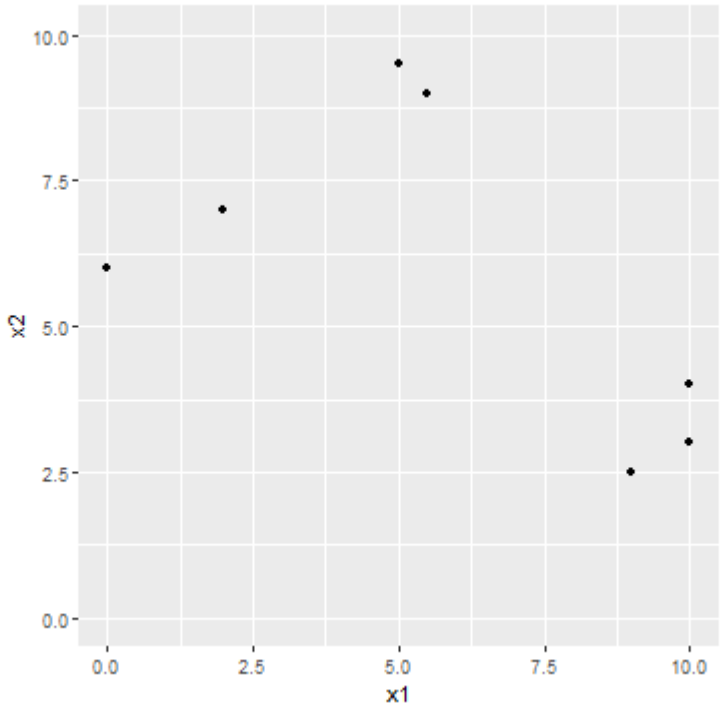
Hierarchical Clustering

Son Nguyen

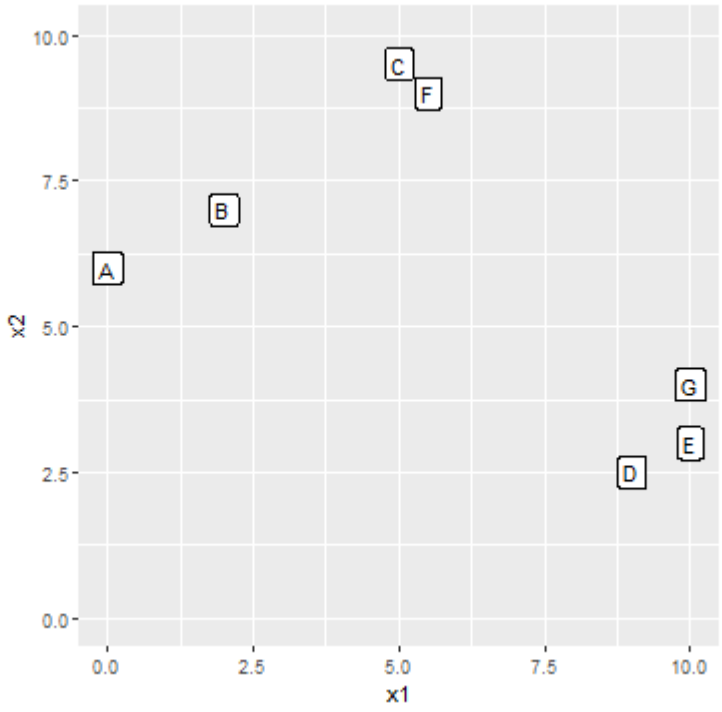
Hierarchical clustering - Centroid Linkage

cluster	x1	x2
A	0.0	6.0
B	2.0	7.0
C	5.0	9.5
D	9.0	2.5
E	10.0	3.0
F	5.5	9.0
G	10.0	4.0

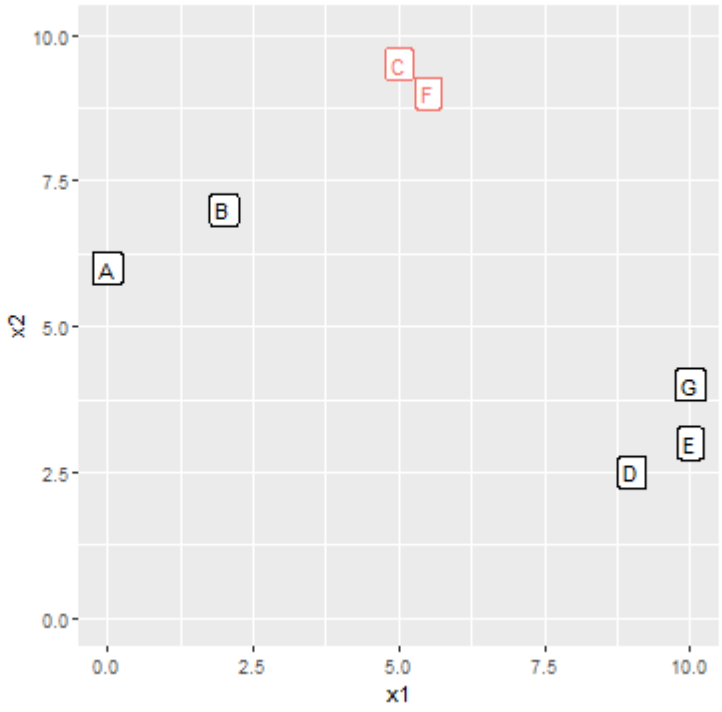
Hierarchical clustering - Centroid Linkage



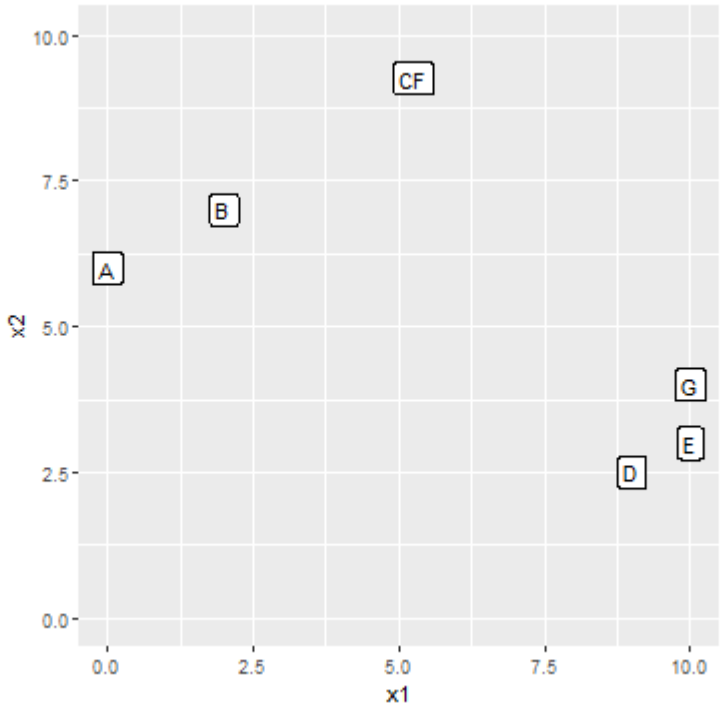
Label the Points



Pair with the smallest distance.



Group the pair



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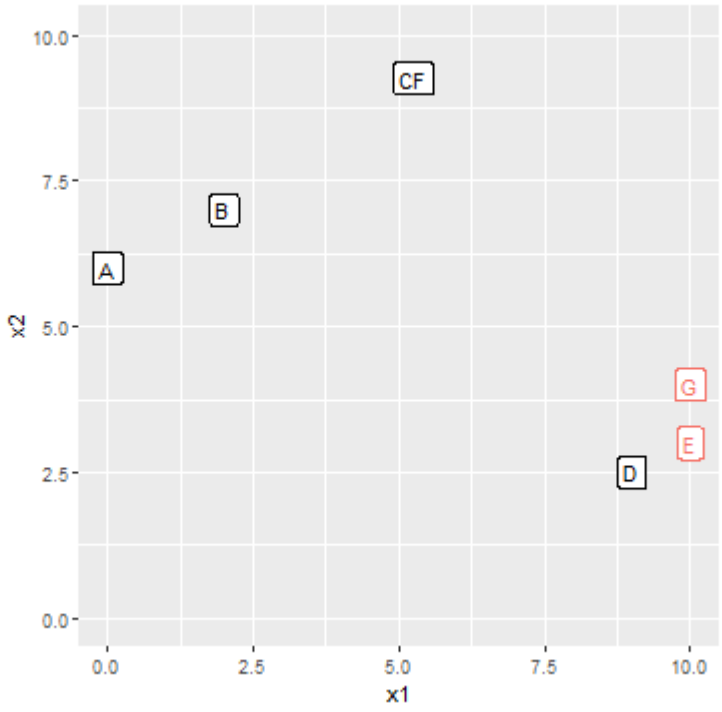

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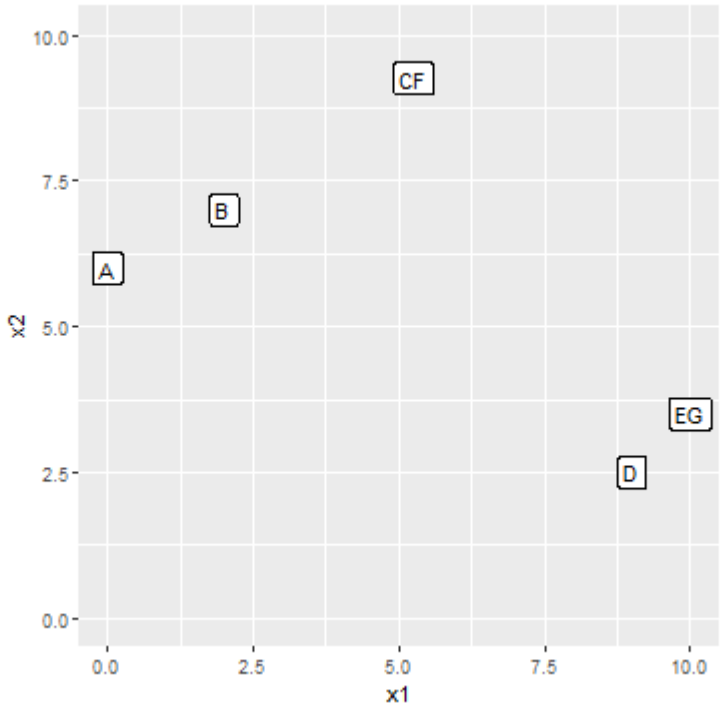

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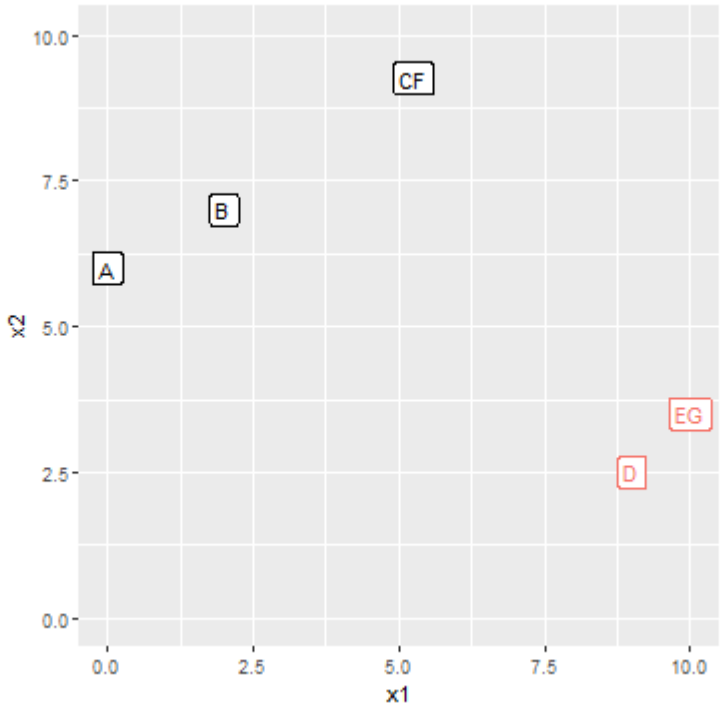

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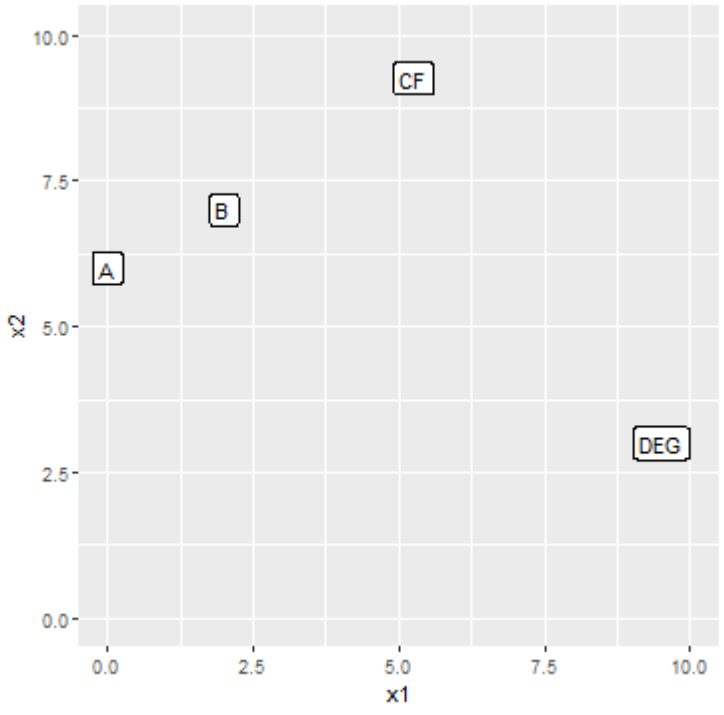

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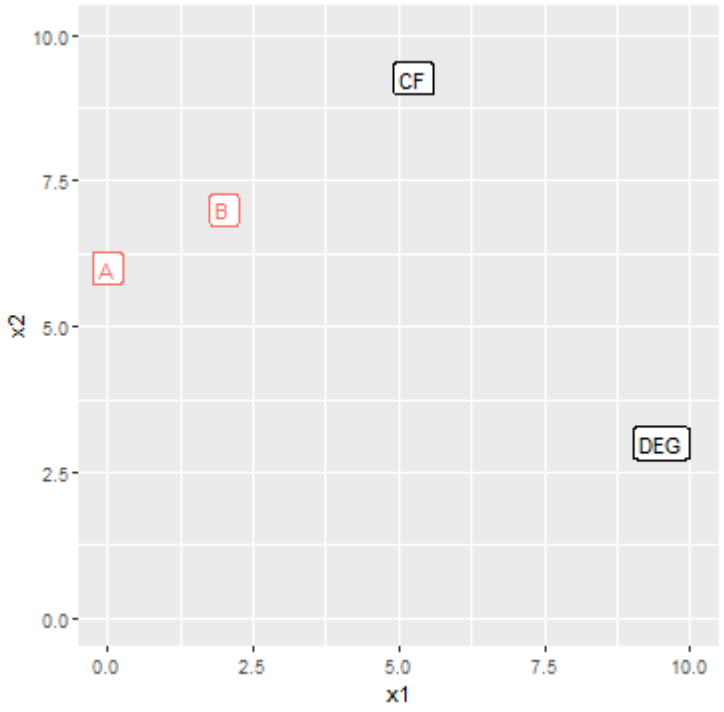

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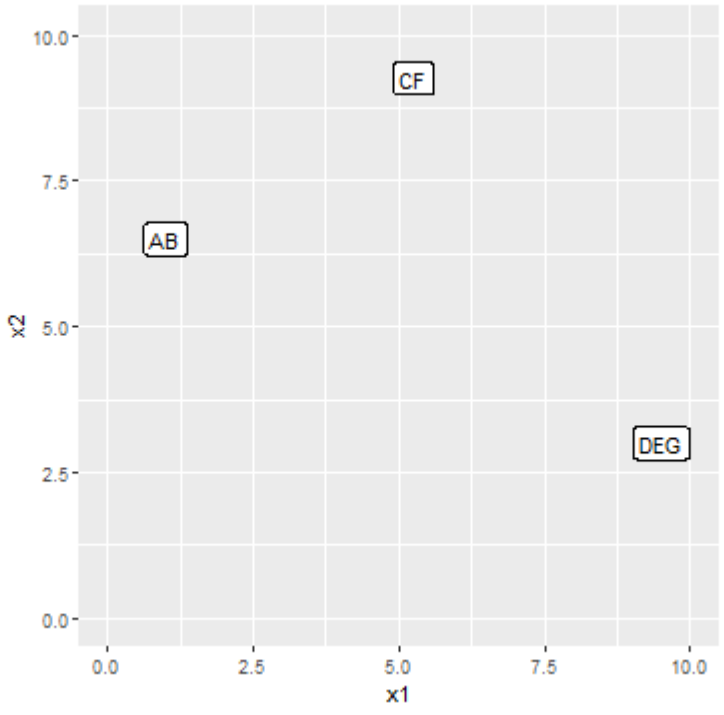

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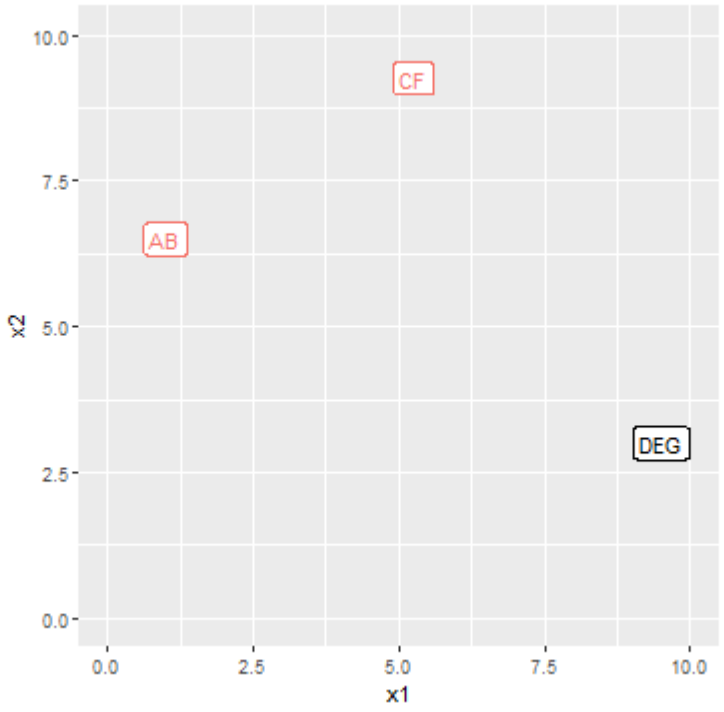
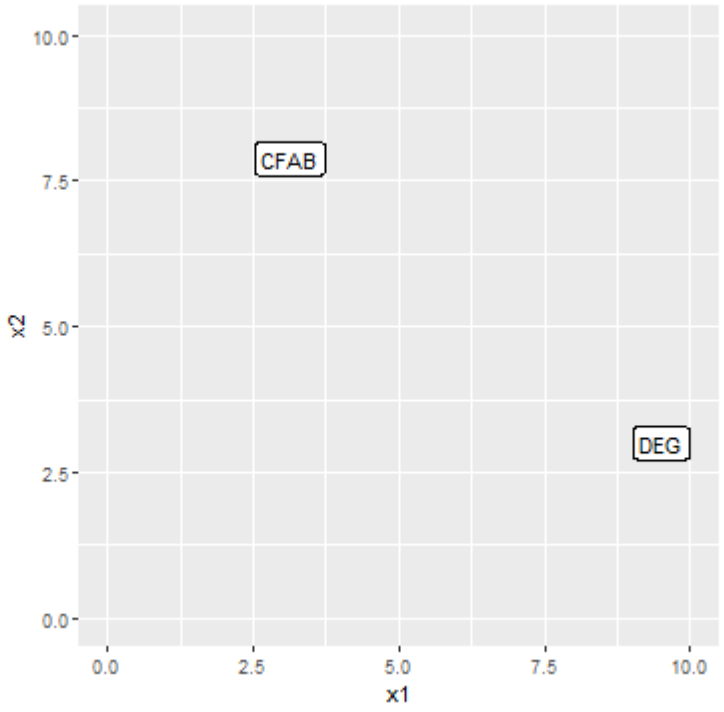


Group the pair



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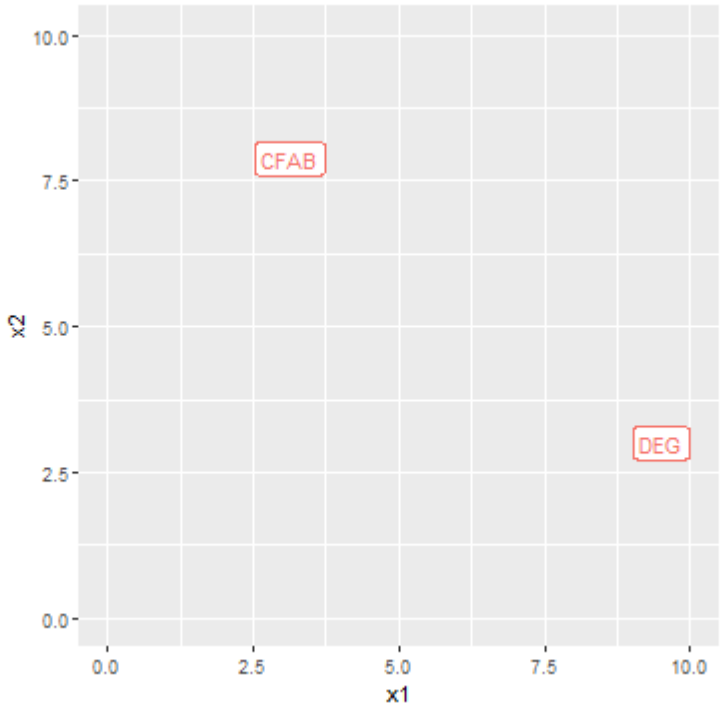
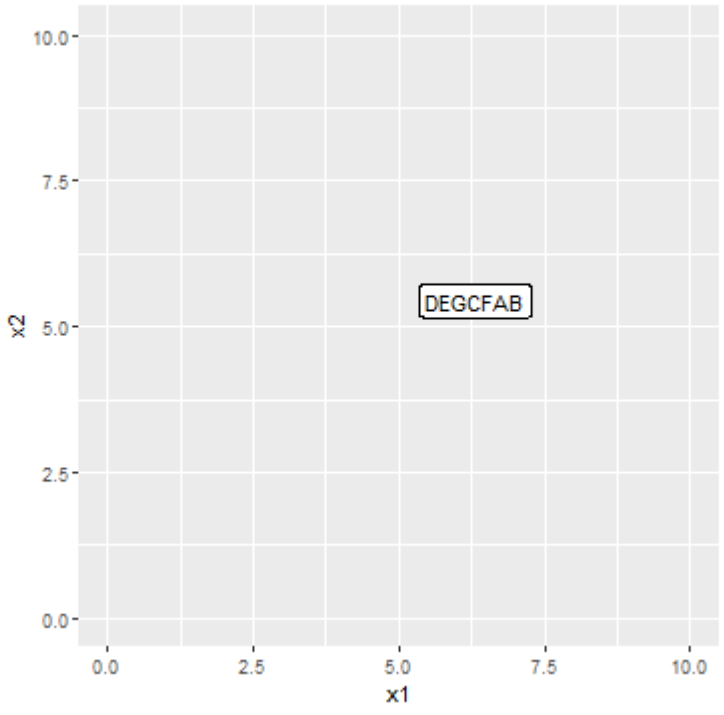
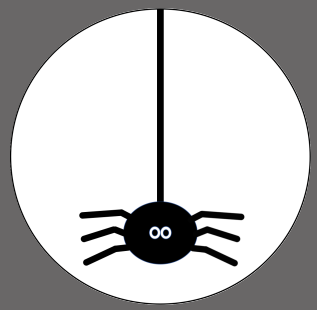


Group the pair



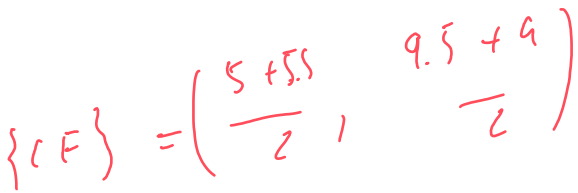
Detail Calculation



Detail Calculation

- The original data

cluster	x1	x2
A	0.0	6.0
B	2.0	7.0
C	5.0	9.5
D	9.0	2.5
E	10.0	3.0
F	5.5	9.0
G	10.0	4.0



Detail Calculation

- Calculate all the possible pair distances

	A	B	C	D	E	F	G
A	0.00	2.24	6.10	9.66	10.44	6.26	10.20
B	2.24	0.00	3.91	8.32	8.94	4.03	8.54
C	6.10	3.91	0.00	8.06	8.20	0.71	7.43
D	9.66	8.32	8.06	0.00	1.12	7.38	1.80
E	10.44	8.94	8.20	1.12	0.00	7.50	1.00
F	6.26	4.03	0.71	7.38	7.50	0.00	6.73
G	10.20	8.54	7.43	1.80	1.00	6.73	0.00

- Example: $AB = \sqrt{(0-2)^2 + (6-7)^2} = 2.24$
- The minimum distance is 0.71
- CF has the minimum distance
- Thus, group CF into one cluster

Detail Calculation

- The updated data after merging C and F

cluster	x1	x2
A	0.00	6.00
B	2.00	7.00
D	9.00	2.50
E	10.00	3.00
G	10.00	4.00
CF	5.25	9.25

- Notice that $CF = \left(\frac{5+5.5}{2}, \frac{9.5+9.0}{2}\right) = (5.25, 9.25)$

Detail Calculation

- Calculate all the possible pair distances

	A	B	D	E	G	CF
A	0.00	2.24	9.66	10.44	10.20	6.17
B	2.24	0.00	8.32	8.94	8.54	3.95
D	9.66	8.32	0.00	1.12	1.80	7.72
E	10.44	8.94	1.12	0.00	1.00	7.85
G	10.20	8.54	1.80	1.00	0.00	7.08
CF	6.17	3.95	7.72	7.85	7.08	0.00

- The minimum distance is 1
- EG has the minimum distance
- Thus, group EG together

Detail Calculation

- The updated data after merging EG together

cluster	x1	x2
A	0.00	6.00
B	2.00	7.00
D	9.00	2.50
CF	5.25	9.25
EG	10.00	3.50

Detail Calculation

- Calculate all the possible pair distances

	A	B	D	CF	EG
A	0.00	2.24	9.66	6.17	10.31
B	2.24	0.00	8.32	3.95	8.73
D	9.66	8.32	0.00	7.72	1.41
CF	6.17	3.95	7.72	0.00	7.46
EG	10.31	8.73	1.41	7.46	0.00

- The minimum distance is 1.41
- D - EG has the minimum distance
- Thus, group D-EG together

Detail Calculation

- The updated data after merging D-EG together

cluster	x1	x2
A	0.00	6.00
B	2.00	7.00
CF	5.25	9.25
DEG	9.50	3.00

Detail Calculation

- Calculate all the possible pair distances

	A	B	CF	DEG
A	0.00	2.24	6.17	9.96
B	2.24	0.00	3.95	8.50
CF	6.17	3.95	0.00	7.56
DEG	9.96	8.50	7.56	0.00

- The minimum distance is 2.24
- AB has the minimum distance
- Thus, group AB together

Detail Calculation

- The updated data after merging AB together

cluster	x1	x2
CF	5.25	9.25
DEG	9.50	3.00
AB	1.00	6.50

Detail Calculation

- Calculate all the possible pair distances

	CF	DEG	AB
CF	0.00	7.56	5.06
DEG	7.56	0.00	9.19
AB	5.06	9.19	0.00

- The minimum distance is 5.06
- CF-AB has the minimum distance
- Thus, group CF-AB together

Detail Calculation

- The updated data after merging CF-AB together

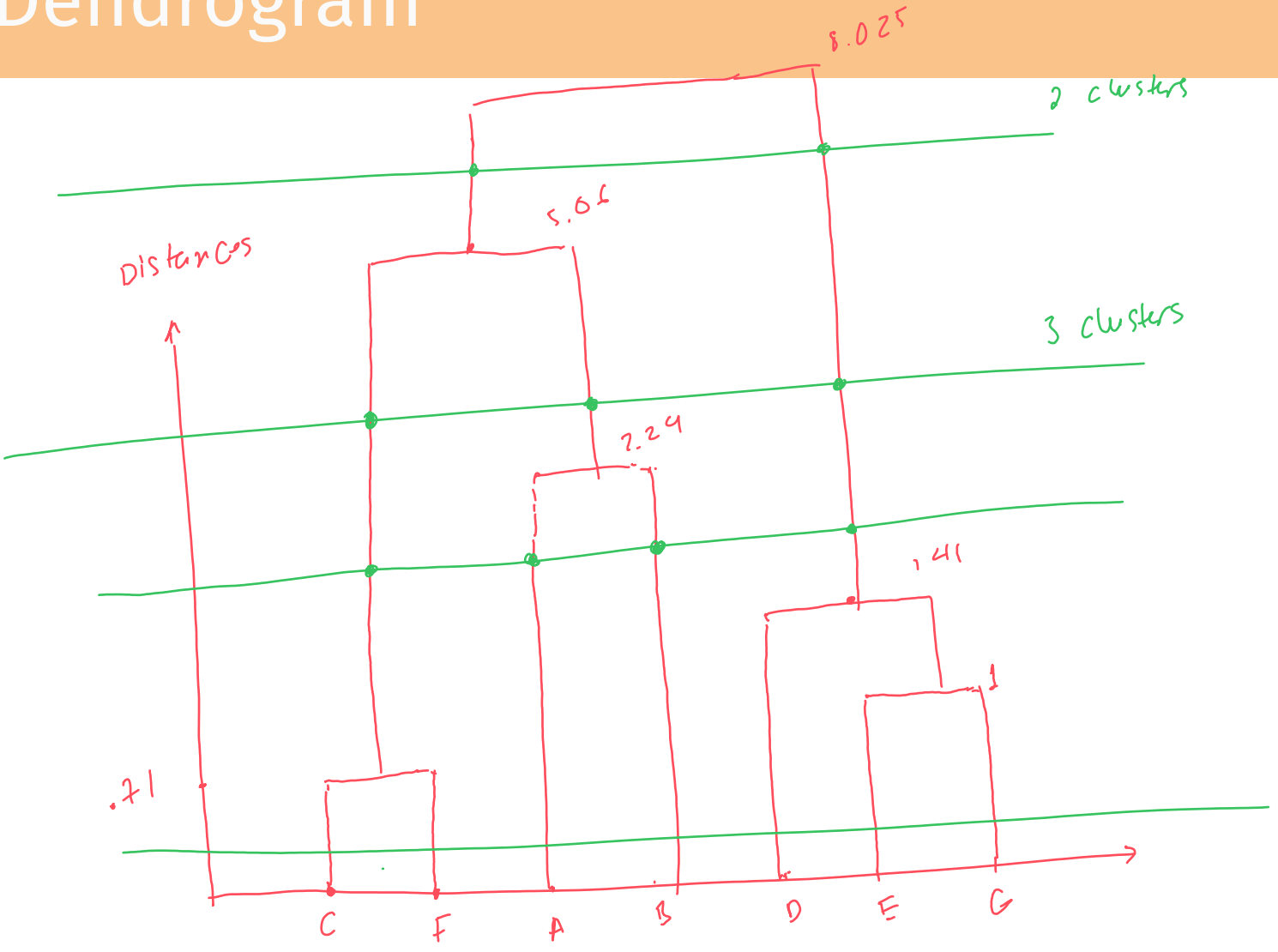
cluster	x1	x2
DEG	9.500	3.000
CFAB	3.125	7.875

Detail Calculation

- There are only two clusters left
- Just need to group them together

cluster	x1	x2
DEGCFAB	6.3125	5.4375

Dendrogram


8.025
2 clusters
5.05
Distances
3 clusters
2.24
1.41
1
.71
C
F
A
B
D
E
G

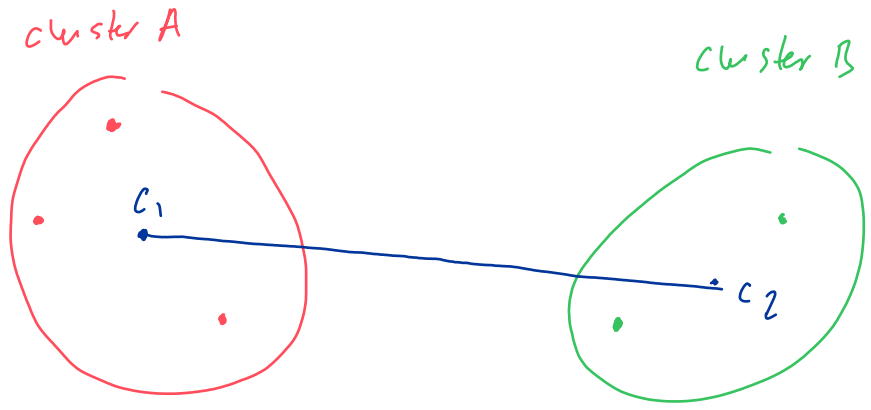
Problem

Point	x1	x2
A	0	6
B	2	7
C	5	9
D	9	2
E	1	3

- Calculate H-Clustering for the data and plot the Dendrogram

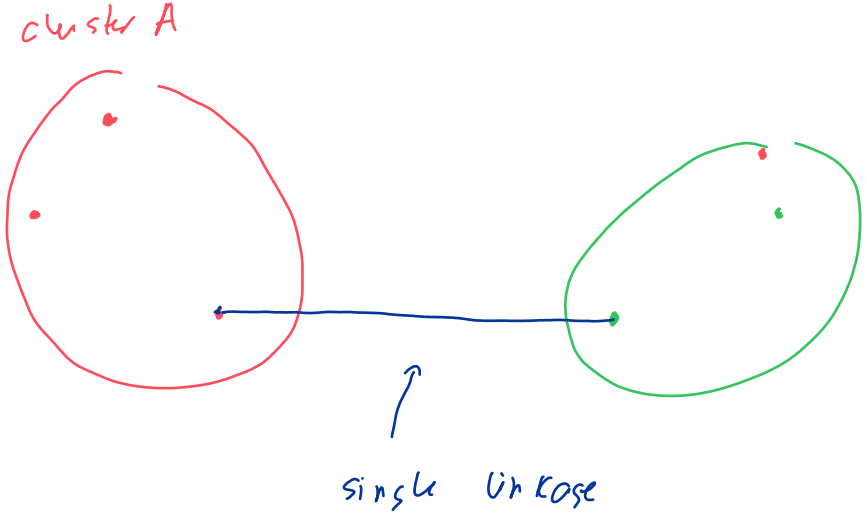
Linkages

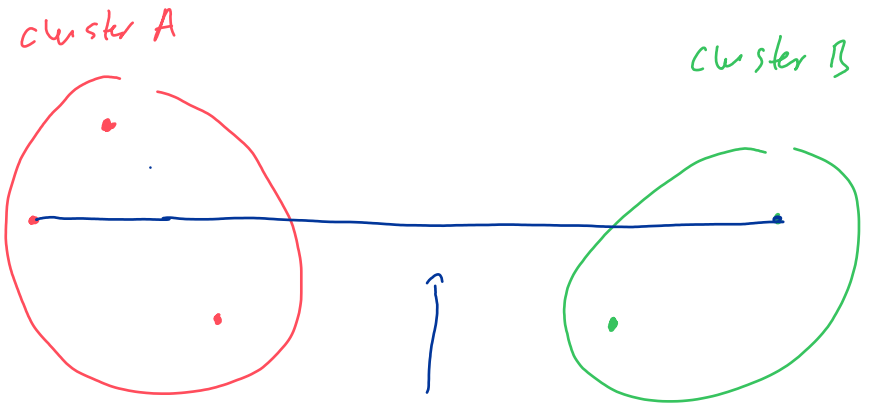
Linkage	*Description*
Complete	Maximal intercluster dissimilarity. Compute all pairwise dissimilarities between the observations in cluster A and the observations in cluster B, and record the *largest* of these dissimilarities.
Single	Minimal intercluster dissimilarity. Compute all pairwise dissimilarities between the observations in cluster A and the observations in cluster B, and record the *smallest* of these dissimilarities. Single linkage can result in extended, trailing clusters in which single observations are fused one-at-a-time.
Average	Mean intercluster dissimilarity. Compute all pairwise dissimilarities between the observations in cluster A and the observations in cluster B, and record the *average* of these dissimilarities.
Centroid	Dissimilarity between the centroid for cluster A (a mean vector of length p) and the centroid for cluster B. Centroid linkage can result in undesirable *inversions*.



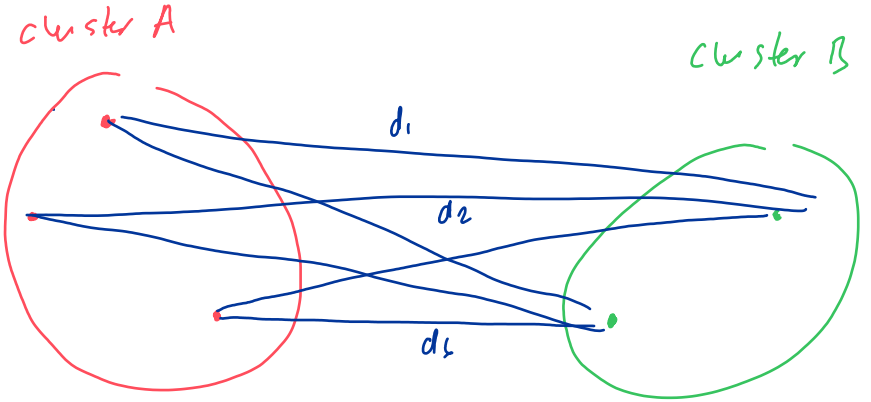
① Centroid Linkage : Distance (A, B) = $C_1 C_2$ cluster A

②





complete
Linkage



Average Linkage $= \frac{d_1 + \dots + d_L}{6}$