

ST3011 ASSIGNMENT

Q1. Single linkage between two clusters A and B defined as

$$d(A, B) = \min_{x \in A, y \in B} d(x, y)$$

$$d(A, B) \geq 0$$

$$d(A, B) = \min |B - a| = |B - A| = d(A, B) \geq 0$$

If the two points are not the same the value will be ≥ 0 .
 If points are the same, $d(A, B) = 0$.

$$d(A, B) = 0 \Leftrightarrow A = B$$

If $A = B$ then A and B are on the same point.

$$\text{So } d(A, B) = d(A, A) = d(B, B) = |A - A| = |B - B| = |0| = 0$$

$$d(A, B) = d(B, A)$$

$$d(A, B) = |B - A|$$

$$d(B, A) = |A - B|$$

These values are equal \rightarrow property satisfied

For any other cluster $C = \{z_1, \dots, z_m\}$ $d(A, C) \leq d(A, B) + d(B, C)$

Three examples.

1.

A

C

$$\text{Clearly } d(A, C) \leq d(A, B) + d(B, C)$$

2.

A

B

C

Again, ^{shortest} distance from A to C is equal to shortest distance from A to B added to shortest distance from B to C.

3.

A, B, C

All (A, B, C) all the same point. All shortest distances are zero. Equality holds
 $0 \leq 0 + 0$

Q2 Euclidean Dissimilarity and Average Linkage

$$E.O. = \sqrt{(y_2 - y_1)^2 + (x_2 - x_1)^2} \quad A.L. = \frac{1}{\sum_{x \in A} \sum_{y \in B} d(x, y)}$$

$$d(A, A) = d \left\{ \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ 2 \end{pmatrix} \right\}$$

$$\sqrt{(1-1)^2 + (2-1)^2} = \sqrt{1} \quad A.L. = \frac{\sqrt{1} + 0 + 0}{(2)(2)} = \frac{1}{4}$$

$$\sqrt{(1-1)^2 + (1-1)^2} = \sqrt{0} = 0$$

$$\sqrt{(2-2)^2 + (1-1)^2} = \sqrt{0} = 0$$

$$d(B, B) = d \left\{ \begin{pmatrix} 2 \\ 3 \end{pmatrix}, \begin{pmatrix} 2 \\ 3 \end{pmatrix}, \begin{pmatrix} 3 \\ 4 \end{pmatrix} \right\}$$

$$\sqrt{(4-3)^2 + (3-2)^2} = \sqrt{2}$$

$$\sqrt{(3-3)^2 + (2-2)^2} = \sqrt{0} = 0$$

$$\sqrt{(4-4)^2 + (4-4)^2} = \sqrt{0} = 0$$

$$A.L. = \frac{\sqrt{2} + 0 + 0}{(2)(2)} = \frac{\sqrt{2}}{4}$$

$$d(C, C) = d \left\{ \begin{pmatrix} 4 \\ 5 \end{pmatrix}, \begin{pmatrix} 5 \\ 6 \end{pmatrix}, \begin{pmatrix} 2 \\ 2 \end{pmatrix}, \begin{pmatrix} 4 \\ 6 \end{pmatrix}, \begin{pmatrix} 4 \\ 5 \end{pmatrix}, \begin{pmatrix} 6 \\ 2 \end{pmatrix} \right\}$$

$$\sqrt{(5-5)^2 + (4-4)^2} = \sqrt{0} = 0$$

$$\sqrt{(6-6)^2 + (5-5)^2} = \sqrt{0} = 0$$

$$\sqrt{(2-2)^2 + (1-1)^2} = \sqrt{0} = 0$$

$$\sqrt{(6-5)^2 + (5-4)^2} = \sqrt{2}$$

$$\sqrt{(2-5)^2 + (1-4)^2} = \sqrt{18}$$

$$\sqrt{(2-6)^2 + (1-5)^2} = \sqrt{32}$$

$$A.L. = \frac{0 + 0 + 0 + \sqrt{2} + \sqrt{18} + \sqrt{32}}{(3)(3)} = \frac{4 + 4\sqrt{2}}{9}$$

$$= \frac{8\sqrt{2}}{9} = 1.257$$

$$d(A, B) = d \left\{ \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ 2 \end{pmatrix}, \begin{pmatrix} 2 \\ 3 \end{pmatrix}, \begin{pmatrix} 1 \\ 3 \end{pmatrix}, \begin{pmatrix} 2 \\ 4 \end{pmatrix} \right\}$$

$$\sqrt{(3-1)^2 + (2-1)^2} = \sqrt{5}$$

$$\sqrt{(4-1)^2 + (3-1)^2} = \sqrt{13}$$

$$\sqrt{(3-2)^2 + (2-1)^2} = \sqrt{2}$$

$$\sqrt{(4-2)^2 + (3-1)^2} = \sqrt{8}$$

$$A.L. = \frac{\sqrt{5} + \sqrt{13} + \sqrt{2} + \sqrt{8}}{(2)(2)} = 2.52$$

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cont..

$$d(A,C) = d \left\{ \begin{pmatrix} 1 \\ 1 \end{pmatrix} \begin{pmatrix} 4 \\ 4 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \begin{pmatrix} 6 \\ 6 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \begin{pmatrix} 2 \\ 2 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \begin{pmatrix} 2 \\ 2 \end{pmatrix} \right\}$$

$$\sqrt{(5-1)^2 + (4-1)^2} = \sqrt{25} = 5$$

$$\sqrt{(6-1)^2 + (5-1)^2} = \sqrt{41}$$

$$\sqrt{(2-1)^2 + (1-1)^2} = \sqrt{1} = 1$$

$$\sqrt{(5-2)^2 + (4-1)^2} = \sqrt{18}$$

$$\sqrt{(6-2)^2 + (5-1)^2} = \sqrt{32}$$

$$\sqrt{(2-2)^2 + (1-1)^2} = \sqrt{0} = 0$$

$$A.L = (2)(3)$$

$$5 + \sqrt{41} + 1 + \sqrt{18} + \sqrt{32} + 0 = 3.717$$

$$d(B,C) = d \left\{ \begin{pmatrix} 2 \\ 3 \end{pmatrix} \begin{pmatrix} 4 \\ 5 \end{pmatrix} \begin{pmatrix} 2 \\ 3 \end{pmatrix} \begin{pmatrix} 6 \\ 6 \end{pmatrix} \begin{pmatrix} 2 \\ 3 \end{pmatrix} \begin{pmatrix} 4 \\ 5 \end{pmatrix} \begin{pmatrix} 3 \\ 4 \end{pmatrix} \begin{pmatrix} 6 \\ 6 \end{pmatrix} \begin{pmatrix} 3 \\ 4 \end{pmatrix} \begin{pmatrix} 2 \\ 3 \end{pmatrix} \right\}$$

$$\sqrt{(5-3)^2 + (4-2)^2} = \sqrt{8}$$

$$\sqrt{(6-3)^2 + (5-2)^2} = \sqrt{18}$$

$$\sqrt{(2-3)^2 + (1-2)^2} = \sqrt{2}$$

$$\sqrt{(5-4)^2 + (4-3)^2} = \sqrt{2}$$

$$\sqrt{(6-4)^2 + (5-3)^2} = \sqrt{8}$$

$$\sqrt{(2-4)^2 + (1-3)^2} = \sqrt{8}$$

$$\sqrt{8} + \sqrt{18} + \sqrt{2} + \sqrt{2} + \sqrt{8} + \sqrt{8} = \frac{11\sqrt{2}}{6} = 2.59$$

$$A.L = (2)(3)$$

Resulting Dissimilarity matrix

	A	B	C
A	0.25	2.52	3.717
B	2.52	0.35	2.59
C	3.717	2.59	1.257

Q3 Rand Index =
$$\frac{\binom{n}{2} + 2 \sum_{i=1}^{C_1} \sum_{j=1}^{C_2} \binom{n_{ij}}{2} - \left[\sum_{i=1}^{C_1} \binom{n_{i.}}{2} + \sum_{j=1}^{C_2} \binom{n_{.j}}{2} \right]}{\binom{n}{2}}$$

		Cluster A		
		Group 1	Group 2	
Cluster B	Group 1	25	3	28
	Group 2	4	36	40
	Group 3	6	7	13
		35	46	81

$$\frac{\binom{81}{2} + 2 \left[\binom{25}{2} \binom{3}{2} \binom{4}{2} \binom{36}{2} \binom{6}{2} \binom{7}{2} \right] - \left[\binom{28}{2} \binom{40}{2} \binom{13}{2} \binom{35}{2} \binom{46}{2} \right]}{\binom{81}{2}}$$

~~3240 + 2[300 + 3 + 6 + 630 + 15 + 21]~~

~~3240 + 2[300 + 3 + 6 + 630 + 15 + 21]~~

$$\frac{3240 + 2[300 + 3 + 6 + 630 + 15 + 21]}{3240} - \frac{[378 + 780 + 78 + 595 + 1035]}{3240}$$

$$\frac{3240 + 1950 - 2866}{3240} = \frac{2324}{3240} = 0.71728$$

Rand Index = 0.71728

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Q2 Euclidean Dissimilarity and Average Linkage

$$ED = \sqrt{(y_2 - y_1)^2 + (x_2 - x_1)^2}$$

$$A.L = \frac{1}{n(n-1)} \sum_{x \in X} \sum_{y \in X} d(x, y)$$

$$d(A, A) = d \left\{ (1|1), (1|2), (2|1), (2|2) \right\}$$

$$\sqrt{(1-1)^2 + (1-1)^2} = \sqrt{0} = 0$$

$$\sqrt{(1-1)^2 + (2-1)^2} = \sqrt{1} = 1$$

$$\sqrt{(1-2)^2 + (1-1)^2} = \sqrt{1} = 1$$

$$\sqrt{(2-2)^2 + (1-1)^2} = \sqrt{0} = 0$$

$$A.L = \frac{0+1+1+0}{4} = \frac{2}{4} = \frac{1}{2}$$

$$d(B, B) = d \left\{ (3|3), (3|4), (4|3), (4|4) \right\}$$

$$\sqrt{(3-3)^2 + (3-3)^2} = \sqrt{0} = 0$$

$$\sqrt{(4-3)^2 + (3-3)^2} = \sqrt{1} = 1$$

$$\sqrt{(3-4)^2 + (3-3)^2} = \sqrt{1} = 1$$

$$\sqrt{(4-4)^2 + (3-3)^2} = \sqrt{0} = 0$$

$$A.L = \frac{0+\sqrt{2}+\sqrt{2}+0}{(2)(2)} = \frac{\sqrt{2}}{2} = 0.71$$

$$d(C, C) = d \left\{ (4|4), (4|5), (5|4), (5|5), (6|6), (6|7), (7|6), (7|7), (8|8), (8|9), (9|8), (9|9) \right\}$$

$$\sqrt{(5-4)^2 + (4-4)^2} = \sqrt{1} = 1$$

$$\sqrt{(6-4)^2 + (4-4)^2} = \sqrt{4} = 2$$

$$\sqrt{(7-4)^2 + (4-4)^2} = \sqrt{9} = 3$$

$$\sqrt{(8-4)^2 + (4-4)^2} = \sqrt{16} = 4$$

$$\sqrt{(9-4)^2 + (4-4)^2} = \sqrt{25} = 5$$

$$\sqrt{(6-5)^2 + (5-5)^2} = \sqrt{1} = 1$$

$$\sqrt{(7-5)^2 + (5-5)^2} = \sqrt{4} = 2$$

$$\sqrt{(8-5)^2 + (5-5)^2} = \sqrt{9} = 3$$

$$\sqrt{(9-5)^2 + (5-5)^2} = \sqrt{16} = 4$$

$$\sqrt{(6-6)^2 + (6-6)^2} = \sqrt{0} = 0$$

$$\sqrt{(7-6)^2 + (6-6)^2} = \sqrt{1} = 1$$

$$\sqrt{(8-6)^2 + (6-6)^2} = \sqrt{4} = 2$$

$$\sqrt{(9-6)^2 + (6-6)^2} = \sqrt{9} = 3$$

$$\sqrt{(7-7)^2 + (7-7)^2} = \sqrt{0} = 0$$

$$\sqrt{(8-7)^2 + (7-7)^2} = \sqrt{1} = 1$$

$$\sqrt{(9-7)^2 + (7-7)^2} = \sqrt{4} = 2$$

$$\sqrt{(8-8)^2 + (8-8)^2} = \sqrt{0} = 0$$

$$\sqrt{(9-8)^2 + (8-8)^2} = \sqrt{1} = 1$$

$$\sqrt{(9-9)^2 + (9-9)^2} = \sqrt{0} = 0$$

$$A.L = \frac{0+\sqrt{2}+\sqrt{18}+\sqrt{2}+0+\sqrt{32}+\sqrt{18}+\sqrt{32}+0}{(3)(3)} = \frac{16\sqrt{2}}{9} = 2.51$$

$$d(A, B) = d \left\{ (1|3), (1|4), (2|3), (2|4) \right\}$$

$$\sqrt{(3-1)^2 + (2-1)^2} = \sqrt{5}$$

$$\sqrt{(4-1)^2 + (2-1)^2} = \sqrt{13}$$

$$\sqrt{(3-2)^2 + (2-1)^2} = \sqrt{2}$$

$$\sqrt{(4-2)^2 + (2-1)^2} = \sqrt{8}$$

$$A.L = \frac{\sqrt{5} + \sqrt{13} + \sqrt{2} + \sqrt{8}}{(2)(2)} = 2.52$$

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Q2 cont.

$$d(A,C) = d \left\{ (1|1/5), (1|1/8), (1|1/2), (2|1/5), (2|1/6), (2|1/2) \right\}$$

$$\sqrt{(5-1)^2 + (4-1)^2} = \sqrt{20} = 5$$

$$\sqrt{(6-1)^2 + (5-1)^2} = \sqrt{41} \approx 6.4$$

$$\sqrt{(2-1)^2 + (1-1)^2} = \sqrt{1} = 1$$

$$\sqrt{(5-2)^2 + (4-1)^2} = \sqrt{18} \approx 4.2$$

$$\sqrt{(6-2)^2 + (5-1)^2} = \sqrt{32} \approx 5.7$$

$$\sqrt{(2-2)^2 + (1-1)^2} = \sqrt{0} = 0$$

$$A.L. = \frac{5 + \sqrt{41} + 1 + \sqrt{18} + \sqrt{32} + 0}{(2)(3)} = 3.717$$

$$d(B,C) = d \left\{ (2|1/5), (2|1/8), (2|1/2), (3|1/5), (4|1/8), (4|1/2) \right\}$$

$$\sqrt{(5-3)^2 + (4-2)^2} = \sqrt{8} \approx 2.8$$

$$\sqrt{(6-3)^2 + (5-2)^2} = \sqrt{18} \approx 4.2$$

$$\sqrt{(2-3)^2 + (1-2)^2} = \sqrt{2} \approx 1.4$$

$$\sqrt{(5-4)^2 + (4-3)^2} = \sqrt{2} \approx 1.4$$

$$\sqrt{(6-4)^2 + (5-3)^2} = \sqrt{8} \approx 2.8$$

$$\sqrt{(2-4)^2 + (1-3)^2} = \sqrt{8} \approx 2.8$$

$$A.L. = \frac{\sqrt{8} + \sqrt{18} + \sqrt{2} + \sqrt{2} + \sqrt{8} + \sqrt{8}}{(2)(3)} = \frac{11\sqrt{2}}{6} \approx 2.59$$

Resulting Dissimilarity Matrix:

	A	(B,C)	C
A	0.5	2.52	3.717
B	2.52	0.71	2.59
C	3.717	2.59	2.51

Single Linkage

$$d(A, B) = \min_{x \in A, y \in B} d(x, y)$$

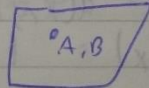
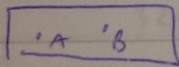
total shortest distance

- In beginning each element is in cluster of its own
- Clusters are then sequentially combined into larger clusters until all elements end up being in the same cluster
- At each step, the two clusters separated by the shortest distance are combined

$$d(A, B) \geq 0$$

A and B are any two points. Then distance will always be ≥ 0 as shown in graph

if $A=B$ distance $= 0$



Satisfies properties

$$d(A, B) = 0 \text{ if and only if } x=y$$

If $x \neq y$ then distance will be > 0 , that is, the distance of 0, A and B must be at the same point

$$d(x, y) = d(y, x)$$

This will always be the case with single linkage, as distance will not change depending on which point comes first/second

12/12/14 Assignment Correction

$$1. d(A, B) = \min_{x \in A, y \in B} (d(x, y)) \leftarrow \text{minimum of non negative} \Rightarrow \text{so non negative itself.}$$

$$d(x, y) \geq 0$$

$$A = \{(0), (1)\} \neq B = \{(8), (1)\}$$

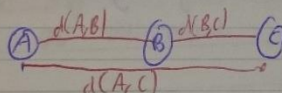
$$\text{But } d(A, B) = d(\{(8), (8)\}) = 0$$

$x=y$ part of property is NOT true

$$i. d(A, B) = d(x, y) = d(y, x) = \min_{x \in A, y \in B} (d(y, x)) = d(B, A)$$

ii. Third property is false for single links

Counter example



$$d(A, C) \geq d(A, B) + d(B, C)$$

$$2. d(A, A) \quad A = \{(1), (1)\}$$

$$\frac{d(\{(1), (1)\}) + d(\{(1), (1)\}) + d(\{(1), (1)\}) + d(\{(1), (1)\})}{4} = \frac{2}{4}$$

$$D(A, B) \quad A = \{(1), (1)\} \\ B = \{(3), (4)\}$$

$$\frac{d(\{(1), (3)\}) + d(\{(1), (4)\}) + d(\{(1), (3)\}) + d(\{(1), (4)\})}{4} = \frac{\sqrt{5} + \sqrt{13} + \sqrt{2} + \sqrt{8}}{4}$$

$$d(B, B) = \frac{2\sqrt{2}}{4}$$

$$d(C, C) = \frac{(2\sqrt{2} + 2\sqrt{18} + 2\sqrt{32})}{9}$$

$$d(A, C) = d(C, A) = \frac{(\sqrt{25} + \sqrt{41} + 1 + \sqrt{18} + \sqrt{32})}{6}$$

$$d(B, C) = d(C, B) = \frac{(\sqrt{8} + \sqrt{18} + \sqrt{2} + \sqrt{8} + \sqrt{2} + \sqrt{2})}{6}$$

2

$$3. \frac{\binom{81}{2} + 2 \left[\binom{23}{2} + \binom{4}{2} + \binom{6}{2} + \binom{3}{2} + \binom{6}{2} + \binom{7}{2} \right] - \left[\binom{33}{2} + \binom{40}{2} + \binom{28}{2} + \binom{40}{2} + \binom{13}{2} \right]}{\binom{81}{2}} \approx 0.72$$

- 4
 - 1m Follow report guideline
 - 1m Standardise the data
 - 1m Was a PCA performed?
 - 1.5m First PC interpreted
 - 1.5m Second PC interpreted
 - 1 How many PC's to include
 - 1.5 Compare results with non standardised data
 - 1 Was clustering performed?
 - 1.5 Choice of dissimilarity / effect of dissimilarity
 - 1.5 Choice / effect of linkage, after conclusion
 - 1 How many clusters should be used?
 - 1.5 For chosen clusters, what are they like? What makes it different?
 - 3 Consider cluster analysis on the lower dimensional PCA results
 - 1 Looking at Rand Index
 - 1 Relating back to motivating story