into a distance matrix
2) Set each object as a cluster (thus if we have *N* objects, we will have *N* clusters at the beginning)
3) Repeat until number of cluster is one (or known # of clusters)
   - Merge two closest clusters
   - Update "distance matrix"



Example



	X1	X2
A	1	1
B	1.5	1.5
C	5	5
D	3	4
E	4	4
F	3	3.5

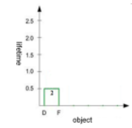
$$d_{AB} = \left((1-1.5)^2 + (1-1.5)^2\right)^{\frac{1}{2}} = \sqrt{\tfrac{1}{2}} = 0.7071$$

$$d_{DF} = \left((3-3)^2 + (4-3.5)^2\right)^{\frac{1}{2}} = 0.5$$

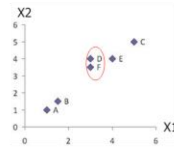
Euclidean distance

Dist	A	B	C	D	E	F
A	0.00	0.71	5.66	3.61	4.24	3.20
B	0.71	0.00	4.95	2.92	3.54	2.50
C	5.66	4.95	0.00	2.24	1.41	2.50
D	3.61	2.92	2.24	0.00	1.00	0.50
E	4.24	3.54	1.41	1.00	0.00	1.12
F	3.20	2.50	2.50	0.50	1.12	0.00

Example



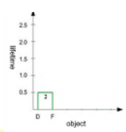
- Merge two closest clusters (iteration 1)



Dist	A	B	C	D	E	F
A	0.00	0.71	5.66	3.61	4.24	3.20
B	0.71	0.00	4.95	2.92	3.54	2.50
C	5.66	4.95	0.00	2.24	1.41	2.50
D	3.61	2.92	2.24	0.00	1.00	0.50
E	4.24	3.54	1.41	1.00	0.00	1.12
F	3.20	2.50	2.50	0.50	1.12	0.00

Dist	A	B	C	D, F	E
A	0.00	0.71	5.66	?	4.24
B	0.71	0.00	4.95	?	3.54
C	5.66	4.95	0.00	?	1.41
D, F	?	?	?	0.00	?
E	4.24	3.54	1.41	?	0.00

Example



Dist	A	B	C	D	E	F
A	0.00	0.71	5.66	3.61	4.24	3.20
B	0.71	0.00	4.95	2.92	3.54	2.50
C	5.66	4.95	0.00	2.24	1.41	2.50
D	3.61	2.92	2.24	0.00	1.00	0.50
E	4.24	3.54	1.41	1.00	0.00	1.12
F	3.20	2.50	2.50	0.50	1.12	0.00

$$d_{(D,F)\to A} = \min(d_{DA}, d_{FA}) = \min(3.61, 3.20) = 3.20$$

$$d_{(D,F)\to B} = \min(d_{DB}, d_{FB}) = \min(2.92, 2.50) = 2.50$$

$$d_{(D,F)\to C} = \min(d_{DC}, d_{FC}) = \min(2.24, 2.50) = 2.24$$

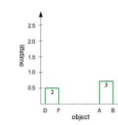
$$d_{E\to(D,F)} = \min(d_{ED}, d_{EF}) = \min(1.00, 1.12) = 1.00$$

Dist	A	B	C	D, F	E
A	0.00	0.71	5.66	?	4.24
B	0.71	0.00	4.95	?	3.54
C	5.66	4.95	0.00	?	1.41
D, F	?	?	?	0.00	?
E	4.24	3.54	1.41	?	0.00

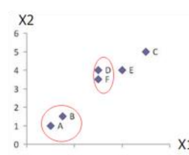
Min Distance (Single Linkage)

Dist	A	B	C	D, F	E
A	0.00	0.71	5.66	3.20	4.24
B	0.71	0.00	4.95	2.50	3.54
C	5.66	4.95	0.00	2.24	1.41
D, F	**3.20**	**2.50**	**2.24**	0.00	1.00
E	4.24	3.54	1.41	**1.00**	0.00

Example



- Merge two closest clusters (iteration 2)

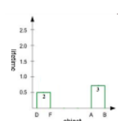


Min Distance (Single Linkage)

Dist	A	B	C	D, F	E
A	0.00	0.71	5.66	3.20	4.24
B	0.71	0.00	4.95	2.50	3.54
C	5.66	4.95	0.00	2.24	1.41
D, F	**3.20**	**2.50**	**2.24**	0.00	1.00
E	4.24	3.54	1.41	**1.00**	0.00

Dist	A,B	C	(D, F)	E
A,B	0	?	?	?
C	?	0	2.24	1.41
(D, F)	?	2.24	0	1.00
E	?	1.41	1.00	0

Example



- Update distance matrix (iteration 2)

Min Distance (Single Linkage)

Dist	A	B	C	D, F	E
A	0.00	0.71	5.66	3.20	4.24
B	0.71	0.00	4.95	2.50	3.54
C	5.66	4.95	0.00	2.24	1.41
D, F	**3.20**	**2.50**	**2.24**	0.00	1.00
E	4.24	3.54	1.41	**1.00**	0.00

$$d_{C\to(A,B)} = \min(d_{CA}, d_{CB}) = \min(5.66, 4.95) = 4.95$$

$$d_{(D,F)\to(A,B)} = \min(d_{DA}, d_{DB}, d_{FA}, d_{FB}) = \min(3.61, 2.92, 3.20, 2.50) = 2.50$$

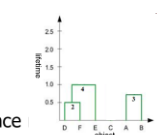
$$d_{E\to(A,B)} = \min(d_{EA}, d_{EB}) = \min(4.24, 3.54) = 3.54$$

Dist	A,B	C	(D, F)	E
A,B	0	?	?	?
C	?	0	2.24	1.41
(D, F)	?	2.24	0	1.00
E	?	1.41	1.00	0

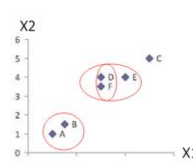
Min Distance (Single Linkage)

Dist	A,B	C	(D, F)	E
A,B	0	4.95	2.50	3.54
C	**4.95**	0	2.24	1.41
(D, F)	**2.50**	2.24	0	1.00
E	**3.54**	1.41	1.00	0

Example



- Merge two closest clusters/update distance (iteration 3)



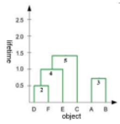
Min Distance (Single Linkage)

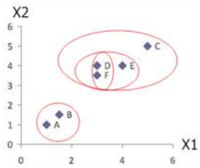
Dist	A,B	C	(D, F)	E
A,B	0	4.95	2.50	3.54
C	**4.95**	0	2.24	1.41
(D, F)	**2.50**	2.24	0	1.00
E	**3.54**	1.41	1.00	0

Min Distance (Single Linkage)

Dist	(A,B)	C	(D, F), E
(A,B)	0.00	4.95	2.50
C	4.95	0.00	1.41
(D, F), E	**2.50**	**1.41**	0.00

Example





Min Distance (Single Linkage)

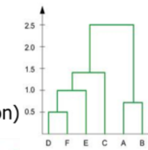
Dist	(A,B)	C	(D, F), E
(A,B)	0.00	4.95	2.50
C	4.95	0.00	1.41
(D, F), E	2.50	1.41	0.00

Min Distance (Single Linkage)

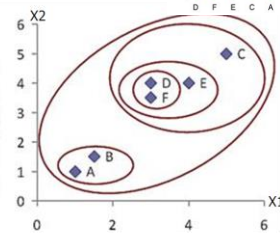
Dist	(A,B)	((D, F), E),C
(A,B)	0.00	2.50
((D, F), E),C	2.50	0.00

Example

- Final result (meeting termination condition)

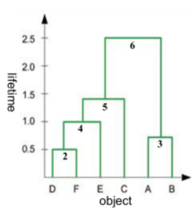


	X1	X2
A	1	1
B	1.5	1.5
C	5	5
D	3	4
E	4	4
F	3	3.5



Lifetime

- Lifetime vs *K*-cluster Lifetime



- **Lifetime**
  The distance between that a cluster is created and that it disappears (merges with other clusters during clustering).
  e.g. lifetime of A, B, C, D, E and F are 0.71, 0.71, 1.41, 0.50, 1.00 and 0.50, respectively, the life time of (A, B) is 2.50 – 0.71 = 1.79, ……
- ***K*-cluster Lifetime**
  The distance from that *K* clusters emerge to that *K* clusters vanish (due to the reduction to *K-1* clusters).
  e.g.
  5-cluster lifetime is 0.71 - 0.50 = 0.21
  4-cluster lifetime is 1.00 – 0.71 = 0.29
  3-cluster lifetime is 1.41 – 1.00 = 0.41
  2-cluster lifetime is 2.50 – 1.41 = 1.09

Conclusion

- How to determine the number of clusters
  - If the number of clusters known, termination condition is given!
  - The *K*-cluster lifetime as the range of threshold value on the dendrogram tree that leads to the identification of *K* clusters
  - Heuristic rule: cut a dendrogram tree with maximum life time to find a "proper" *K*
- Major weakness of agglomerative clustering methods
  - Can never undo what was done previously
  - Sensitive to cluster distance measures and noise/outliers
  - Less efficient: $O(n^2 \log n)$, where n is the number of total objects