

Agglomerative Hierarchical Clustering

James Loomis & Paul Romanczyk

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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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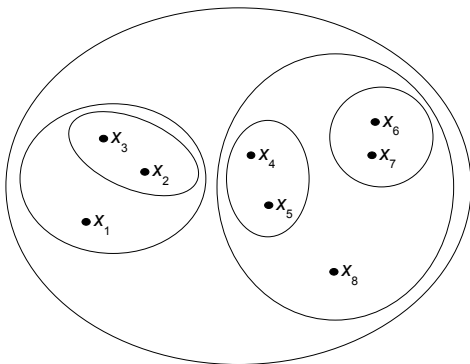
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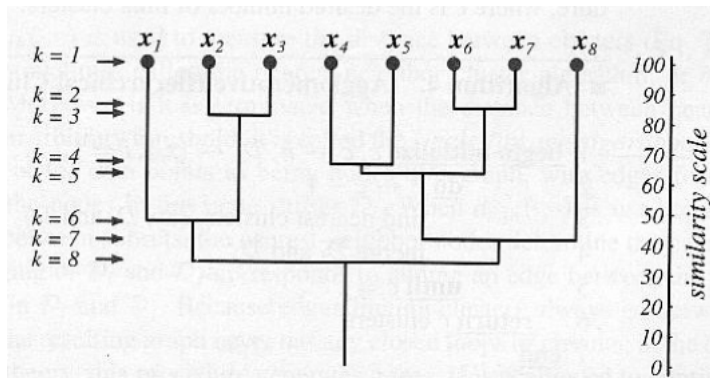
Hierarchical Clustering

Hierarchical clustering:

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



[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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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
- ▶ Divisive (*top down, splitting*)
 - ▶ Start with one cluster
 - ▶ Successively split clusters
 - ▶ Single iteration is more expensive
 - ▶ With fewer clusters, fewer iterations

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Agglomerative Clustering Algorithm

Agglomerative
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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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```

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	$d_c(\vec{x}_1, \vec{x}_2) = \frac{\vec{x}_1^T \vec{x}_2}{\ \vec{x}_1\ \cdot \ \vec{x}_2\ }$
Chebyshev	$d_C(\vec{x}_1, \vec{x}_2) = \max(x_{1,i} - x_{2,i})$

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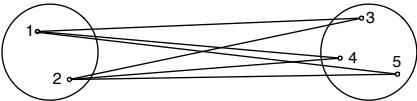
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Distance Measures—Between Clusters

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

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Data

x	y
-1.3508	0.9010
-0.3674	1.1548
-1.5895	-0.0732
-1.3615	0.1443
-0.7088	0.3324
0.3155	-0.3220
1.6638	0.2567
0.4751	0.2582
2.0778	0.2848
1.3015	-1.0126

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Example

Cluster distances using single linkage. Iteration: 1

	1	2	3	4	5	6	7	8	9	10
1	0.00	1.02	1.00	0.76	0.86	2.07	3.08	1.94	3.48	3.27
2	1.02	0.00	1.73	1.42	0.89	1.63	2.22	1.23	2.60	2.74
3	1.00	1.73	0.00	0.32	0.97	1.92	3.27	2.09	3.68	3.04
4	0.76	1.42	0.32	0.00	0.68	1.74	3.03	1.84	3.44	2.90
5	0.86	0.89	0.97	0.68	0.00	1.22	2.37	1.19	2.79	2.42
6	2.07	1.63	1.92	1.74	1.22	0.00	1.47	0.60	1.86	1.20
7	3.08	2.22	3.27	3.03	2.37	1.47	0.00	1.19	0.41	1.32
8	1.94	1.23	2.09	1.84	1.19	0.60	1.19	0.00	1.60	1.52
9	3.48	2.60	3.68	3.44	2.79	1.86	0.41	1.60	0.00	1.51
10	3.27	2.74	3.04	2.90	2.42	1.20	1.32	1.52	1.51	0.00

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Cluster distances using single linkage. Iteration: 2

	1	2	5	6	7	8	9	10	11
1	0.00	1.02	0.86	2.07	3.08	1.94	3.48	3.27	0.76
2	1.02	0.00	0.89	1.63	2.22	1.23	2.60	2.74	1.42
5	0.86	0.89	0.00	1.22	2.37	1.19	2.79	2.42	0.68
6	2.07	1.63	1.22	0.00	1.47	0.60	1.86	1.20	1.74
7	3.08	2.22	2.37	1.47	0.00	1.19	0.41	1.32	3.03
8	1.94	1.23	1.19	0.60	1.19	0.00	1.60	1.52	1.84
9	3.48	2.60	2.79	1.86	0.41	1.60	0.00	1.51	3.44
10	3.27	2.74	2.42	1.20	1.32	1.52	1.51	0.00	2.90
11	0.76	1.42	0.68	1.74	3.03	1.84	3.44	2.90	0.00

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Cluster distances using single linkage. Iteration: 3

	1	2	5	6	8	10	11	12
1	0.00	1.02	0.86	2.07	1.94	3.27	0.76	3.08
2	1.02	0.00	0.89	1.63	1.23	2.74	1.42	2.22
5	0.86	0.89	0.00	1.22	1.19	2.42	0.68	2.37
6	2.07	1.63	1.22	0.00	0.60	1.20	1.74	1.47
8	1.94	1.23	1.19	0.60	0.00	1.52	1.84	1.19
10	3.27	2.74	2.42	1.20	1.52	0.00	2.90	1.32
11	0.76	1.42	0.68	1.74	1.84	2.90	0.00	3.03
12	3.08	2.22	2.37	1.47	1.19	1.32	3.03	0.00

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Cluster distances using single linkage. Iteration: 4

	1	2	5	10	11	12	13
1	0.00	1.02	0.86	3.27	0.76	3.08	1.94
2	1.02	0.00	0.89	2.74	1.42	2.22	1.23
5	0.86	0.89	0.00	2.42	0.68	2.37	1.19
10	3.27	2.74	2.42	0.00	2.90	1.32	1.20
11	0.76	1.42	0.68	2.90	0.00	3.03	1.74
12	3.08	2.22	2.37	1.32	3.03	0.00	1.19
13	1.94	1.23	1.19	1.20	1.74	1.19	0.00

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Cluster distances using single linkage. Iteration: 5

	1	2	10	12	13	14
1	0.00	1.02	3.27	3.08	1.94	0.76
2	1.02	0.00	2.74	2.22	1.23	0.89
10	3.27	2.74	0.00	1.32	1.20	2.42
12	3.08	2.22	1.32	0.00	1.19	2.37
13	1.94	1.23	1.20	1.19	0.00	1.19
14	0.76	0.89	2.42	2.37	1.19	0.00

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Cluster distances using single linkage. Iteration: 6

	2	10	12	13	15
2	0.00	2.74	2.22	1.23	0.89
10	2.74	0.00	1.32	1.20	2.42
12	2.22	1.32	0.00	1.19	2.37
13	1.23	1.20	1.19	0.00	1.19
15	0.89	2.42	2.37	1.19	0.00

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Cluster distances using single linkage. Iteration: 7

	10	12	13	16
10	0.00	1.32	1.20	2.42
12	1.32	0.00	1.19	2.22
13	1.20	1.19	0.00	1.19
16	2.42	2.22	1.19	0.00

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Cluster distances using single linkage. Iteration: 8

	10	12	17
10	0.00	1.32	1.20
12	1.32	0.00	1.19
17	1.20	1.19	0.00

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Cluster distances using single linkage. Iteration: 9

	10	18
10	0.00	1.20
18	1.20	0.00

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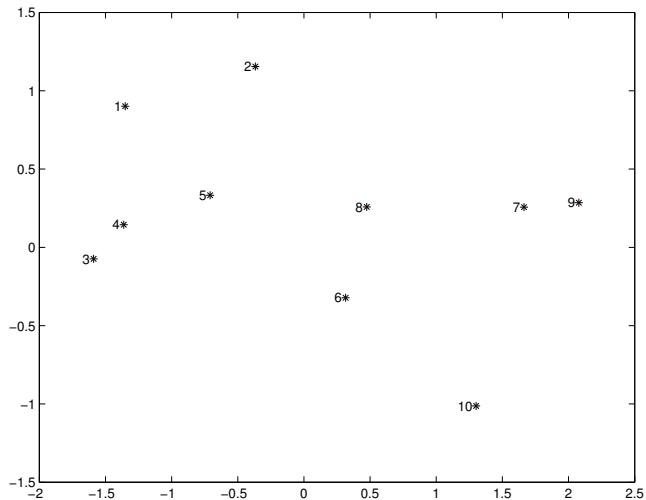
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Example—Linkage Step 1

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Single Linkage Complete Linkage Average Linkage

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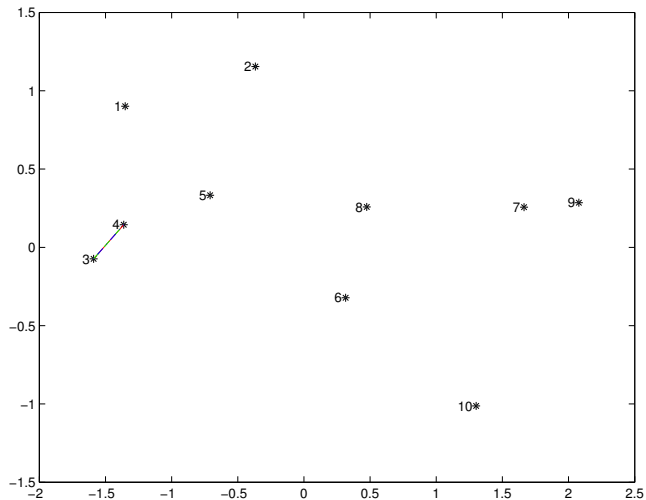
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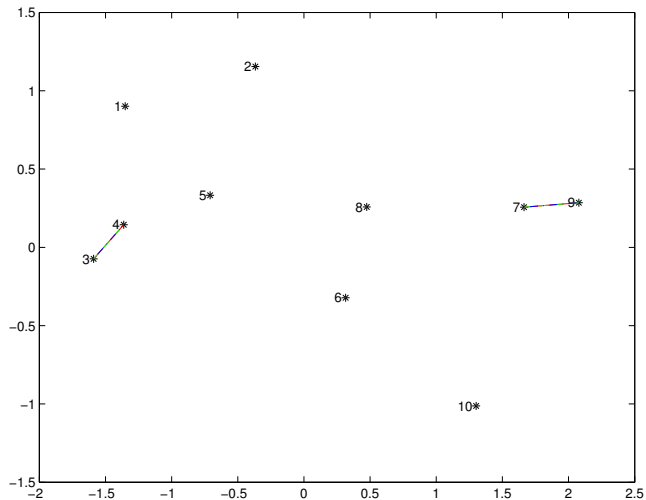
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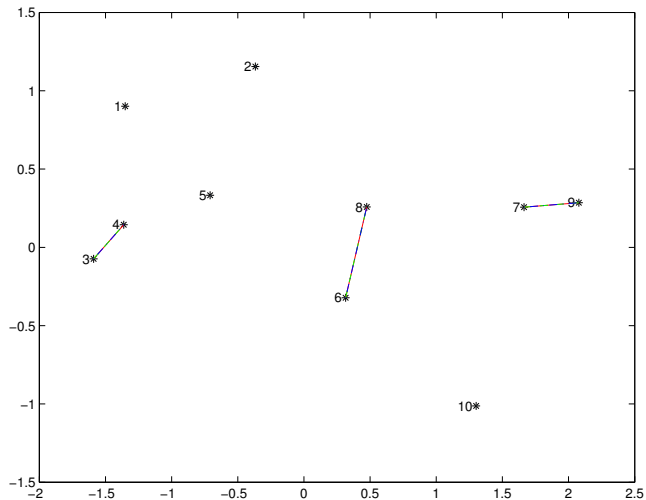
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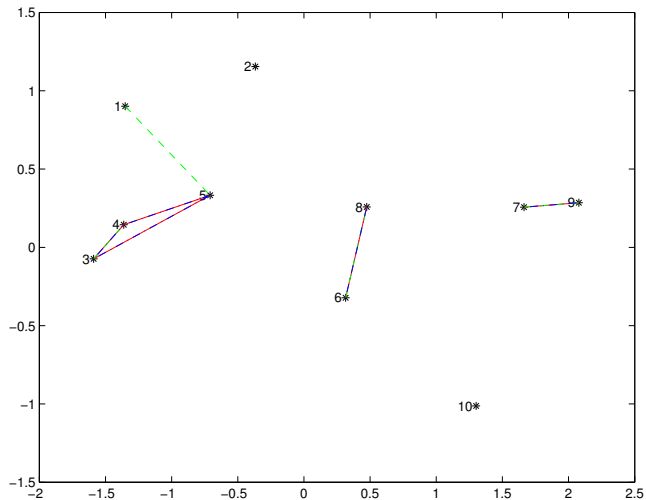
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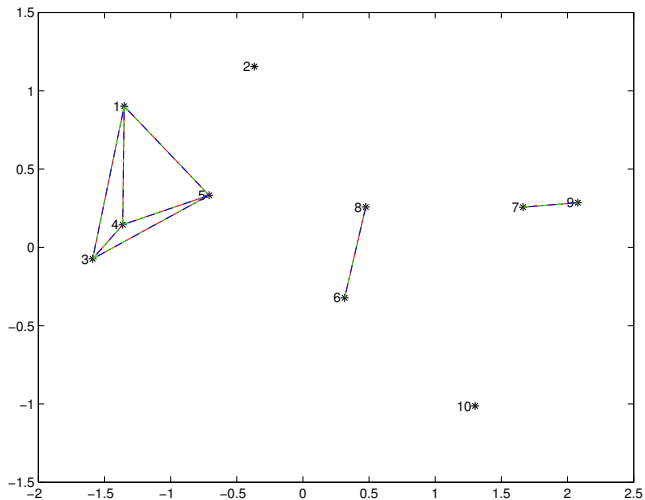
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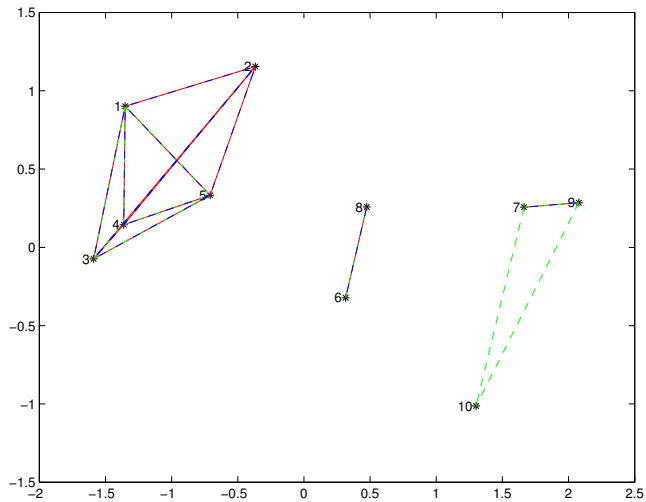


Single Linkage Complete Linkage Average Linkage

Example—Linkage Step 7

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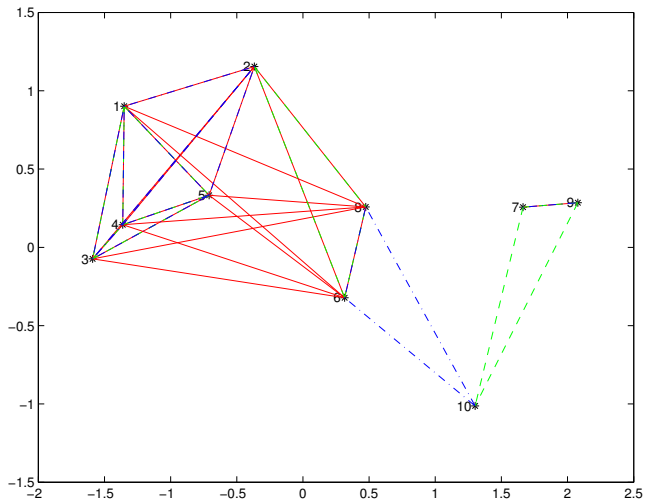
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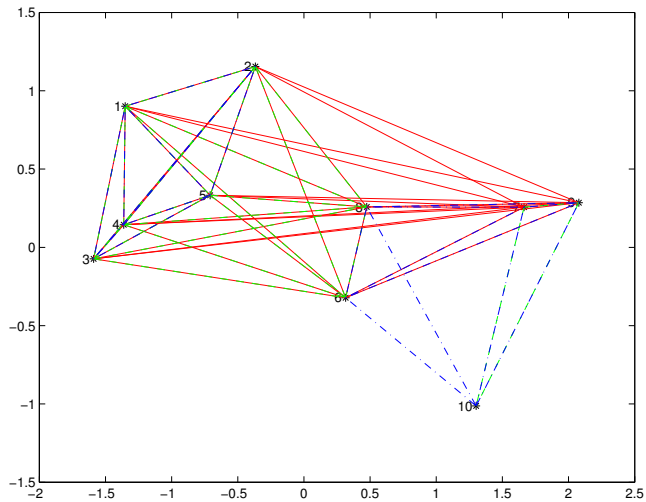
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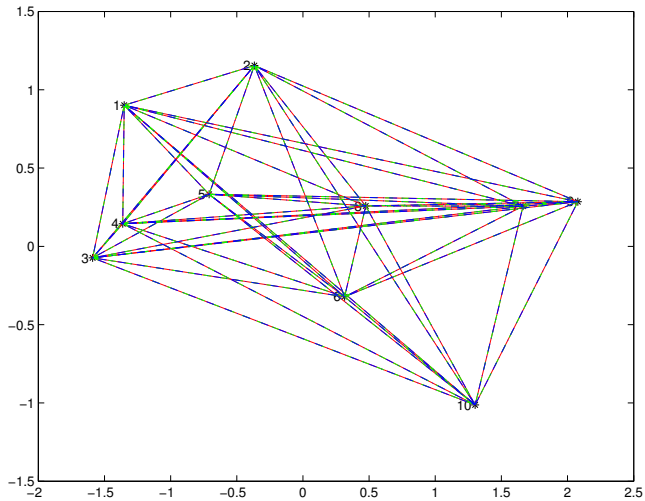
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Example—Linkage Step 10



Single Linkage Complete Linkage Average Linkage

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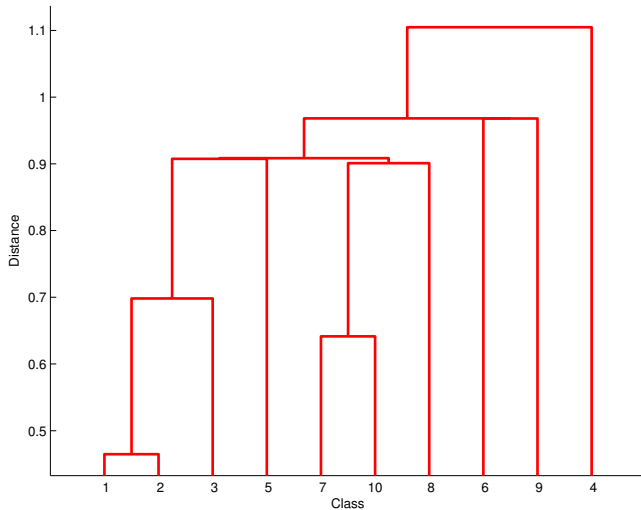
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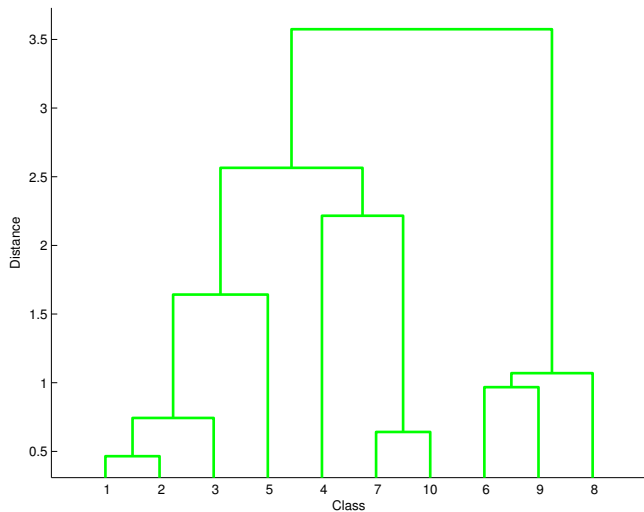
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Example–Dendrogram



Example–Dendrogram



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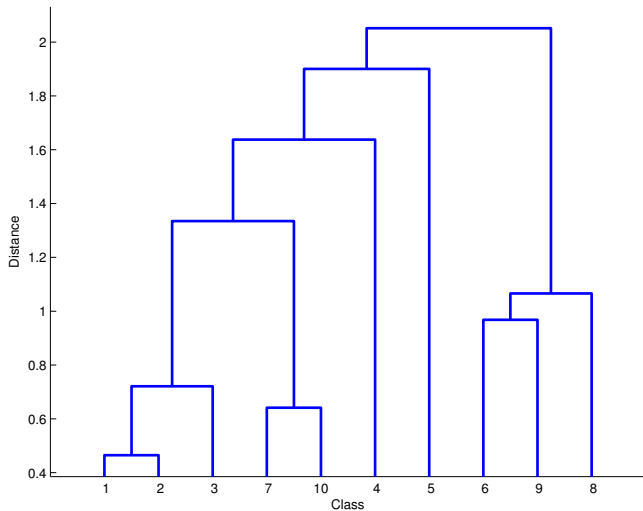
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Example–Dendrogram



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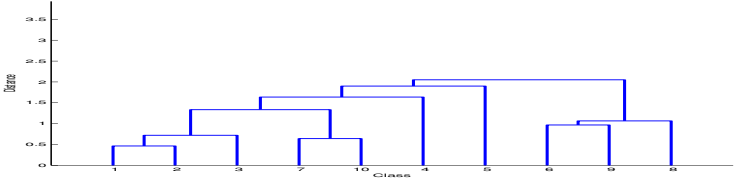
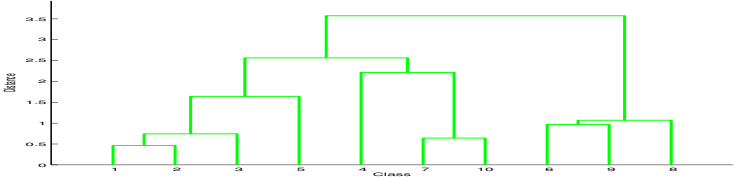
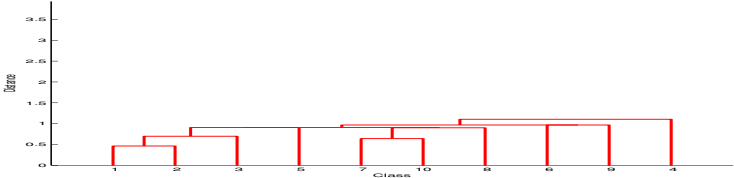
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Example–Dendrogram



Single Linkage Complete Linkage Average Linkage

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Example

Single Linkage		Complete Linkage		Average Linkage	
dist.	action	dist.	action	dist.	action
0.3151	{4, 3} → 11	0.3151	{4, 3} → 11	0.3151	{4, 3} → 11
0.4149	{9, 7} → 12	0.4149	{9, 7} → 12	0.4149	{9, 7} → 12
0.6018	{8, 6} → 13	0.6018	{8, 6} → 13	0.6018	{8, 6} → 13
0.6792	{11, 5} → 14	0.8576	{5, 1} → 14	0.8244	{11, 5} → 14
0.7568	{14, 1} → 15	1.0030	{14, 11} → 15	0.8724	{14, 1} → 15
0.8904	{15, 2} → 16	1.5119	{12, 10} → 16	1.2640	{15, 2} → 16
1.1862	{16, 13} → 17	1.6271	{13, 2} → 17	1.3598	{13, 10} → 17
1.1887	{17, 12} → 18	2.0910	{17, 15} → 18	1.4924	{17, 12} → 18
1.2038	{10, 18} → 19	3.2706	{16, 18} → 19	2.4476	{16, 18} → 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	1.02	1.00	0.76	0.86	2.07	3.08	1.94	3.48	3.27
2	1.02	0.00	1.73	1.42	0.89	1.63	2.22	1.23	2.60	2.74
3	1.00	1.73	0.00	0.32	0.97	1.92	3.27	2.09	3.68	3.04
4	0.76	1.42	0.32	0.00	0.68	1.74	3.03	1.84	3.44	2.90
5	0.86	0.89	0.97	0.68	0.00	1.22	2.37	1.19	2.79	2.42
6	2.07	1.63	1.92	1.74	1.22	0.00	1.47	0.60	1.86	1.20
7	3.08	2.22	3.27	3.03	2.37	1.47	0.00	1.19	0.41	1.32
8	1.94	1.23	2.09	1.84	1.19	0.60	1.19	0.00	1.60	1.52
9	3.48	2.60	3.68	3.44	2.79	1.86	0.41	1.60	0.00	1.51
10	3.27	2.74	3.04	2.90	2.42	1.20	1.32	1.52	1.51	0.00

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Example

Cluster distances using total linkage. Iteration: 2

	1	2	5	6	7	8	9	10	11
1	0.00	1.02	0.86	2.07	3.08	1.94	3.48	3.27	1.00
2	1.02	0.00	0.89	1.63	2.22	1.23	2.60	2.74	1.73
5	0.86	0.89	0.00	1.22	2.37	1.19	2.79	2.42	0.97
6	2.07	1.63	1.22	0.00	1.47	0.60	1.86	1.20	1.92
7	3.08	2.22	2.37	1.47	0.00	1.19	0.41	1.32	3.27
8	1.94	1.23	1.19	0.60	1.19	0.00	1.60	1.52	2.09
9	3.48	2.60	2.79	1.86	0.41	1.60	0.00	1.51	3.68
10	3.27	2.74	2.42	1.20	1.32	1.52	1.51	0.00	3.04
11	1.00	1.73	0.97	1.92	3.27	2.09	3.68	3.04	0.32

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Cluster distances using total linkage. Iteration: 3

	1	2	5	6	8	10	11	12
1	0.00	1.02	0.86	2.07	1.94	3.27	1.00	3.48
2	1.02	0.00	0.89	1.63	1.23	2.74	1.73	2.60
5	0.86	0.89	0.00	1.22	1.19	2.42	0.97	2.79
6	2.07	1.63	1.22	0.00	0.60	1.20	1.92	1.86
8	1.94	1.23	1.19	0.60	0.00	1.52	2.09	1.60
10	3.27	2.74	2.42	1.20	1.52	0.00	3.04	1.51
11	1.00	1.73	0.97	1.92	2.09	3.04	0.32	3.68
12	3.48	2.60	2.79	1.86	1.60	1.51	3.68	0.41

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Example

Cluster distances using total linkage. Iteration: 4

	1	2	5	10	11	12	13
1	0.00	1.02	0.86	3.27	1.00	3.48	2.07
2	1.02	0.00	0.89	2.74	1.73	2.60	1.63
5	0.86	0.89	0.00	2.42	0.97	2.79	1.22
10	3.27	2.74	2.42	0.00	3.04	1.51	1.52
11	1.00	1.73	0.97	3.04	0.32	3.68	2.09
12	3.48	2.60	2.79	1.51	3.68	0.41	1.86
13	2.07	1.63	1.22	1.52	2.09	1.86	0.60

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Cluster distances using total linkage. Iteration: 5

	2	10	11	12	13	14
2	0.00	2.74	1.73	2.60	1.63	1.02
10	2.74	0.00	3.04	1.51	1.52	3.27
11	1.73	3.04	0.32	3.68	2.09	1.00
12	2.60	1.51	3.68	0.41	1.86	3.48
13	1.63	1.52	2.09	1.86	0.60	2.07
14	1.02	3.27	1.00	3.48	2.07	0.86

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Cluster distances using total linkage. Iteration: 6

	2	10	12	13	15
2	0.00	2.74	2.60	1.63	1.73
10	2.74	0.00	1.51	1.52	3.27
12	2.60	1.51	0.41	1.86	3.68
13	1.63	1.52	1.86	0.60	2.09
15	1.73	3.27	3.68	2.09	1.00

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Cluster distances using total linkage. Iteration: 7

	2	13	15	16
2	0.00	1.63	1.73	2.74
13	1.63	0.60	2.09	1.86
15	1.73	2.09	1.00	3.68
16	2.74	1.86	3.68	1.51

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Cluster distances using total linkage. Iteration: 8

	15	16	17
15	1.00	3.68	2.09
16	3.68	1.51	2.74
17	2.09	2.74	1.63

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Cluster distances using total linkage. Iteration: 9

	16	18
16	0.00	3.27
18	3.27	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	1.02	1.00	0.76	0.86	2.07	3.08	1.94	3.48	3.27
2	1.02	0.00	1.73	1.42	0.89	1.63	2.22	1.23	2.60	2.74
3	1.00	1.73	0.00	0.32	0.97	1.92	3.27	2.09	3.68	3.04
4	0.76	1.42	0.32	0.00	0.68	1.74	3.03	1.84	3.44	2.90
5	0.86	0.89	0.97	0.68	0.00	1.22	2.37	1.19	2.79	2.42
6	2.07	1.63	1.92	1.74	1.22	0.00	1.47	0.60	1.86	1.20
7	3.08	2.22	3.27	3.03	2.37	1.47	0.00	1.19	0.41	1.32
8	1.94	1.23	2.09	1.84	1.19	0.60	1.19	0.00	1.60	1.52
9	3.48	2.60	3.68	3.44	2.79	1.86	0.41	1.60	0.00	1.51
10	3.27	2.74	3.04	2.90	2.42	1.20	1.32	1.52	1.51	0.00

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Example

Cluster distances using average linkage. Iteration: 2

	1	2	5	6	7	8	9	10	11
1	0.00	1.02	0.86	2.07	3.08	1.94	3.48	3.27	0.88
2	1.02	0.00	0.89	1.63	2.22	1.23	2.60	2.74	1.58
5	0.86	0.89	0.00	1.22	2.37	1.19	2.79	2.42	0.82
6	2.07	1.63	1.22	0.00	1.47	0.60	1.86	1.20	1.83
7	3.08	2.22	2.37	1.47	0.00	1.19	0.41	1.32	3.15
8	1.94	1.23	1.19	0.60	1.19	0.00	1.60	1.52	1.97
9	3.48	2.60	2.79	1.86	0.41	1.60	0.00	1.51	3.56
10	3.27	2.74	2.42	1.20	1.32	1.52	1.51	0.00	2.97
11	0.88	1.58	0.82	1.83	3.15	1.97	3.56	2.97	0.16

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Example

Cluster distances using average linkage. Iteration: 3

	1	2	5	6	8	10	11	12
1	0.00	1.02	0.86	2.07	1.94	3.27	0.88	3.28
2	1.02	0.00	0.89	1.63	1.23	2.74	1.58	2.41
5	0.86	0.89	0.00	1.22	1.19	2.42	0.82	2.58
6	2.07	1.63	1.22	0.00	0.60	1.20	1.83	1.67
8	1.94	1.23	1.19	0.60	0.00	1.52	1.97	1.40
10	3.27	2.74	2.42	1.20	1.52	0.00	2.97	1.42
11	0.88	1.58	0.82	1.83	1.97	2.97	0.16	3.36
12	3.28	2.41	2.58	1.67	1.40	1.42	3.36	0.21

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Example

Cluster distances using average linkage. Iteration: 4

	1	2	5	10	11	12	13
1	0.00	1.02	0.86	3.27	0.88	3.28	2.00
2	1.02	0.00	0.89	2.74	1.58	2.41	1.43
5	0.86	0.89	0.00	2.42	0.82	2.58	1.20
10	3.27	2.74	2.42	0.00	2.97	1.42	1.36
11	0.88	1.58	0.82	2.97	0.16	3.36	1.90
12	3.28	2.41	2.58	1.42	3.36	0.21	1.53
13	2.00	1.43	1.20	1.36	1.90	1.53	0.30

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Example

Cluster distances using average linkage. Iteration: 5

	1	2	10	12	13	14
1	0.00	1.02	3.27	3.28	2.00	0.87
2	1.02	0.00	2.74	2.41	1.43	1.35
10	3.27	2.74	0.00	1.42	1.36	2.79
12	3.28	2.41	1.42	0.21	1.53	3.10
13	2.00	1.43	1.36	1.53	0.30	1.67
14	0.87	1.35	2.79	3.10	1.67	0.44

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Example

Cluster distances using average linkage. Iteration: 6

	2	10	12	13	15
2	0.00	2.74	2.41	1.43	1.26
10	2.74	0.00	1.42	1.36	2.91
12	2.41	1.42	0.21	1.53	3.14
13	1.43	1.36	1.53	0.30	1.75
15	1.26	2.91	3.14	1.75	0.57

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Example

Cluster distances using average linkage. Iteration: 7

	10	12	13	16
10	0.00	1.42	1.36	2.87
12	1.42	0.21	1.53	3.00
13	1.36	1.53	0.30	1.69
16	2.87	3.00	1.69	0.77

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Example

Cluster distances using average linkage. Iteration: 8

	12	16	17
12	0.21	3.00	1.49
16	3.00	0.77	2.08
17	1.49	2.08	0.74

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Cluster distances using average linkage. Iteration: 9

	16	18
16	0.00	2.45
18	2.45	0.00

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