



CS 4104 APPLIED MACHINE LEARNING

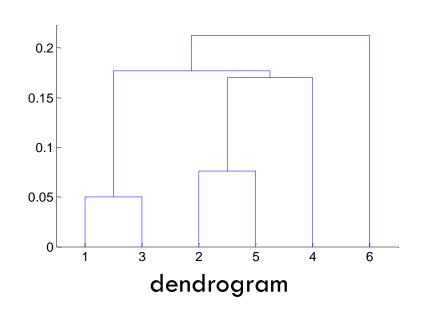
Dr. Hashim Yasin

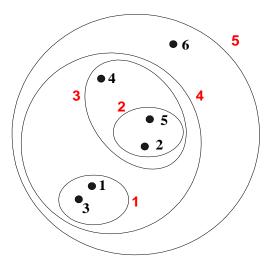
National University of Computer and Emerging Sciences,

Faisalabad, Pakistan.

HIERARCHICAL CLUSTERING

- Produces a set of nested clusters organized as a hierarchical tree
 - Can be visualized as a <u>dendrogram</u>
 - A tree like diagram that records the sequences of merges or splits

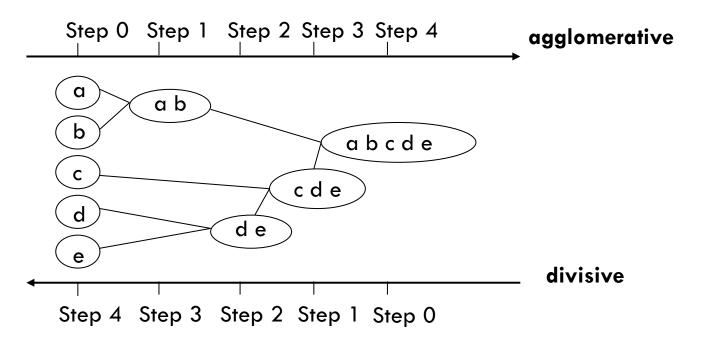




Venn diagram

- Two main types of hierarchical clustering
 - Agglomerative:
 - Start with the points as individual clusters
 - At each step, merge the closest pair of clusters until only one cluster (or k clusters) left
 - **□** Divisive:
 - Start with one, all-inclusive cluster
 - At each step, split a cluster until each cluster contains a point (or there are k clusters)
- Traditional hierarchical algorithms use a similarity or distance matrix
 - Merge or split one cluster at a time

□ Use <u>distance matrix</u> as clustering criteria. This method does not require the number of clusters **k** as an input but needs a termination condition.



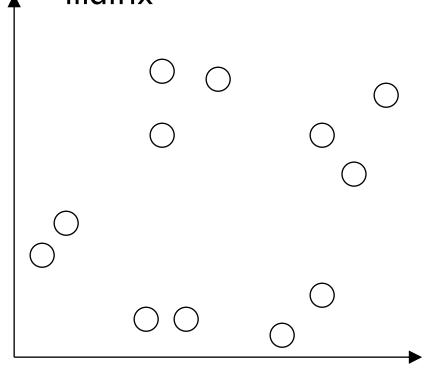
AGGLOMERATIVE HIERARCHICAL CLUSTERING

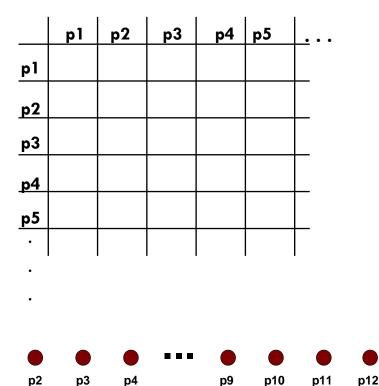
Agglomerative Hierarchical Clustering

- More popular hierarchical clustering technique
- Basic algorithm is straightforward
 - Compute the proximity matrix
 - Let each data point be a cluster
 - 3. Repeat
 - 4. Merge the two closest clusters
 - Update the proximity matrix
 - 6. Until only a single cluster remains
- Key operation is the computation of the proximity of two clusters
 - Different approaches to define the distance between clusters distinguish the different algorithms

Agglomerative Hierarchical Clustering

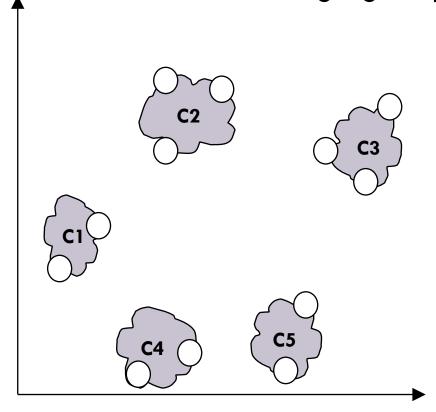
 Start with clusters of individual points and a proximity matrix



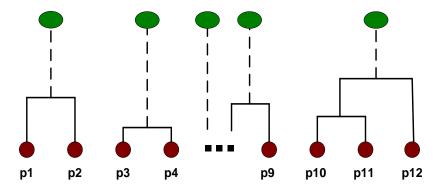


Agglomerative Hierarchical Clustering

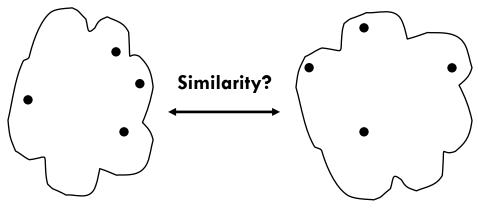
□ After some merging steps, we have some clusters



	C 1	C2	C 3	C4	C 5
C1					
C2					
C 3					
C4					
C 5					

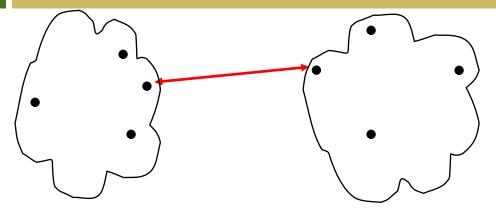


Applied Machine Learning (CS4104)



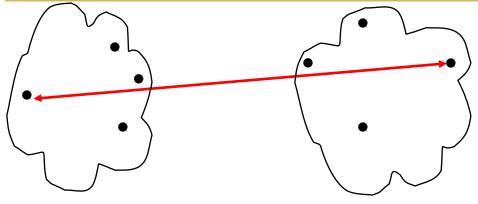
	p1	p2	р3	р4	р5	<u> </u>
рl						
p2						
рЗ						
p4						
р5						

- MIN
- MAX
- Group Average
- Distance Between Centroids
- Other methods driven by an objective function
 - Ward's Method uses squared error



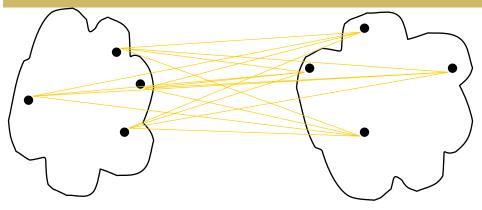
	p1	p2	р3	р4	р5	<u> </u>
p1						
p2						
p3						
p4						
р5						

- MIN
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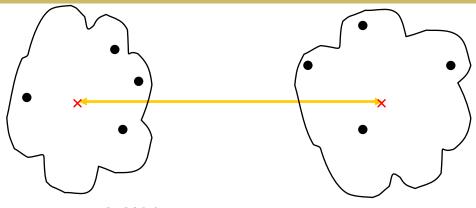
	рl	p2	р3	р4	р5	<u> </u>
pl						
p2						
р3						
p4						
p5						
•						

- MIN
- MAX
- Group Average
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 - Ward's Method uses squared error



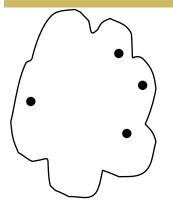
	p1	p2	р3	р4	р5	<u>.</u> .
pl						
p2						
р3						
p4						
p5						
•						

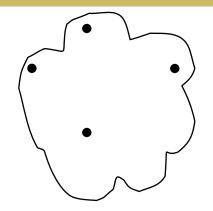
- MIN
- MAX
- Group Average
- Distance Between Centroids
- Other methods driven by an objective function
 - Ward's Method uses squared error



	p1	p2	р3	р4	р5	<u> </u>
pl						
p2						
р3						
p4						
p5						

- MIN
- MAX
- Group Average
- Distance Between Centroids
- Other methods driven by an objective function
 - Ward's Method uses squared error



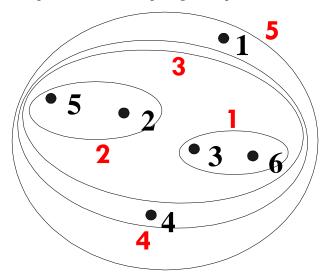


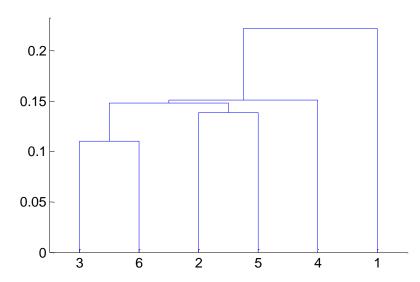
	рl	p2	р3	р4	р5	<u> </u>
рl						
p2						
р3						
p4						
р5						

- MIN
- MAX
- **Group Average**
- **Distance Between Centroids**
- Other methods driven by an objective function
 - Ward's Method uses squared error

MIN or Single Link Linkage

- Similarity of two clusters is based on the two most similar (closest) points in the different clusters
 - Determined by one pair of points, i.e., by one link in the proximity graph.

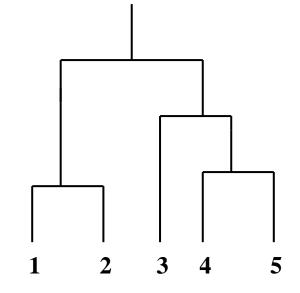




MAX or Complete Linkage

- Similarity of two clusters is based on the two least similar (most distant) points in the different clusters
 - Determined by the all pairs of points in the two clusters

_	I 1	12	13	l 4	1 5
11	0.00	0.90	0.10	0.65	0.20
12	0.90	0.00	0.70	0.60	0.50
13	0.10	0.70	0.00	0.40	0.30
14	0.65	0.60	0.40	0.00	0.80
15	0.20	0.50	0.30	0.80	0.20 0.50 0.30 0.80 0.00



Group Average Linkage

Proximity of two clusters is the average of pairwise proximity
 between points in the two clusters.

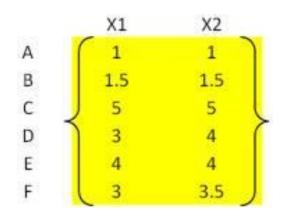
$$proximity(Cluster_{i}, Cluster_{j}) = \frac{\sum_{\substack{p_{i} \in Cluster_{i} \\ p_{j} \in Cluster_{j}}} \sum_{\substack{p_{i} \in Cluster_{j} \\ p_{j} \in Cluster_{j}}} \frac{\sum_{\substack{p_{i} \in Cluster_{i} \\ p_{j} \in Cluster_{i}}} |Cluster_{i}| * |Cluster_{j}|}{|Cluster_{i}|}$$

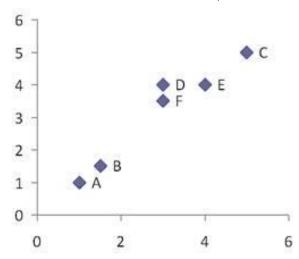
- Need to use average connectivity for scalability since total proximity favors large clusters
- Compromise between Single and Complete Link
- Strengths --- Less susceptible to noise and outliers

- \square All the algorithms are at least $O(n^2)$.
 - n is the number of data points.
- \square Single link can be done in $O(n^2)$.
- □ Complete and average links can be done in $O(n^2 \log n)$.
- Due the complexity, hard to use for large data sets.
 - Sampling may be the solution

SINGLE LINKAGE CLUSTERING EXAMPLE

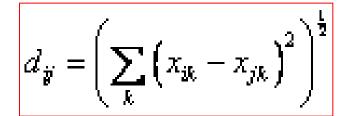
- □ Consider there are 6 objects (A, B, C, D, E, F).
- Our target is to group them into single one cluster at the end of the iteration.
- In each step of iteration, find the closest pair cluster.
- First, we must compute the distance matrix,

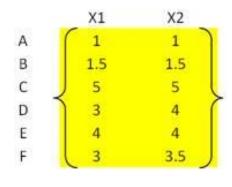


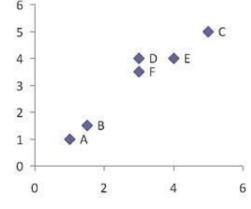


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Applied Machine Learning (CS4104)



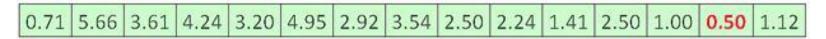




$$d_{AB} = \left(\left(1 - 1.5 \right)^2 + \left(1 - 1.5 \right)^2 \right)^{\frac{1}{2}} = \sqrt{\frac{1}{2}} = 0.7071$$

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





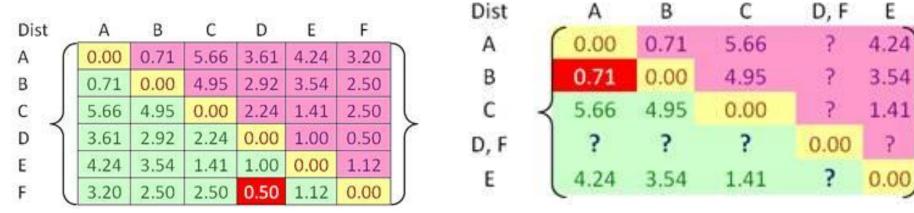
Dist	Α	В	С	D	E	F	299
A	0.00	0.71	5.66	3.61	4.24	3.20	n
В	0.71	0.00	4.95	2.92	3.54	2.50	Ш
c J	5.66	4.95	0.00	2.24	1.41	2.50	
D	3.61	2.92	2.24	0.00	1.00	0.50	1
E	4.24	3.54	1.41	1.00	0.00	1.12	
F	3.20	2.50	2.50	0.50	1.12	0.00	U

 The shortest (min) distance is between pair F and D which is 0.50. Then we update the distance matrix like, Min Distance (Single Linkage)

Dist	Α	В	C	D, F	E	
Α	0.00	0.71	5.66	?	4.24	
В	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	

The distance between cluster {D,F} and other cluster is:

Min Distance (Single Linkage)



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

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

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

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

Min Distance (Single Linkage)

The updated distance matrix would be:

Min Distance (Single Linkage)



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

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

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

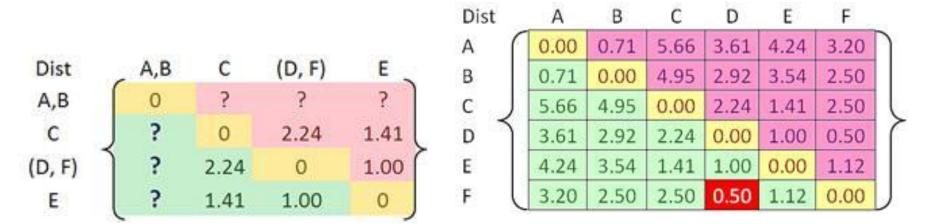
$$d_{E\to(D,F)} = \min (d_{ED}, d_{EF}) = \min (1.00, 1.12) = 1.00$$

The next closest distance is between A and B is 0.71.

Dist 3.20 0.00 0.71 5.66 4.24 0.00 4.95 3.54 5.66 4.95 0.00 2.24 1.41 3.20 2.50 2.24 0.00 1.00 E 4.24 3.54 1.41 1.00 0.00

Applied Machine Learning (CS4104)

The distance between cluster {A,B} and other cluster is:

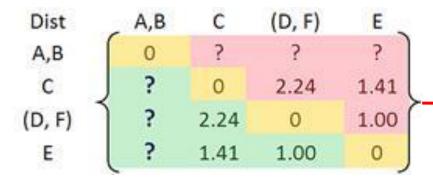


$$d_{C \to (A,B)} = \min (d_{CA}, d_{CB}) = \min (5.66, 4.95) = 4.95$$

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

$$d_{B \to (A,B)} = \min (d_{BA}, d_{BB}) = \min (4.24, 3.54) = 3.54$$

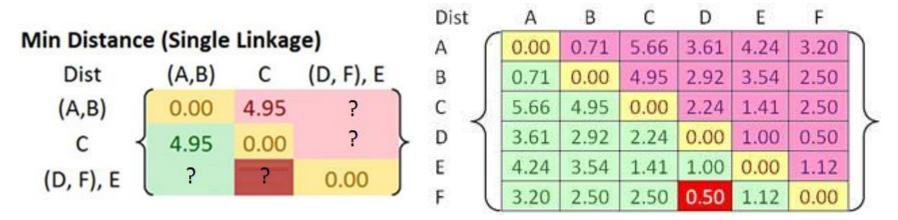
□ The updated distance matrix would be:



The next closest distance is between {D,F} and E which is 1.00.

Min Distance (Single Linkage)

The <u>distance computations</u> would be:

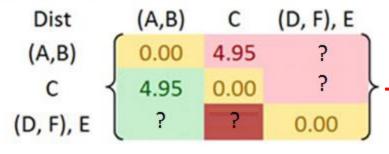


$$d_{((D,F),E) \to (A,E)} = \min \left(d_{DA}, d_{DB}, d_{FA}, d_{FB}, d_{EA}, d_{EB} \right) = \min \left(3.61, 2.92, 3.20, 2.50, 4.24, 3.54 \right) = 2.50$$

$$d_{((D,F),E)\to C} = \min(d_{DC}, d_{FC}, d_{EC}) = \min(2.24, 2.50, 1.41) = 1.41$$

The updated distance matrix would be:

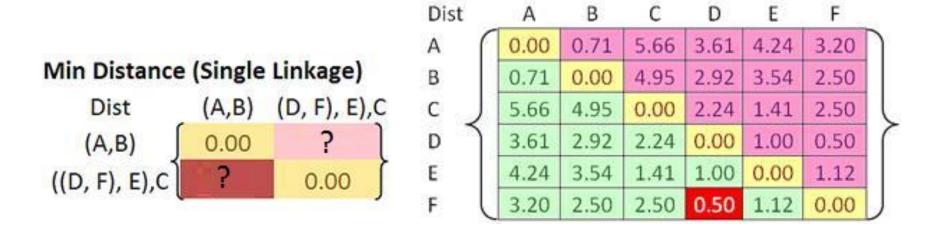
Min Distance (Single Linkage)



The next closest distance is between {(D,F),E} and C.

Min Distance (Single Linkage)

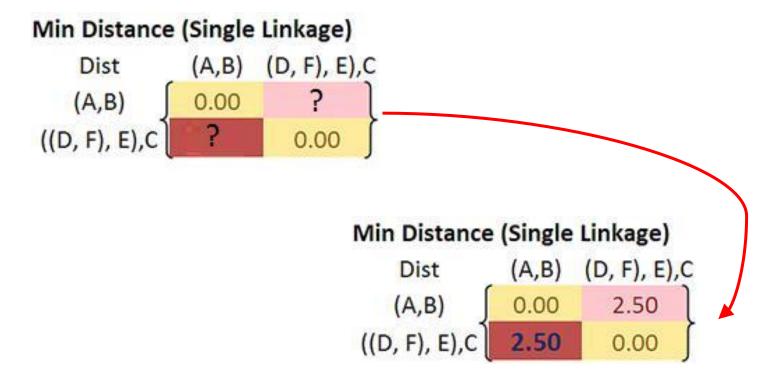
The distance computations would be:



$$d_{(((D,F),E),C) \to (A,B)} = \min \left(d_{DA}, d_{DB}, d_{FA}, d_{FB}, d_{EA}, d_{EB}, d_{CA}, d_{CB} \right)$$

$$d_{(((D,F),E),C)\to(A,B)} = \min (3.61, 2.92, 3.20, 2.50, 4.24, 3.54, 5.66, 4.95) = 2.50$$

□ The updated distance matrix would be:



□ In the beginning we have 6 clusters:

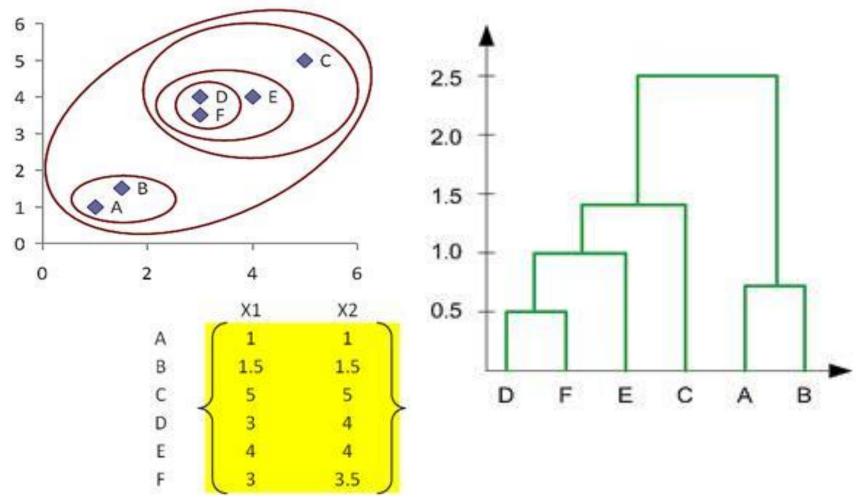
A, B, C, D, E and F

- We merge cluster **D** and **F** into cluster (**D**, **F**) at distance **0.50**
- □ We merge cluster A and cluster B into (A, B) at distance 0.71
- □ We merge cluster E and (D, F) into ((D, F), E) at distance 1.00

We merge cluster ((D, F), E) and C into (((D, F), E),
 C) at distance 1.41

We merge cluster (((D, F), E), C) and (A, B) into ((((D, F), E), C), (A, B)) at distance 2.50

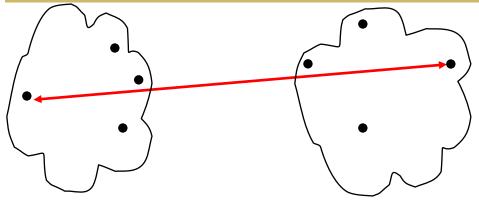
The last cluster contain all the objects, thus conclude the computation.



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COMPLETE LINKAGE CLUSTERING



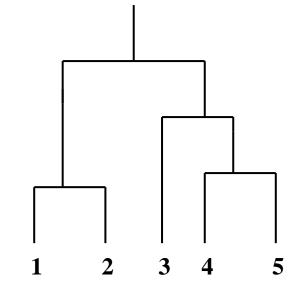
	p1	p2	р3	р4	р5	<u>.</u>
pl						
p2						
р3						
p4						
p5						
•						

- MIN
- MAX
- Group Average
- Distance Between Centroids
- Other methods driven by an objective function
 - Ward's Method uses squared error

MAX or Complete Linkage

- Similarity of two clusters is based on the two least similar (most distant) points in the different clusters
 - Determined by the all pairs of points in the two clusters

_	I 1	12	13	l 4	1 5
11	0.00	0.90	0.10	0.65	0.20
12	0.90	0.00	0.70	0.60	0.50
13	0.10	0.70	0.00	0.40	0.30
14	0.65	0.60	0.40	0.00	0.80
15	0.20	0.50	0.30	0.80	0.20 0.50 0.30 0.80 0.00



- Consider the following data points,
- Assume the Manhattan distance metric

Points	x-coordinate	y-coordinate
P1	3	5
P2	5	6
Р3	1	7
P4	2	2
P5	8	3

Points	x-coordinate	y-coordinate
P1	3	5
P2	5	6
P3	1	7
P4	2	2
P5	8	3

	P1	P2	P3	P4	P5
P1	0	3	4	4	7
P2	3	0	5	7	6
P3	4	5	0	6	11
P4	4	7	6	0	7
P5	7	6	11	7	0

	P1	P2	P3	P4	P5
P1	0	3	4	4	7
P2	3	0	5	7	6
P3	4	5	0	6	11
P4	4	7	6	0	7
P5	7	6	11	7	0

	(P1, P2)	P3	P4	P5
(P1, P2)	0	5	7	7
P3	5	0	6	11
P4	7	6	0	7
P5	7	11	7	0

$$D_{(P1,P2)\to P3} = \max(D_{P1\to P3}, D_{P2\to P3})$$

 $= \max(4,5) = 5$
 $D_{(P1,P2)\to P4} = \max(D_{P1\to P4}, D_{P2\to P4})$
 $= \max(4,7) = 7$
 $D_{(P1,P2)\to P5} = \max(D_{P1\to P5}, D_{P2\to P5})$
 $= \max(7,6) = 7$

	P1	P2	P3	P4	P5
P1	0	3	4	4	7
P2	3	0	5	7	6
P3	4	5	0	6	11
P4	4	7	6	0	7
P5	7	6	11	7	0

	(P1, P2, P3)	P4	P5
(P1, P2, P3)	0	7	11
P4	7	0	7
P5	11	7	0

$$\begin{aligned} D_{(P1,P2,P3)\to P4} &= \max(D_{P1\to P4},D_{P2\to P4},D_{P3\to P4}) \\ &= \max(4,7,6) = 7 \\ D_{(P1,P2,P3)\to P5} &= \max(D_{P1\to P5},D_{P2\to P5},D_{P3\to P5}) \\ &= \max(7,6,11) = 11 \end{aligned}$$

	P1	P2	P3	P4	P5
P1	0	3	4	4	7
P2	3	0	5	7	6
P3	4	5	0	6	11
P4	4	7	6	0	7
P5	7	6	11	7	0

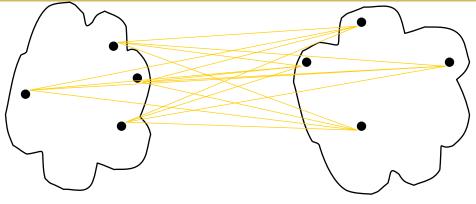
	(P1, P2, P3, P4)	P5
(P1, P2,P3, P4)	0	11
P5	11	0

$$D_{(P1,P2,P3,P4)\to P5} =$$

= max $(D_{P1\to P5}, D_{P2\to P5}, D_{P3\to P5}, D_{P4\to P5})$
= max $(7,6,11,7) = 11$

AVERAGE LINKAGE CLUSTERING EXAMPLE

Inter-Cluster Similarity



	p1	p2	р3	р4	р5	<u>.</u> .
p1						
p2						
рЗ						
p4						
р5						

Proximity Matrix

- MIN
- MAX
- Group Average
- Distance Between Centroids
- Other methods driven by an objective function
 - Ward's Method uses squared error

- Consider the following data points,
- □ Assume the **Manhattan distance** metric

Points	x-coordinate	y-coordinate
P1	3	5
P2	5	6
Р3	1	7
P4	2	2
P5	8	3

Points	x-coordinate	y-coordinate
P1	3	5
P2	5	6
P3	1	7
P4	2	2
P5	8	3

	P1	P2	P3	P4	P5
P1	0	3	4	4	7
P2	3	0	5	7	6
P3	4	5	0	6	11
P4	4	7	6	0	7
P5	7	6	11	7	0

	P1	P2	P3	P4	P5
P1	0	3	4	4	7
P2	3	0	5	7	6
P3	4	5	0	6	11
P4	4	7	6	0	7
P5	7	6	11	7	0

	(P1, P2)	P3	P4	P5
(P1, P2)	0	?	?	?
P3	?	0	6	11
P4	?	6	0	7
P5	?	11	7	0

$$\frac{\sum_{p_i \in Cluster_i} proximity(p_i, p_j)}{p_i \in Cluster_i}$$

$$proximity(Cluster_i, Cluster_j) = \frac{p_i \in Cluster_i}{p_j \in Cluster_j}$$

$$| Cluster_i | * | Cluster_j |$$

	P1	P2	P3	P4	P5
P1	0	3	4	4	7
P2	3	0	5	7	6
P3	4	5	0	6	11
P4	4	7	6	0	7
P5	7	6	11	7	0

	(P1, P2)	P3	P4	P5
(P1, P2)	0	4.5	5.5	6.5
P3	4.5	0	6	11
P4	5.5	6	0	7
P5	6.5	11	7	0

$$D_{(P1,P2)\to P3} = \frac{(D_{P1\to P3} + D_{P2\to P3})}{2 \times 1} = \frac{4+5}{2}$$

$$D_{(P1,P2)\to P4} = \frac{(D_{P1\to P4} + D_{P2\to P4})}{2 \times 1} = \frac{4+7}{2}$$

$$= 5.5$$

$$D_{(P1,P2)\to P5} = \frac{(D_{P1\to P5} + D_{P2\to P5})}{2 \times 1} = \frac{7+6}{2}$$

$$= 6.5$$

	P1	P2	P3	P4	P5
P1	0	3	4	4	7
P2	3	0	5	7	6
P3	4	5	0	6	11
P4	4	7	6	0	7
P5	7	6	11	7	0

	(P1, P2, P3)	P4	P5
(P1, P2, P3)	0	5.7	8
P4	5.7	0	7
P5	8	7	0

$$D_{(P1,P2,P3)\to P4} = \frac{(D_{P1\to P4} + D_{P2\to P4} + D_{P3\to P4})}{3\times1}$$

$$= \frac{4+7+6}{3\times1} = 5.7$$

$$D_{(P1,P2,P3)\to P5} = \frac{(D_{P1\to P5} + D_{P2\to P5} + D_{P3\to P5})}{3\times1}$$

$$= \frac{7+6+11}{3\times1} = 8$$

	P1	P2	P3	P4	P5
P1	0	3	4	4	7
P2	3	0	5	7	6
P3	4	5	0	6	11
P4	4	7	6	0	7
P5	7	6	11	7	0

	(P1, P2, P3, P4)	P5
(P1, P2,P3, P4)	0	7.75
P5	7.75	0

$$D_{(P1,P2,P3,P4)\to P5} = \frac{(D_{P1\to P5} + D_{P2\to P5} + D_{P3\to P5} + D_{P4\to P5})}{4 \times 1}$$

$$= \frac{\frac{7+6+11+7}{4\times 1}}{4\times 1} = \frac{31}{4} = 7.75$$

Group Average Linkage

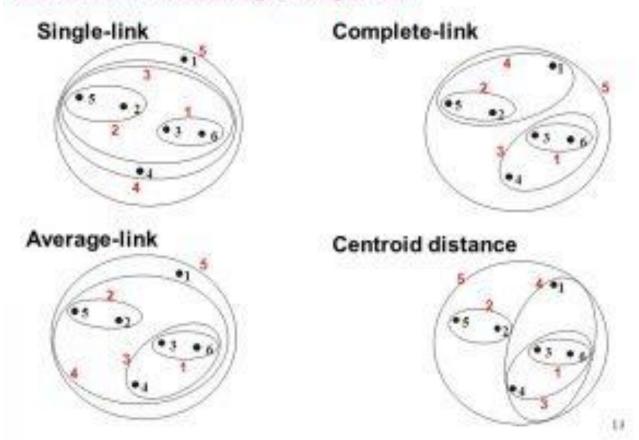
Proximity of two clusters is the average of pairwise proximity
 between points in the two clusters.

$$proximity(Cluster_{i}, Cluster_{j}) = \frac{\sum_{\substack{p_{i} \in Cluster_{i} \\ p_{j} \in Cluster_{j}}} \sum_{\substack{p_{i} \in Cluster_{j} \\ p_{j} \in Cluster_{j}}} \frac{\sum_{\substack{p_{i} \in Cluster_{i} \\ p_{j} \in Cluster_{i}}} |Cluster_{i}| * |Cluster_{i}|}{|Cluster_{i}|}$$

- Need to use average connectivity for scalability since total proximity favors large clusters
- □ Compromise between Single and Complete Link
- Strengths --- Less susceptible to noise and outliers

Comparison

Hierarchical Clustering: Comparison



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