

Broad classification

- There are various types of clustering algorithms and they all use different approaches to cluster.
- Broadly classified in three categories:
 - Partitioning algorithm
 - Hierarchical algorithm
 - Graph based algorithm

Example: Single-linkage algorithm

Question 01: Perform a hierarchical clustering of five samples using the single-linkage algorithm and two features x and y .

	x	y
1	4	4
2	8	4
3	15	8
4	24	4
5	24	12

	1	2	3	4	5
1	—	4.0	11.7	20.0	21.5
2	4.0	—	8.1	16.0	17.9
3	11.7	8.1	—	9.8	9.8
4	20.0	16.0	9.8	—	8.0
5	21.5	17.9	9.8	8.0	—

- Combine 1 and 2 in single cluster

$$\{1, 2\}, \{3\}, \{4\}, \{5\}$$

Complete-linkage algorithm

- The *Complete-linkage algorithm* is obtained by defining the distance between two clusters to be the maximum distance between two points such that one point is in each cluster.
- If C_i and C_j are two clusters then distance between cluster is defined as

$$D_{CL}(C_i, C_j) = \max_{a \in C_i, b \in C_j} d(a, b)$$

where $d(a, b)$ – distance between data sample a and b

Example: Complete-linkage algorithm

Question 02: Perform a hierarchical clustering of five samples using the complete-linkage algorithm and two features x and y .

	x	y
1	4	4
2	8	4
3	15	8
4	24	4
5	24	12

	1	2	3	4	5
1	—	4.0	11.7	20.0	21.5
2	4.0	—	8.1	16.0	17.9
3	11.7	8.1	—	9.8	9.8
4	20.0	16.0	9.8	—	8.0
5	21.5	17.9	9.8	8.0	—

- Combine 1 and 2 in single cluster

$$\{1, 2\}, \{3\}, \{4\}, \{5\}$$

Example: Complete-linkage algorithm

	{1,2}	3	4	5
{1,2}	—	11.7	20.0	21.5
3	11.7	—	9.8	9.8
4	20.0	9.8	—	8.0
5	21.5	9.8	8.0	—

- Minimum value is 8.0 so merge cluster {4} and {5}.

$\{1, 2\}, \{3\}, \{4, 5\}$

Example: Complete-linkage algorithm

	{1,2}	3	{4,5}
{1,2}	—	11.7	21.5
3	11.7	—	9.8
{4,5}	21.5	9.8	—

- Minimum value is 9.8 so merge cluster {4,5} and {3}.

{1,2}, {3,4,5}

- In next step will merge the two remaining clusters.

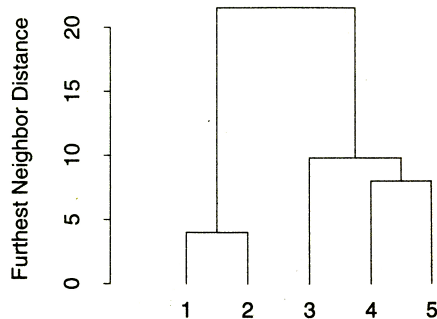


Figure: Dendrogram of Hierarchical clustering using complete-linkage algorithm

Average-linkage algorithm

- The *Average-linkage algorithm* is obtained by taking the average distance of all possible pair of clusters such that one point is in each cluster.
- If C_i and C_j are two clusters then distance between cluster is defined as

$$D_{AL}(C_i, C_j) = \text{avg}_{a \in C_i, b \in C_j} d(a, b)$$

where $d(a, b)$ – distance between data sample a and b

Example: Average-linkage algorithm

Question 03: Perform a hierarchical clustering of five samples using the average-linkage algorithm and two features x and y .

	x	y
1	4	4
2	8	4
3	15	8
4	24	4
5	24	12

	1	2	3	4	5
1	—	4.0	11.7	20.0	21.5
2	4.0	—	8.1	16.0	17.9
3	11.7	8.1	—	9.8	9.8
4	20.0	16.0	9.8	—	8.0
5	21.5	17.9	9.8	8.0	—

- Combine 1 and 2 in single cluster

$$\{1, 2\}, \{3\}, \{4\}, \{5\}$$

Example: Average-linkage algorithm

	{1,2}	3	4	5
{1,2}	—	9.9	18.0	19.7
3	9.9	—	9.8	9.8
4	18	9.8	—	8.0
5	19.7	9.8	8.0	—

- Minimum value is 8.0 so merge cluster {4} and {5}.

{1, 2}, {3}, {4, 5}

Example: Average-linkage algorithm

	{1,2}	3	{4,5}
{1,2}	—	9.9	18.9
3	9.9	—	9.8
{4,5}	18.9	9.8	—

- Minimum value is 9.8 so merge cluster {4,5} and {3}.

{1,2}, {3,4,5}

- In next step will merge the two remaining clusters.

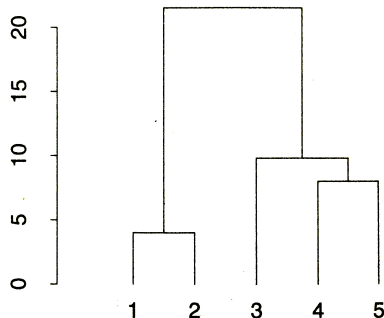


Figure: Dendrogram of Hierarchical clustering using average-linkage algorithm

Ward's Algorithm

- The hierarchical clustering based on variance.
- also called minimum-variance method
- Consider C_j class has k no. of feature vectors x_1, x_2, \dots, x_k
- Error within j^{th} cluster

$$E_j = \sum_{i=1}^k \|x_i - \mu\|^2 = k\sigma^2$$

we need to minimize the variance

- Total error

$$E = \sum_{j=1}^c E_j$$

- Computationally expensive because need to check all combination of samples.

Example: Ward's algorithm

Question: Perform Ward's algorithm to cluster the following data samples.

	x	y
1	4	4
2	8	4
3	15	8
4	24	4
5	24	12

Clusters	Squared Error, E
$\{1,2\},\{3\},\{4\},\{5\}$	8.0
$\{1,3\},\{2\},\{4\},\{5\}$	68.5
$\{1,4\},\{2\},\{3\},\{5\}$	200.0
$\{1,5\},\{2\},\{3\},\{4\}$	232.0
$\{2,3\},\{1\},\{4\},\{5\}$	32.5
$\{2,4\},\{1\},\{3\},\{5\}$	128.0
$\{2,5\},\{1\},\{3\},\{4\}$	160.0
$\{3,4\},\{1\},\{2\},\{5\}$	48.5
$\{3,5\},\{1\},\{2\},\{4\}$	48.5
$\{4,5\},\{1\},\{2\},\{3\}$	32.0

- Minimum Squared Error is 8.0 so form the cluster $\{1, 2\}, \{3\}, \{4\}, \{5\}$

Example: Ward's algorithm

Clusters	Squared Error, E
$\{1,2,3\},\{4\},\{5\}$	72.7
$\{1,2,4\},\{3\},\{5\}$	224.0
$\{1,2,5\},\{3\},\{4\}$	266.7
$\{1,2\},\{3,4\},\{5\}$	56.5
$\{1,2\},\{3,5\},\{4\}$	56.5
$\{1,2\},\{4,5\},\{3\}$	40.0

- Minimum Squared Error is 40.0 so form the cluster $\{1, 2\}, \{3\}, \{4, 5\}$

Example: Ward's algorithm

Clusters	Squared Error, E
$\{1,2,3\}, \{4,5\}$	104.7
$\{1,2,4,5\}, \{3\}$	380.0
$\{1,2\}, \{3,4,5\}$	94.0

- Minimum value is 94.0 so form the cluster $\{1, 2\}, \{3, 4, 5\}$
- In next step will merge the two remaining clusters.

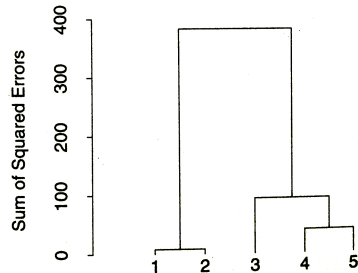
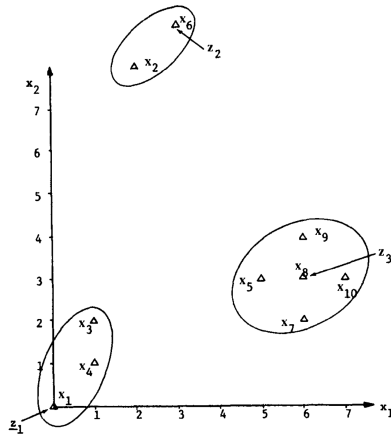


Figure: Dendrogram of Ward's algorithm

Batchelor and Wilkins' Algorithm

- Heuristic procedure for clustering also called *maximum distance algorithm*



Example: Batchelor and Wilkins' Algorithm

Question:

Perform the Batchelor and Wilkins' algorithm to cluster the following data samples.

Distance matrix

	A	B	C	D	E	F	G	H	I	J	K
$A \rightarrow (1, 1)$	0.0	1.0	2.2	2.8	7.0	7.8	7.8	8.5	6.0	7.0	8.0
$B \rightarrow (1, 2)$		0.0	2.0	2.2	6.4	7.0	7.0	7.8	6.0	7.0	8.1
$C \rightarrow (3, 2)$			0.0	1.0	5.0	4.9	5.6	6.4	4.1	5.0	6.1
$D \rightarrow (3, 3)$				0.0	4.2	5.0	5.0	5.6	4.5	5.1	6.3
$E \rightarrow (6, 6)$					0.0	1.0	1.0	1.4	5.1	4.5	5.8
$F \rightarrow (6, 7)$						0.0	1.4	1.0	6.1	5.4	6.7
$G \rightarrow (7, 6)$							0.0	1.0	5.0	4.1	5.4
$H \rightarrow (7, 6)$								0.0	6.0	5.1	6.3
$I \rightarrow (7, 1)$									0.0	1.4	2.0
$J \rightarrow (8, 2)$										0.0	1.4
$K \rightarrow (9, 1)$											0.0

Batchelor and Wilkins' Algorithm

Solution

	A	B	C	D	E	F	G	H	I	J	K
A	0.0	1.0	2.2	2.8	7.0	7.8	7.8	8.5	6.0	7.0	8.0
B		0.0	2.0	2.2	6.4	7.0	7.0	7.8	6.0	7.0	8.1
C			0.0	1.0	5.0	4.9	5.6	6.4	4.1	5.0	6.1
D				0.0	4.2	5.0	5.0	5.6	4.5	5.1	6.3
E					0.0	1.0	1.0	1.4	5.1	4.5	5.8
F						0.0	1.4	1.0	6.1	5.4	6.7
G							0.0	1.0	5.0	4.1	5.4
H								0.0	6.0	5.1	6.3
I									0.0	1.4	2.0
J										0.0	1.4
K											0.0

Batchelor and Wilkins' Algorithm

Solution

	A	B	C	D	E	F	G	H	I	J	K
A	0.0	1.0	2.2	2.8	7.0	7.8	7.8	8.5	6.0	7.0	8.0
B		0.0	2.0	2.2	6.4	7.0	7.0	7.8	6.0	7.0	8.1
C			0.0	1.0	5.0	4.9	5.6	6.4	4.1	5.0	6.1
D				0.0	4.2	5.0	5.0	5.6	4.5	5.1	6.3
E					0.0	1.0	1.0	1.4	5.1	4.5	5.8
F						0.0	1.4	1.0	6.1	5.4	6.7
G							0.0	1.0	5.0	4.1	5.4
H								0.0	6.0	5.1	6.3
I									0.0	1.4	2.0
J										0.0	1.4
K											0.0

