

Agglomerative Hierarchical Clustering

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Hierarchical Clustering

Hierarchical clustering:

- ▶ Clustering using a hierarchy of clusters
- ▶ May be represented in a tree structure (*dendrogram*)
- ▶ Root - a single cluster containing all observations
- ▶ Leaves - individual observations.

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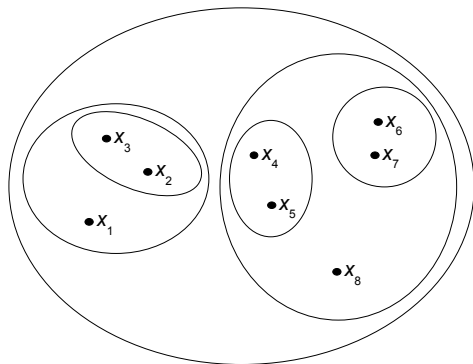
T.L. Dist. Matrices

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Hierarchical Clustering

Hierarchical clustering:

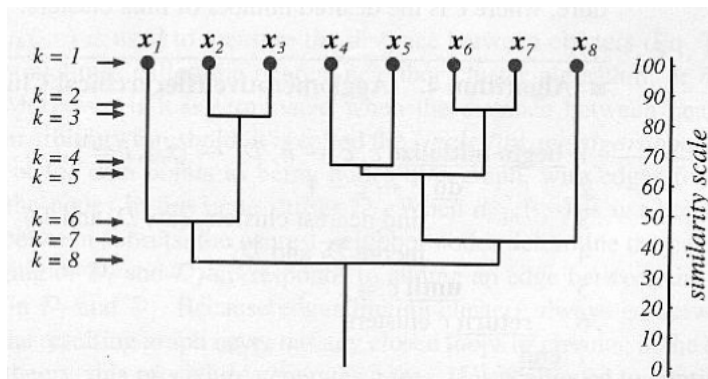
- ▶ Clustering using a hierarchy of clusters
- ▶ May be represented in a tree structure (*dendrogram*)
- ▶ Root - a single cluster containing all observations
- ▶ Leaves - individual observations.



Dendrogram

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[Duda et al., 2001] Figure 10.11

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Two Distinct Approaches:

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Two Distinct Approaches:

- ▶ Agglomerative (*bottom up, clumping*)
 - ▶ Start with n *singleton* clusters
 - ▶ Successively merge ("*clump*") clusters
 - ▶ Computation from one level to another generally simpler
 - ▶ For small number of clusters, takes many iterations

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Agglomerative Clustering Algorithm

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```
1   $c, \hat{c} \leftarrow n$ 
2   $D_i \leftarrow \{\mathbf{x}_i\}$  where  $i = 1, \dots, n$ 

3      do  $\hat{c} \leftarrow \hat{c} - 1$ 
4          find nearest clusters  $D_i, D_j$ 
5          merge  $D_i$  and  $D_j$ 
6      until  $c = \hat{c}$ 

7  return  $c$  clusters
```

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5          merge  $D_i$  and  $D_j$ 
6      until  $c = \hat{c}$ 

7  return  $c$  clusters
```

How do we determine which two clusters are *nearest*?

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Properties of Distance

- ▶ Distance is non-negative.
 - ▶ $D(x, y) \geq 0$
- ▶ $D(x, y) = 0$ if and only if $x = y$.
- ▶ Distance is symmetric.
 - ▶ $D(x, y) = D(y, x)$
- ▶ Distance satisfies the triangle inequality
 - ▶ $D(x, z) \leq D(x, y) + D(y, z)$

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Distance Measures—Between Points

Let $\vec{x}_1 = [x_{1,1} \ x_{1,2} \ \cdots \ x_{1,n}]^T$ and
 $\vec{x}_2 = [x_{2,1} \ x_{2,2} \ \cdots \ x_{2,n}]^T$

Name	Formula
Manhattan	$d_1(\vec{x}_1, \vec{x}_2) = \sum_{i=1}^n x_{1,i} - x_{2,i} $
Euclidian	$d_2(\vec{x}_1, \vec{x}_2) = \sqrt{\sum_{i=1}^n x_{1,i} - x_{2,i} ^2}$
P-norm	$d_p(\vec{x}_1, \vec{x}_2) = \sqrt[p]{\sum_{i=1}^n x_{1,i} - x_{2,i} ^p}$
Statistical	$d_s(\vec{x}_1, \vec{x}_2) = \sqrt{\sum_{i=1}^n \left(\frac{x_{1,i} - x_{2,i}}{\sigma_i} \right)^2}$
Mahalanobis	$d_m(\vec{x}_1, \vec{x}_2) = \sqrt{(\vec{x}_1 - \vec{\mu}) \Sigma^{-1} (\vec{x}_2 - \vec{\mu})^T}$
Cosine	$d_c(\vec{x}_1, \vec{x}_2) = \frac{\vec{x}_1^T \vec{x}_2}{\ \vec{x}_2\ \cdot \ \vec{x}_1\ }$
Chebyshev	$d_C(\vec{x}_1, \vec{x}_2) = \max(x_{1,i} - x_{2,i})$

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Distance Measures—Between Clusters

Single Linkage	$d_{(U,V),W} = \min\{d_{U,W}, d_{V,W}\}$
$d_{2,4}$	
Complete Linkage	$d_{(U,V),W} = \max\{d_{U,W}, d_{V,W}\}$
$d_{1,5}$	
Average Linkage	$d_{(U,V),W} = \frac{\sum_i \sum_j d_{i,j}}{N_{U,V} N_W}$
$\frac{\sum_{i=1}^2 \sum_{j=3}^5 d_{i,j}}{2 \cdot 3}$	

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x	y
-1.4833	-0.5745
-1.0573	-0.7131
-1.8613	-0.1988
-0.0784	-0.3186
-1.1796	-0.3535
1.4692	0.0054
1.2185	0.1419
1.2315	0.1564
0.9236	0.4333
1.4556	-0.2758

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Cluster distances using single linkage. Iteration: 1

	1	2	3	4	5	6	7	8	9	10
1	0.00	0.45	0.53	1.43	0.38	3.01	2.80	2.81	2.61	2.95
2	0.45	0.00	0.95	1.06	0.38	2.63	2.43	2.45	2.29	2.55
3	0.53	0.95	0.00	1.79	0.70	3.34	3.10	3.11	2.86	3.32
4	1.43	1.06	1.79	0.00	1.10	1.58	1.38	1.39	1.25	1.53
5	0.38	0.38	0.70	1.10	0.00	2.67	2.45	2.46	2.25	2.64
6	3.01	2.63	3.34	1.58	2.67	0.00	0.29	0.28	0.69	0.28
7	2.80	2.43	3.10	1.38	2.45	0.29	0.00	0.02	0.41	0.48
8	2.81	2.45	3.11	1.39	2.46	0.28	0.02	0.00	0.41	0.49
9	2.61	2.29	2.86	1.25	2.25	0.69	0.41	0.41	0.00	0.89
10	2.95	2.55	3.32	1.53	2.64	0.28	0.48	0.49	0.89	0.00

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Cluster distances using single linkage. Iteration: 2

	1	2	3	4	5	6	9	10	11
1	0.00	0.45	0.53	1.43	0.38	3.01	2.61	2.95	2.80
2	0.45	0.00	0.95	1.06	0.38	2.63	2.29	2.55	2.43
3	0.53	0.95	0.00	1.79	0.70	3.34	2.86	3.32	3.10
4	1.43	1.06	1.79	0.00	1.10	1.58	1.25	1.53	1.38
5	0.38	0.38	0.70	1.10	0.00	2.67	2.25	2.64	2.45
6	3.01	2.63	3.34	1.58	2.67	0.00	0.69	0.28	0.28
9	2.61	2.29	2.86	1.25	2.25	0.69	0.00	0.89	0.41
10	2.95	2.55	3.32	1.53	2.64	0.28	0.89	0.00	0.48
11	2.80	2.43	3.10	1.38	2.45	0.28	0.41	0.48	0.00

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Cluster distances using single linkage. Iteration: 3

	1	2	3	4	5	9	11	12
1	0.00	0.45	0.53	1.43	0.38	2.61	2.80	2.95
2	0.45	0.00	0.95	1.06	0.38	2.29	2.43	2.55
3	0.53	0.95	0.00	1.79	0.70	2.86	3.10	3.32
4	1.43	1.06	1.79	0.00	1.10	1.25	1.38	1.53
5	0.38	0.38	0.70	1.10	0.00	2.25	2.45	2.64
9	2.61	2.29	2.86	1.25	2.25	0.00	0.41	0.69
11	2.80	2.43	3.10	1.38	2.45	0.41	0.00	0.28
12	2.95	2.55	3.32	1.53	2.64	0.69	0.28	0.00

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Cluster distances using single linkage. Iteration: 4

	1	2	3	4	5	9	13
1	0.00	0.45	0.53	1.43	0.38	2.61	2.80
2	0.45	0.00	0.95	1.06	0.38	2.29	2.43
3	0.53	0.95	0.00	1.79	0.70	2.86	3.10
4	1.43	1.06	1.79	0.00	1.10	1.25	1.38
5	0.38	0.38	0.70	1.10	0.00	2.25	2.45
9	2.61	2.29	2.86	1.25	2.25	0.00	0.41
13	2.80	2.43	3.10	1.38	2.45	0.41	0.00

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Cluster distances using single linkage. Iteration: 5

	2	3	4	9	13	14
2	0.00	0.95	1.06	2.29	2.43	0.38
3	0.95	0.00	1.79	2.86	3.10	0.53
4	1.06	1.79	0.00	1.25	1.38	1.10
9	2.29	2.86	1.25	0.00	0.41	2.25
13	2.43	3.10	1.38	0.41	0.00	2.45
14	0.38	0.53	1.10	2.25	2.45	0.00

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Cluster distances using single linkage. Iteration: 6

	3	4	9	13	15
3	0.00	1.79	2.86	3.10	0.53
4	1.79	0.00	1.25	1.38	1.06
9	2.86	1.25	0.00	0.41	2.25
13	3.10	1.38	0.41	0.00	2.43
15	0.53	1.06	2.25	2.43	0.00

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Cluster distances using single linkage. Iteration: 7

	3	4	15	16
3	0.00	1.79	0.53	2.86
4	1.79	0.00	1.06	1.25
15	0.53	1.06	0.00	2.25
16	2.86	1.25	2.25	0.00

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Cluster distances using single linkage. Iteration: 8

	4	16	17
4	0.00	1.25	1.06
16	1.25	0.00	2.25
17	1.06	2.25	0.00

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Cluster distances using single linkage. Iteration: 9

	16	18
16	0.00	1.25
18	1.25	0.00

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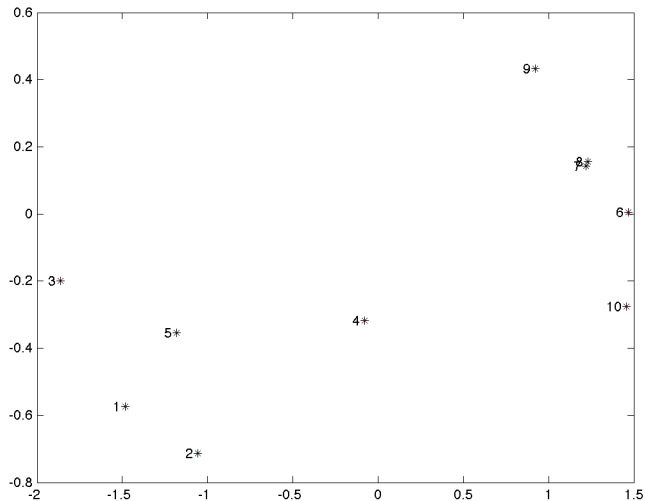
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Example—Linkage Step 1

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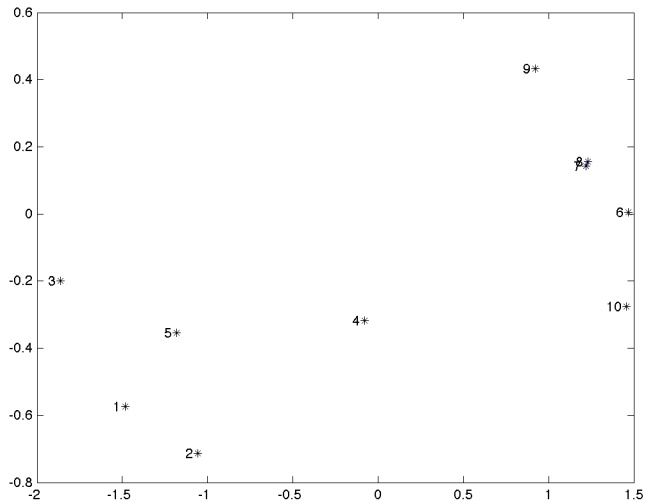
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Single Linkage Complete Linkage Average Linkage

Example—Linkage Step 2



Single Linkage Complete Linkage Average Linkage

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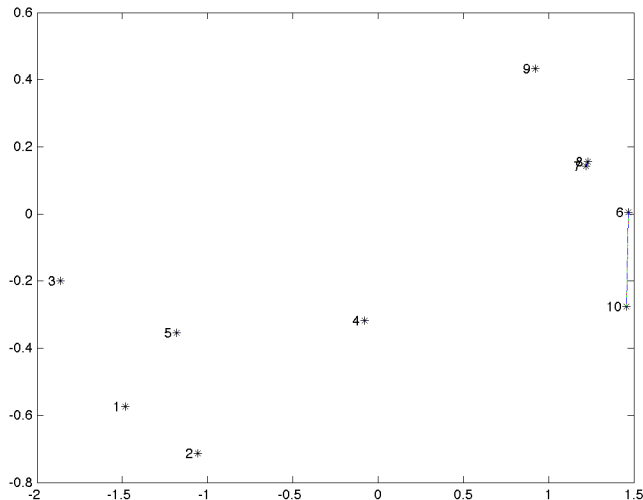
T.L. Dist. Matrices

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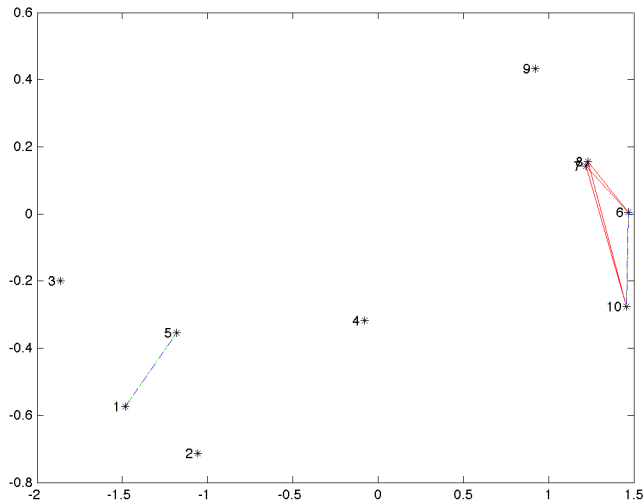
A.L. Dist. Matrices

Single Linkage Complete Linkage Average Linkage

Example—Linkage Step 4

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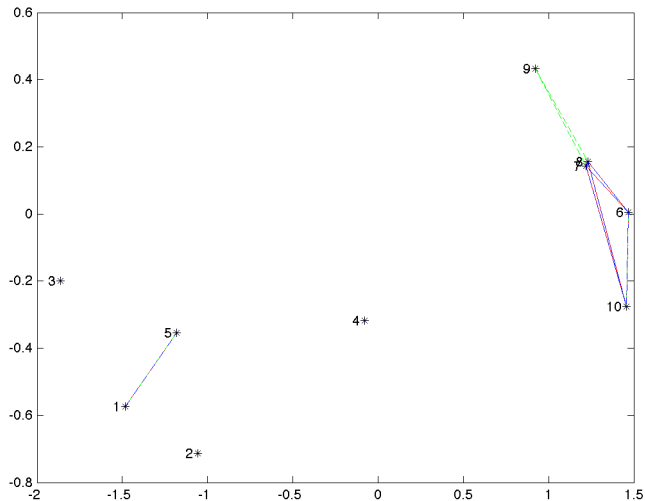
A.L. Dist. Matrices

Single Linkage Complete Linkage Average Linkage

Example—Linkage Step 5

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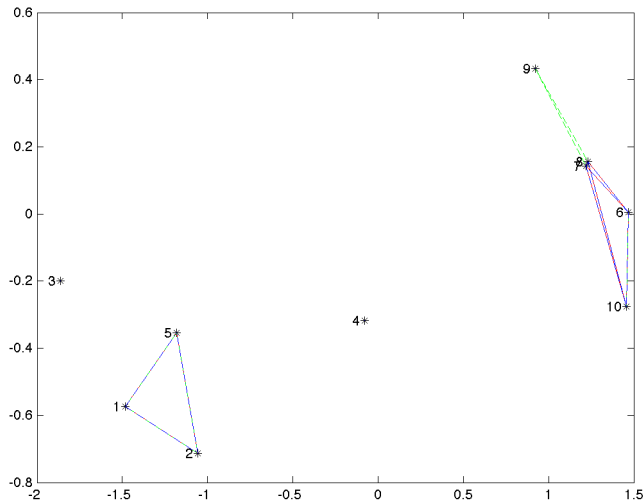
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Single Linkage Complete Linkage Average Linkage

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Single Linkage Complete Linkage Average Linkage

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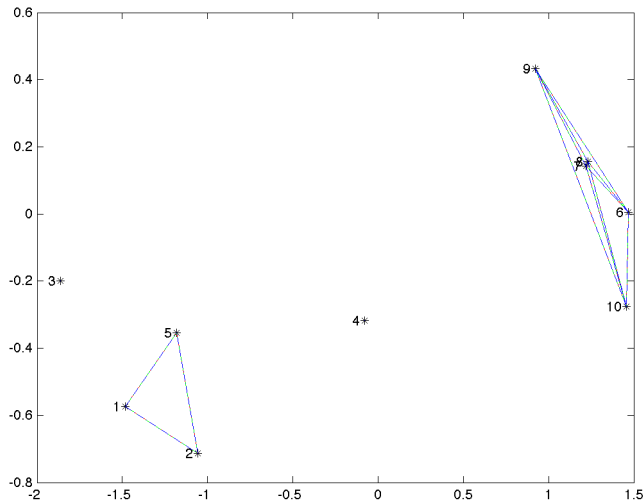
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Example—Linkage Step 7

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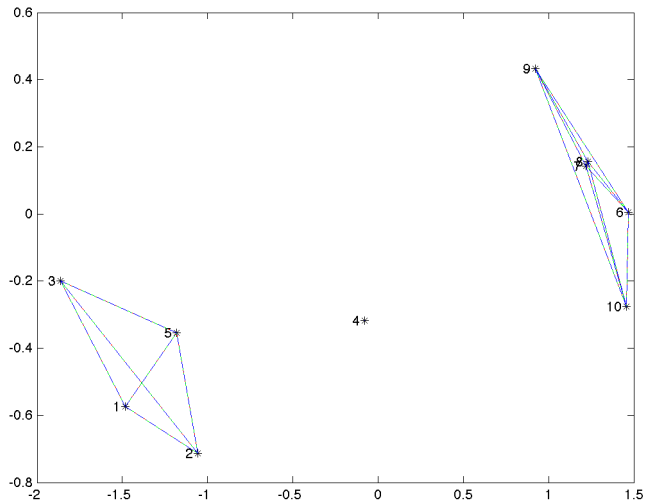
Extra Stuff

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Single Linkage Complete Linkage Average Linkage

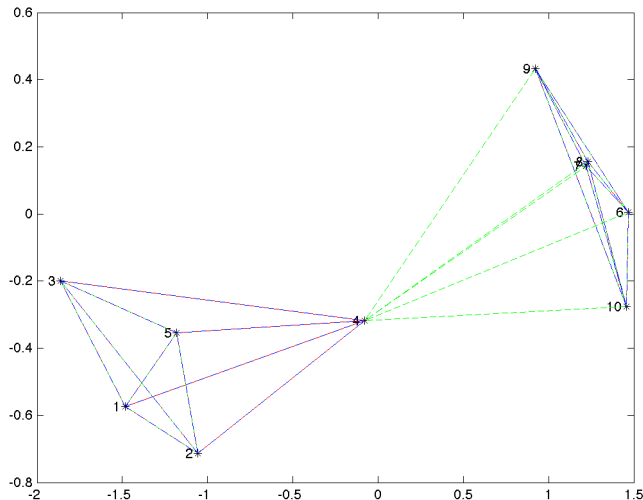
Example—Linkage Step 8



Example—Linkage Step 9

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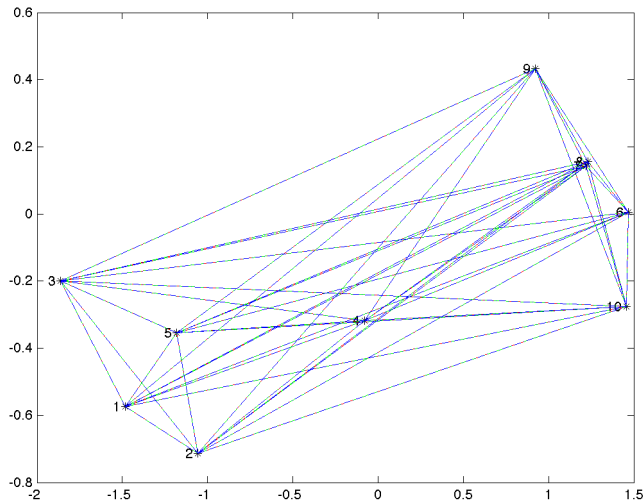
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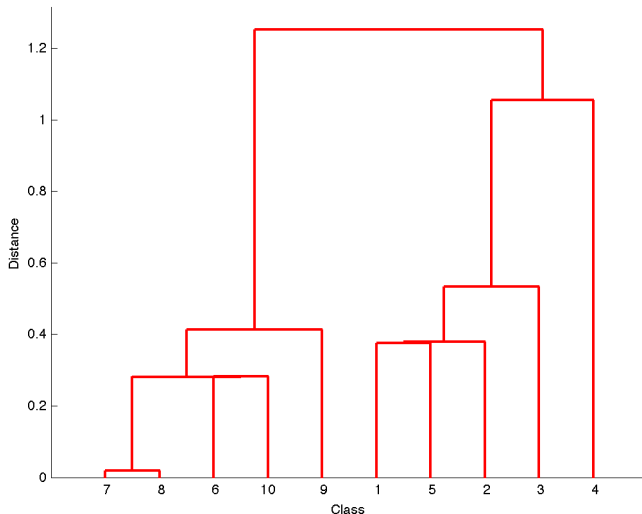
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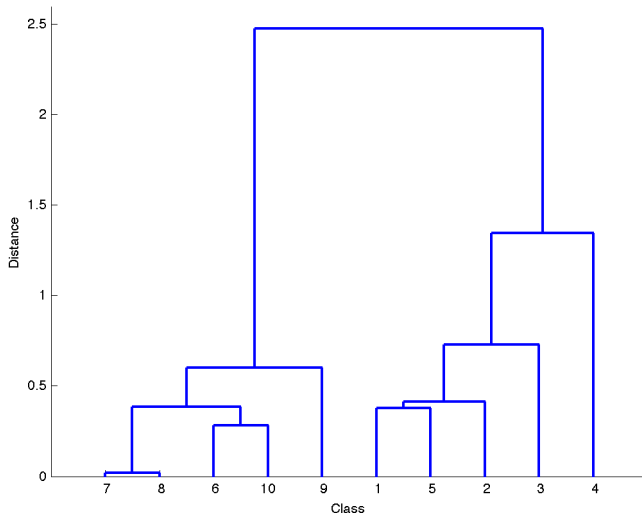
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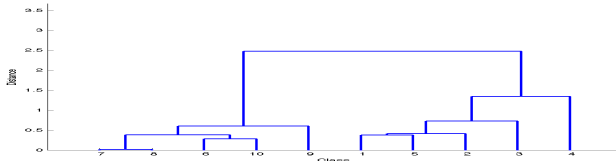
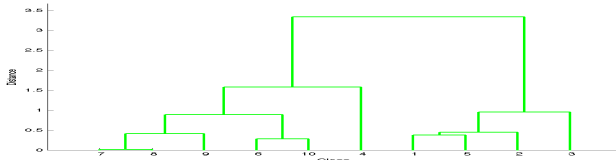
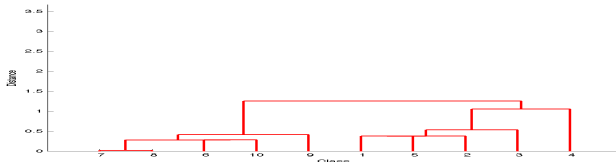
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Single Linkage Complete Linkage Average Linkage

Example

Single Linkage		Complete Linkage		Average Linkage	
dist.	action	dist.	action	dist.	action
0.0195	$\{8, 7\} \rightarrow 11$	0.0195	$\{8, 7\} \rightarrow 11$	0.0195	$\{8, 7\} \rightarrow 11$
0.2816	$\{10, 6\} \rightarrow 12$	0.2816	$\{10, 6\} \rightarrow 12$	0.2816	$\{10, 6\} \rightarrow 12$
0.2816	$\{12, 11\} \rightarrow 13$	0.3757	$\{5, 1\} \rightarrow 13$	0.3757	$\{5, 1\} \rightarrow 13$
0.3757	$\{5, 1\} \rightarrow 14$	0.4146	$\{11, 9\} \rightarrow 14$	0.3836	$\{12, 11\} \rightarrow 14$
0.3798	$\{14, 2\} \rightarrow 15$	0.4480	$\{13, 2\} \rightarrow 15$	0.4139	$\{13, 2\} \rightarrow 15$
0.4141	$\{13, 9\} \rightarrow 16$	0.8865	$\{14, 12\} \rightarrow 16$	0.6021	$\{14, 9\} \rightarrow 16$
0.5330	$\{15, 3\} \rightarrow 17$	0.9544	$\{15, 3\} \rightarrow 17$	0.7288	$\{15, 3\} \rightarrow 17$
1.0553	$\{17, 4\} \rightarrow 18$	1.5812	$\{16, 4\} \rightarrow 18$	1.3430	$\{17, 4\} \rightarrow 18$
1.2528	$\{16, 18\} \rightarrow 19$	3.3368	$\{17, 18\} \rightarrow 19$	2.4741	$\{16, 18\} \rightarrow 19$

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Example

Cluster distances using total linkage. Iteration: 1

	1	2	3	4	5	6	7	8	9	10
1	0.00	0.45	0.53	1.43	0.38	3.01	2.80	2.81	2.61	2.95
2	0.45	0.00	0.95	1.06	0.38	2.63	2.43	2.45	2.29	2.55
3	0.53	0.95	0.00	1.79	0.70	3.34	3.10	3.11	2.86	3.32
4	1.43	1.06	1.79	0.00	1.10	1.58	1.38	1.39	1.25	1.53
5	0.38	0.38	0.70	1.10	0.00	2.67	2.45	2.46	2.25	2.64
6	3.01	2.63	3.34	1.58	2.67	0.00	0.29	0.28	0.69	0.28
7	2.80	2.43	3.10	1.38	2.45	0.29	0.00	0.02	0.41	0.48
8	2.81	2.45	3.11	1.39	2.46	0.28	0.02	0.00	0.41	0.49
9	2.61	2.29	2.86	1.25	2.25	0.69	0.41	0.41	0.00	0.89
10	2.95	2.55	3.32	1.53	2.64	0.28	0.48	0.49	0.89	0.00

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Example

Cluster distances using total linkage. Iteration: 2

	1	2	3	4	5	6	9	10	11
1	0.00	0.45	0.53	1.43	0.38	3.01	2.61	2.95	2.81
2	0.45	0.00	0.95	1.06	0.38	2.63	2.29	2.55	2.45
3	0.53	0.95	0.00	1.79	0.70	3.34	2.86	3.32	3.11
4	1.43	1.06	1.79	0.00	1.10	1.58	1.25	1.53	1.39
5	0.38	0.38	0.70	1.10	0.00	2.67	2.25	2.64	2.46
6	3.01	2.63	3.34	1.58	2.67	0.00	0.69	0.28	0.29
9	2.61	2.29	2.86	1.25	2.25	0.69	0.00	0.89	0.41
10	2.95	2.55	3.32	1.53	2.64	0.28	0.89	0.00	0.49
11	2.81	2.45	3.11	1.39	2.46	0.29	0.41	0.49	0.02

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Example

Cluster distances using total linkage. Iteration: 3

	1	2	3	4	5	9	11	12
1	0.00	0.45	0.53	1.43	0.38	2.61	2.81	3.01
2	0.45	0.00	0.95	1.06	0.38	2.29	2.45	2.63
3	0.53	0.95	0.00	1.79	0.70	2.86	3.11	3.34
4	1.43	1.06	1.79	0.00	1.10	1.25	1.39	1.58
5	0.38	0.38	0.70	1.10	0.00	2.25	2.46	2.67
9	2.61	2.29	2.86	1.25	2.25	0.00	0.41	0.89
11	2.81	2.45	3.11	1.39	2.46	0.41	0.02	0.49
12	3.01	2.63	3.34	1.58	2.67	0.89	0.49	0.28

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Example

Cluster distances using total linkage. Iteration: 4

	2	3	4	9	11	12	13
2	0.00	0.95	1.06	2.29	2.45	2.63	0.45
3	0.95	0.00	1.79	2.86	3.11	3.34	0.70
4	1.06	1.79	0.00	1.25	1.39	1.58	1.43
9	2.29	2.86	1.25	0.00	0.41	0.89	2.61
11	2.45	3.11	1.39	0.41	0.02	0.49	2.81
12	2.63	3.34	1.58	0.89	0.49	0.28	3.01
13	0.45	0.70	1.43	2.61	2.81	3.01	0.38

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Cluster distances using total linkage. Iteration: 5

	2	3	4	12	13	14
2	0.00	0.95	1.06	2.63	0.45	2.45
3	0.95	0.00	1.79	3.34	0.70	3.11
4	1.06	1.79	0.00	1.58	1.43	1.39
12	2.63	3.34	1.58	0.28	3.01	0.89
13	0.45	0.70	1.43	3.01	0.38	2.81
14	2.45	3.11	1.39	0.89	2.81	0.41

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Example

Cluster distances using total linkage. Iteration: 6

	3	4	12	14	15
3	0.00	1.79	3.34	3.11	0.95
4	1.79	0.00	1.58	1.39	1.43
12	3.34	1.58	0.28	0.89	3.01
14	3.11	1.39	0.89	0.41	2.81
15	0.95	1.43	3.01	2.81	0.45

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Cluster distances using total linkage. Iteration: 7

	3	4	15	16
3	0.00	1.79	0.95	3.34
4	1.79	0.00	1.43	1.58
15	0.95	1.43	0.45	3.01
16	3.34	1.58	3.01	0.89

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Cluster distances using total linkage. Iteration: 8

	4	16	17
4	0.00	1.58	1.79
16	1.58	0.89	3.34
17	1.79	3.34	0.95

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Cluster distances using total linkage. Iteration: 9

	17	18
17	0.00	3.34
18	3.34	0.00

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Example

Cluster distances using average linkage. Iteration: 1

	1	2	3	4	5	6	7	8	9	10
1	0.00	0.45	0.53	1.43	0.38	3.01	2.80	2.81	2.61	2.95
2	0.45	0.00	0.95	1.06	0.38	2.63	2.43	2.45	2.29	2.55
3	0.53	0.95	0.00	1.79	0.70	3.34	3.10	3.11	2.86	3.32
4	1.43	1.06	1.79	0.00	1.10	1.58	1.38	1.39	1.25	1.53
5	0.38	0.38	0.70	1.10	0.00	2.67	2.45	2.46	2.25	2.64
6	3.01	2.63	3.34	1.58	2.67	0.00	0.29	0.28	0.69	0.28
7	2.80	2.43	3.10	1.38	2.45	0.29	0.00	0.02	0.41	0.48
8	2.81	2.45	3.11	1.39	2.46	0.28	0.02	0.00	0.41	0.49
9	2.61	2.29	2.86	1.25	2.25	0.69	0.41	0.41	0.00	0.89
10	2.95	2.55	3.32	1.53	2.64	0.28	0.48	0.49	0.89	0.00

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Example

Cluster distances using average linkage. Iteration: 2

	1	2	3	4	5	6	9	10	11
1	0.00	0.45	0.53	1.43	0.38	3.01	2.61	2.95	2.80
2	0.45	0.00	0.95	1.06	0.38	2.63	2.29	2.55	2.44
3	0.53	0.95	0.00	1.79	0.70	3.34	2.86	3.32	3.11
4	1.43	1.06	1.79	0.00	1.10	1.58	1.25	1.53	1.38
5	0.38	0.38	0.70	1.10	0.00	2.67	2.25	2.64	2.46
6	3.01	2.63	3.34	1.58	2.67	0.00	0.69	0.28	0.28
9	2.61	2.29	2.86	1.25	2.25	0.69	0.00	0.89	0.41
10	2.95	2.55	3.32	1.53	2.64	0.28	0.89	0.00	0.48
11	2.80	2.44	3.11	1.38	2.46	0.28	0.41	0.48	0.01

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Example

Cluster distances using average linkage. Iteration: 3

	1	2	3	4	5	9	11	12
1	0.00	0.45	0.53	1.43	0.38	2.61	2.80	2.98
2	0.45	0.00	0.95	1.06	0.38	2.29	2.44	2.59
3	0.53	0.95	0.00	1.79	0.70	2.86	3.11	3.33
4	1.43	1.06	1.79	0.00	1.10	1.25	1.38	1.56
5	0.38	0.38	0.70	1.10	0.00	2.25	2.46	2.65
9	2.61	2.29	2.86	1.25	2.25	0.00	0.41	0.79
11	2.80	2.44	3.11	1.38	2.46	0.41	0.01	0.38
12	2.98	2.59	3.33	1.56	2.65	0.79	0.38	0.14

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Example

Cluster distances using average linkage. Iteration: 4

	2	3	4	9	11	12	13
2	0.00	0.95	1.06	2.29	2.44	2.59	0.41
3	0.95	0.00	1.79	2.86	3.11	3.33	0.62
4	1.06	1.79	0.00	1.25	1.38	1.56	1.26
9	2.29	2.86	1.25	0.00	0.41	0.79	2.43
11	2.44	3.11	1.38	0.41	0.01	0.38	2.63
12	2.59	3.33	1.56	0.79	0.38	0.14	2.82
13	0.41	0.62	1.26	2.43	2.63	2.82	0.19

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Example

Cluster distances using average linkage. Iteration: 5

	2	3	4	9	13	14
2	0.00	0.95	1.06	2.29	0.41	2.51
3	0.95	0.00	1.79	2.86	0.62	3.22
4	1.06	1.79	0.00	1.25	1.26	1.47
9	2.29	2.86	1.25	0.00	2.43	0.60
13	0.41	0.62	1.26	2.43	0.19	2.72
14	2.51	3.22	1.47	0.60	2.72	0.23

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Example

Cluster distances using average linkage. Iteration: 6

	3	4	9	14	15
3	0.00	1.79	2.86	3.22	0.73
4	1.79	0.00	1.25	1.47	1.20
9	2.86	1.25	0.00	0.60	2.38
14	3.22	1.47	0.60	0.23	2.65
15	0.73	1.20	2.38	2.65	0.27

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Example

Cluster distances using average linkage. Iteration: 7

	3	4	15	16
3	0.00	1.79	0.73	3.14
4	1.79	0.00	1.20	1.43
15	0.73	1.20	0.27	2.60
16	3.14	1.43	2.60	0.34

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Cluster distances using average linkage. Iteration: 8

	4	16	17
4	0.00	1.43	1.34
16	1.43	0.34	2.74
17	1.34	2.74	0.42

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Cluster distances using average linkage. Iteration: 9

	16	18
16	0.00	2.47
18	2.47	0.00

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