Displays for Statistics 5401

Lecture 40

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Class Web Page
http://www.stat.umn.edu/~kb/classes/5401

Hierarchical Agglomerative Algorithm

- At the start (stage 0), the clusters are {1}, {2}, ..., {N}, each object forming a cluster. Inter-cluster distances are $d_{\{i\}\{j\}} = d_{ij}$.

  A cluster with one object is sometimes called a *singleton*.

- At each stage, distances d_{UV} between each pair U and V of clusters are computed. Then the two closest clusters (smallest d_{UV}) are combined to form a larger cluster. This *reduces the number of clusters by 1*.

- At the end (stage N-1), there is just *one* cluster {1,2,...,N} consisting of all N objects.

Question:

How should you define $d_{UV} = d(U,V)$ for *sets* U and V where U and/or V are sets of objects, not individual objects?

Once you can define d_{UV}, all stages of the clustering process are completely specified except for how to deal with tied distances, if ties are possible.

Methods

The "flavors" of hierarchical agglomerative clustering differ only in how d_{UV} is defined.

All the standard methods share features:

- You can compute the (N-k-1)×(N-k-1) matrix $\mathbf{D}^{(k+1)} = [d_{UV}^{(k+1)}]$ for stage k+1 with N-k-1 clusters from $\mathbf{D}^{(k)}$, and for some methods, the cluster sizes N_U, N_V and N_W.
- Distances between non-merged clusters are unchanged.

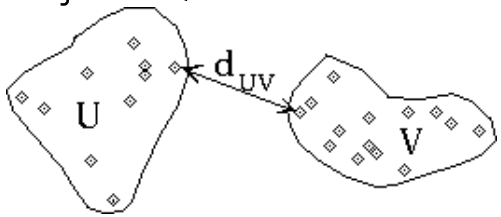
You need at most two (three with Ward, centroid, and median methods) rows and columns of $\mathbf{D}^{(k)}$ to compute a row and column of $\mathbf{D}^{(k+1)}$, plus possibly cluster sizes.

This is the "updating" ($\mathbf{D}^{(k)} \rightarrow \mathbf{D}^{(k+1)}$) step.

- **Single linkage** (minimum distance)

$$d_{UV} = d(U,V) \equiv \min_{i \text{ in } U,\ j \text{ in } V} d_{ij}$$

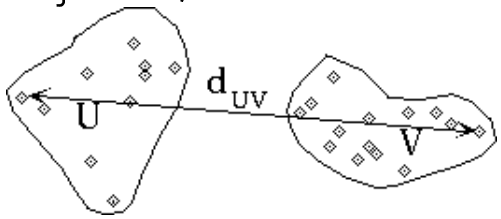
2 clusters are as close as the 2 closest objects, 1 from each cluster.



- **Complete linkage** (maximum distance)

$$d_{UV} \equiv d(U,V) = \max_{i \text{ in } U,\ j \text{ in } V} d_{ij}$$

2 clusters are as close as the 2 most *distant* objects, 1 from each cluster.



In my experience, complete linkage never seems to do a good job of clustering.

Single linkage sometimes does better, but tends to find long thin clusters.

- **Average linkage** (average distance)

$$d_{UV} = d(U,V) \equiv \sum_{i \text{ in } U,\ j \text{ in } V} d_{ij}/(N_U N_V)$$

This is an *average* distance since there are $N_U N_V$ pairs (i,j), $i \in U$, $j \in V$.

This often works well and is a useful default.

Geometrically motivated methods

Suppose you can define cluster "centers" $\mathbf{C}_U$ and $\mathbf{C}_V$. Then when $d_{ij} = d(\mathbf{x}_i, \mathbf{x}_j)$ are distances between data points, a measure of intercluster distance might be

$$d_{UV} = d(U,V) = d(\mathbf{C}_U, \mathbf{C}_V).$$

Or you might use cluster sizes N_U and N_V to adjust raw distances $d(\mathbf{C}_U, \mathbf{C}_V)$.

When distance updating rules don't use the centers explicitly you can use such methods even when "centers" make no sense, as is the case when all you have is a distance matrix $\mathbf{D}$.

- **Centroid method**
  $d_{UV} = d(U,V) = d(\mathbf{C}_U, \mathbf{C}_V)$, where $\mathbf{C}_U$ is the "centroid" of the group.

  When $d_{ij} = \|\mathbf{x}_i - \mathbf{x}_j\|^2$, $\mathbf{C}_U$ is $\overline{\mathbf{x}}_U$ and

  $$d(U,V) = \|\overline{\mathbf{x}}_U - \overline{\mathbf{x}}_V\|^2 = \sum_{1 \le k \le p} (\overline{x}_{kU} - \overline{x}_{kV})^2$$

You need only the formula for $d_{W,\{U,V\}}^{(k+1)}$ so you can use the centroid method in the absence of any centroids.

You can use the same centers and updating formula for a generalized distance

$$d_{ij} = (\mathbf{x}_i - \mathbf{x}_j)' \mathbf{A}^{-1} (\mathbf{x}_i - \mathbf{x}_j),$$

where $\mathbf{A}$ is positive definite.

- **Ward method**

This uses centroids as centers, but the distance between centers is weighted by a factor depending on cluster sizes.

$$d_{UV} = d(U,V) = (N_U N_V/(N_U+N_V))\times d(\mathbf{C}_U, \mathbf{C}_V)$$
$$= d(\mathbf{C}_U, \mathbf{C}_V)/(1/N_U + 1/N_V)$$

When $d_{ij} = \|\mathbf{x}_i - \mathbf{x}_j\|^2$, $\mathbf{C}_U = \overline{\mathbf{x}}_u$,

$d_{UV} = \text{trace } \mathbf{H}_{UV}$

where

$$\mathbf{H}_{UV} \equiv (N_U N_V/(N_U+N_V))(\overline{\mathbf{x}}_U - \overline{\mathbf{x}}_V)(\overline{\mathbf{x}}_U - \overline{\mathbf{x}}_V)'$$

is the *among groups* hypothesis matrix in a <u>two group MANOVA</u>.

Two large clusters are more distant than a pair of smaller clusters whose means are the same distance apart. This helps prevent merges of groups that are "significantly" different.

This works best with "spherical clusters" with $\mathbf{\Sigma}_\ell \cong K\mathbf{I}_p$.

- **Median method**

$d_{UV} = d(U,V) = d(\mathbf{C}_U, \mathbf{C}_V)$, but $\mathbf{C}_{\{U,V\}}$ is half way between the $\mathbf{C}_U$ and $\mathbf{C}_V$ regardless of the size of the clusters.

- **McQuitty method**

There is no clear geometry based on centers. It is defined solely in terms of an updating formula.

$$d_{W,\{U,V\}}^{(k+1)} = (d_{UW}^{(k)} + d_{VW}^{(k)})/2.$$

The distance from W to the new cluster {U,V} is the average of the distances from W to U and from W to V and makes no use of $d_{UV}^{(k)}$.

Example from handout, N = 8, p = 2

Data were generated as samples from 3 bivariate normal populations.

	μ_i	Σ_i	n_i
π_1	$\begin{bmatrix} 10 \\ 30 \end{bmatrix}$	$\begin{bmatrix} 4 & 0 \\ 0 & 4 \end{bmatrix}$	3
π_2	$\begin{bmatrix} 15 \\ 28 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & 2.25 \end{bmatrix}$	3
π_3	$\begin{bmatrix} 20 \\ 31 \end{bmatrix}$	$\begin{bmatrix} 2.25 & 0 \\ 0 & 0.25 \end{bmatrix}$	2

Here are the data

```
Cmd> x # row label is population number
          x1        x2
2     15.606    27.451
1     7.2295     29.53
1     9.9958    30.821
3     17.241     31.21
2     16.212    25.889
1     10.644    28.937
3     20.954    31.244
2     14.528    24.695
```

The row labels are population numbers which you would not have in a real problem.

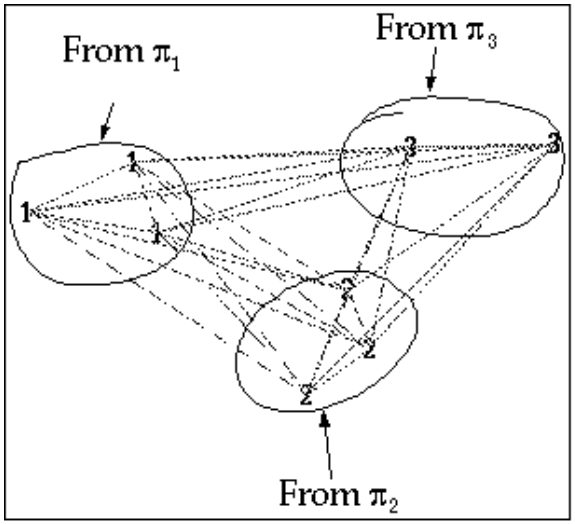
Compute the standardized distances between cases

```
Cmd> d <- matrix(dmat(8,0),\
       labels:structure(getlabels(x,1),getlabels(x,1)))

Cmd> xs <- standardize(x)

Cmd> for(i,1,7){for(j,i+1,8){ # loop over 1 <= i < j <= 8
       d[i,j] <- d[j,i] <- \
          sqrt(sum(vector((xs[i,]-xs[j,]))^2));;}}

Cmd> print(d,format:"6.3f")
d:
       2      1      1      3      2      1      3      2
2  0.000  2.052  1.845  1.551  0.641  1.260  1.936  1.131
1  2.052  0.000  0.807  2.340  2.485  0.800  3.148  2.536
1  1.845  0.807  0.000  1.629  2.418  0.769  2.459  2.658
3  1.551  2.340  1.629  0.000  2.147  1.735  0.831  2.683
2  0.641  2.485  2.418  2.147  0.000  1.746  2.396  0.609
1  1.260  0.800  0.769  1.735  1.746  0.000  2.486  1.911
3  1.936  3.148  2.459  0.831  2.396  2.486  0.000  2.995
2  1.131  2.536  2.658  2.683  0.609  1.911  2.995  0.000
```



Plot with all lines between points.

Reorder distances so that groups are together.

```
Cmd> neworder <- vector(2,3,6,1,5,8,4,7)

Cmd> print(d[neworder, neworder],format:"6.3f")
MATRIX:
```

	1	1	1	2	2	2	3	3
1	0.000	0.807	0.800	2.052	2.485	2.536	2.340	3.148
1	0.807	0.000	0.769	1.845	2.418	2.658	1.629	2.459
1	0.800	0.769	0.000	1.260	1.746	1.911	1.735	2.486
2	2.052	1.845	1.260	0.000	0.641	1.131	1.551	1.936
2	2.485	2.418	1.746	0.641	0.000	0.609	2.147	2.396
2	2.536	2.658	1.911	1.131	0.609	0.000	2.683	2.995
3	2.340	1.629	1.735	1.551	2.147	2.683	0.000	0.831
3	3.148	2.459	2.486	1.936	2.396	2.995	0.831	0.000

Intra-cluster distances are smaller than inter-cluster distances.

That is the basis for most clustering algorithms.

Here's a "magic" way to compute **d**:

```
Cmd> temp <- xs %*% xs'

Cmd> d <- sqrt(diag(temp) + diag(temp)' - 2*temp)

Cmd> print(d,format:"6.3f")
dd:
```

	2	1	1	3	2	1	3	2
2	0.000	2.052	1.845	1.551	0.641	1.260	1.936	1.131
1	2.052	0.000	0.807	2.340	2.485	0.800	3.148	2.536
1	1.845	0.807	0.000	1.629	2.418	0.769	2.459	2.658
3	1.551	2.340	1.629	0.000	2.147	1.735	0.831	2.683
2	0.641	2.485	2.418	2.147	0.000	1.746	2.396	0.609
1	1.260	0.800	0.769	1.735	1.746	0.000	2.486	1.911
3	1.936	3.148	2.459	0.831	2.396	2.486	0.000	2.995
2	1.131	2.536	2.658	2.683	0.609	1.911	2.995	0.000

Distances for standardized data.

	2	1	1	3	2	1	3	2
2	0.000	2.052	1.845	1.551	0.641	1.260	1.936	1.131
1	2.052	0.000	0.807	2.340	2.485	0.800	3.148	2.536
1	1.845	0.807	0.000	1.629	2.418	0.769	2.459	2.658
3	1.551	2.340	1.629	0.000	2.147	1.735	0.831	2.683
2	0.641	2.485	2.418	2.147	0.000	1.746	2.396	0.609
1	1.260	0.800	0.769	1.735	1.746	0.000	2.486	1.911
3	1.936	3.148	2.459	0.831	2.396	2.486	0.000	2.995
2	1.131	2.536	2.658	2.683	0.609	1.911	2.995	0.000

```
Cmd> cluster(x) # cluster using Average Linkage (default)
 Case  Number of Clusters
```

```
No.    2  3  4  5  6  7  8   n - stage number
----  -- -- -- -- -- -- --
  1   1  1  1  1  1  1  1
  2   1  1  3  3  3  3  3      Class Table
  3   1  3  3  3  6  6  6
  4   2  2  2  2  2  2  2    cluster ID
  5   1  1  4  4  4  4  4    numbers
  6   1  3  3  3  6  7  7
  7   2  2  2  5  5  5  5
  8   1  1  4  4  4  4  8
```

Merging from right to left

```
Criterion       Dendrogram (inverted tree)
                +
      2.3442    +-----------------+
      2.1453    +--------+        |
     0.91951    +--+     |        |
     0.83117    |  |     |        +--+
     0.80378    |  |     +--+     |  |
     0.76945    |  |     |  +--+  |  |
     0.60943    |  +--+  |  |  |  |  |
  Cluster No.   1  4  8  3  6  7  2  5
   Clusters 1 to 8 (Top 7 levels of hierarchy).
   Clustering method: Average linkage
   Distance: Euclidian (standardized)
```

Merging from bottom to top

Each step up is a joining of paths reflecting a merge.

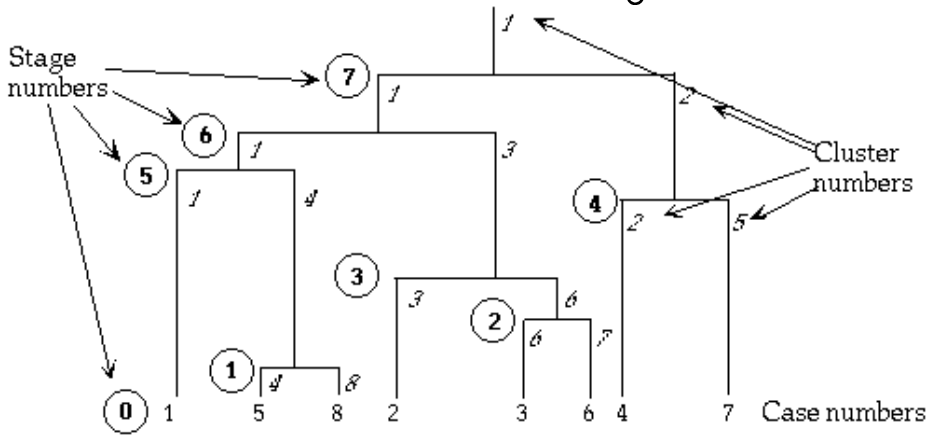
The numbers in the **Criterion** column are the distances between the two clusters being merged at that stage.

A sharp increase going *up* the **Criterion** column suggests the merge may have involved dissimilar clusters that perhaps should *not* be merged. Such jumps are the basis of common ways to choose the number of clusters.

Across the bottom are *cluster* (not case) numbers. The corresponding *case* numbers are (see the class table)

Cluster number	1	2	3	4	5	6	7	8
Case numbers	1	4	2	5	7	3	6	8

A more conventional dendrogram is



Cluster numbers are in *italics*, case numbers at bottom. Numbers in circles ④ are the stage numbers.

Often the vertical dimension in a dendrogram is the distance between the two clusters being merged (**Criterion** in **cluster()** output). That way you can visually identify stages where there are sharp changes in the criterion.

A hard thing to understand in **cluster()** output is recognizing there is no simple matching of case numbers and cluster ID numbers.

You learn the matching *only* from the Class Table where each row goes with a case.

The numbers in the table are cluster numbers which **cluster()** assigns after clustering is complete. This is done in such a way that, at the stage when there are k clusters, cluster k is merged with a cluster with lower number.

Details of average linkage process (**boldface** are cluster numbers; case numbers are in {...}):

- Stage 0 (all cases separate clusters)
  1={1}, **2**={4}, **3**={2}, **4**={5}, **5**={7}, **6**={3}, **7**={6}, **8**={8}
- Stage 1 (merge clusters **4** and **8**)
  1={1}, **2**={4}, **3**={2}, **4**={5,8}, **5**={7}, **6**={3}, **7**={6}

  4={5} and **8**={8} were merged because minimum distance (0.609) is between cases 5 and 8

  Update distances:

  $d(\mathbf{1},\mathbf{4}) = d(\{1\},\{5,8\}) = (d_{1,5}+d_{1,8})/2$
  $= (.641+1.131)/2 = 0.886,$

  $d(\mathbf{2},\mathbf{4}) = d(\{4\},\{5,8\}) = (d_{4,5}+d_{4,8})/2$
  $= (2.147 + 2.683)/2 = 2.415,$

  $d(\mathbf{3},\mathbf{4}) = d(\{2\},\{5,8\}) = (d_{2,5}+d_{2,8})/2$
  $= (2.485 + 2.536)/2 = 2.5105,$

  etc. All exceed .769

- Stage 2 (merge clusters **6** and **7**)
  1={1}, **2**={4}, **3**={2}, **4**={5,8}, **5**={7}, **6**={3,6}

  You merge **6**={3} and **7**={6} because all the new distances as well as $d_{1,4}$, $d_{1,2}$, etc. are larger than $d_{3,6}$ = .769
- Stage 3 (merge clusters **3** and **6**)
  1={1}, **2**={4}, **3**={2,3,6}, **4**={5,8}, **5**={7}
- Stage 4 (merge clusters **2** and **5**)
- Stage 5 (merge clusters **1** and **4**)
  1={1,5,8}, **2**={4,7}, **3**={2,3,6}
- Stage 6 (merge clusters **1** and **3**)
  1={1,2,3,5,6,8}, **2**={4,7}
- Stage 7 **1**={1,2,3,4,5,6,7,8} (merge clusters **1** and **2**; not shown)

This history is summed up in this table

Clus ID	1	2	3	4	5	6	7	8
Stage 0	{1}	{4}	{2}	{5}	{7}	{3}	{6}	{8}
Stage 1	{1}	{4}	{2}	{5,8}	{7}	{3}	{6}	
Stage 2	{1}	{4}	{2}	{5,8}	{7}	{3,6}		
Stage 3	{1}	{4}	{2,3,6}	{5,8}	{7}			
Stage 4	{1}	{4,7}	{2,3,6}	{5,8}				
Stage 5	{1,5,8}	{4,7}	{2,3,6}					
Stage 6	{1,2,3,5,6,8}	{4,7}						
Stage 7	{1,2,3,4,5,6,7,8}							

From the jump in the criterion, the place to stop and accept the clusters found is at stage 5 when there are 3 clusters. In a real problem, it is never this clear.

Updating Formulas

- Single linkage

$$d_{W,\{U,V\}}^{(k+1)} = \min\{d_{WU}^{(k)}, d_{WV}^{(k)}\}$$

- Complete linkage

$$d_{W,\{U,V\}}^{(k+1)} = \max\{d_{WU}^{(k)}, d_{WV}^{(k)}\}$$

- Average linkage

$$d_{W,\{U,V\}}^{(k+1)} = (N_U d_{WU}^{(k)} + N_V d_{WV}^{(k)})/(N_U + N_V)$$

This uses the sizes N_U and N_V of the clusters being merged, but not the size N_W of W or $d_{UV}^{(k)}$.

These "linkage" methods do not make use of $d_{UV}^{(k)}$ in updating.

- Centroid method

$$C_{\{U,V\}}^{(k+1)} = (N_U C_U^{(k)} + N_V C_V^{(k)})/(N_U + N_V)$$

$$d_{W,\{U,V\}}^{(k+1)} = \frac{N_V d_{WU}^{(k)} + N_U d_{WV}^{(k)} - N_U N_V d_{UV}^{(k)}}{N_U + N_V}$$

Since only the formula for $d_{W,\{U,V\}}^{(k+1)}$ is needed, you can use the centroid method in the absence of real centroids.

- Ward method

$$C_{\{U,V\}}^{(k+1)} = (N_U C_U^{(k)} + N_V C_V^{(k)})/(N_U + N_V)$$

$$d_{W,\{U,V\}}^{(k+1)} = \{M_{UW} d_{UW}^{(k)}/N_V + M_{VW} d_{VW}^{(k)}/N_U - d_{UV}^{(k)}/(N_U N_V)\}$$

with $M_{UW} = 1/N_U + 1/N_W$. This uses N_W, and is the only one of these methods that does so.

- Median method

$$C_{\{U,V\}}^{(k+1)} = (C_U^{(k)} + C_V^{(k)})/2$$

$$d_{W,\{U,V\}}^{(k+1)} = (d_{UW}^{(k)} + d_{VW}^{(k)})/2 - d_{UV}^{(k)}/4$$

The new center is half way between the old centers regardless of the size of the clusters.

- McQuitty method is defined purely by the updating formula

$$d_{W,\{U,V\}}^{(k+1)} = (d_{UW}^{(k)} + d_{VW}^{(k)})/2$$

Usage of `cluster()`

`cluster(x,nclust:m,method:"average")`, x a n by p matrix,

- uses average linkage.
- prints the part of the class table describing 2 to m clusters
- prints the dendrogram for stages N-m, N-m+1, ... , N-1 (m down to 1 cluster).

It does the full computation starting with N clusters but prints results only for stages with min(m,N) clusters or fewer.

Instead of `"average"` (the default) you can use `"single"`, `"complete"`, `"ward"`, `"mcquitty"`, `"median"` or `"centroid"` to specify other "flavors".

`cluster(dissim:d,...)` and `cluster(simil:s,...)` do cluster analysis on n by n dissimilarity or similarity matrices.

```
cluster(x,nclust:15,method:"average",\
   reorder:T)
```

prints the class table with *reordered* rows, grouping cases into clusters. This makes it easier to see which cases are in each cluster.

```
Cmd> cluster(x,reorder:T,tree:F)
 Case  Number of Clusters
 No.   2  3  4  5  6  7  8
 ---- -- -- -- -- -- -- --
   1   1  1  1  1  1  1  1
   5   1  1  4  4  4  4  4
   8   1  1  4  4  4  4  8
   2   1  3  3  3  3  3  3
   3   1  3  3  3  6  6  6
   6   1  3  3  3  6  7  7
   4   2  2  2  2  2  2  2
   7   2  2  2  5  5  5  5
```

Cases are not in original order
1st 3 from group 2, next 2 from group 1, last 3 from group 3

I suppressed printing the dendrogram by `tree:F`.

The original groups were

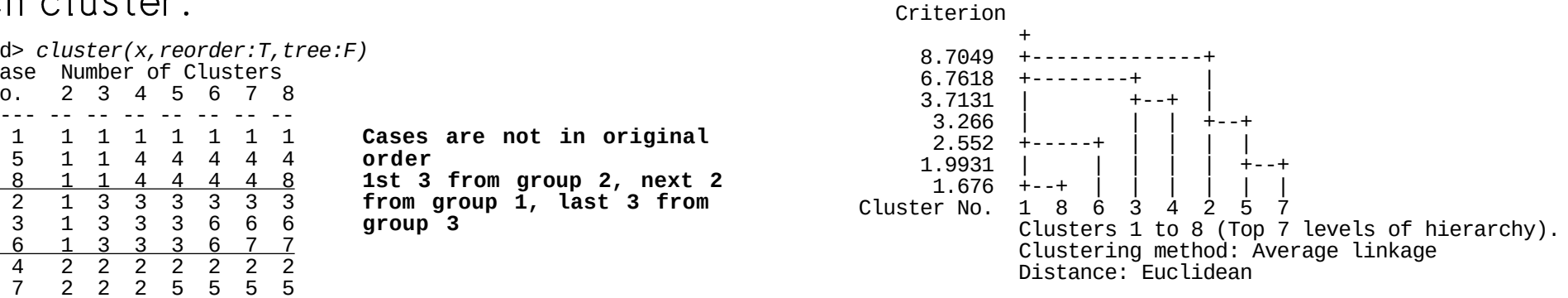
- Group 1: {2, 3, 6} (cluster **3** of 3)
- Group 2: {1, 5, 8} (cluster **1** of 3)
- Group 3: {4, 7} (cluster **2** of 3)

The class table shows that at stage 5 the 3 clusters match these "true" clusters but have different numbers.

If you don't want to standardize before computing distances, use `standard:F`.

If you don't want to print the class table use `class:F`

```
Cmd> cluster(x,standard:F,class:F)
```



This printed only the dendrogram (`class:F`) and used *non-standardized* Euclidean distance (`standard:F`). The biggest jump in the criterion is at the stage when 3 clusters are merged to become 2 clusters.

You can save the values of the criterion, the distances between objects, and the class table.

```
Cmd> stuff <- cluster(x,keep:"all") #prints nothing by default

Cmd> compnames(stuff)
(1) "distances"      8 by 8 symmetric matrix
(2) "classes"        class table
(3) "criterion"      distance apart of merged clusters

Cmd> print(format:"6.3f", stuff)
STRUCTURE:
component: distances    standardized distances
(1,1)  0.000  2.052  1.845  1.551  0.641  1.260  1.936  1.131
(2,1)  2.052  0.000  0.807  2.340  2.485  0.800  3.148  2.536
(3,1)  1.845  0.807  0.000  1.629  2.418  0.769  2.459  2.658
(4,1)  1.551  2.340  1.629  0.000  2.147  1.735  0.831  2.683
(5,1)  0.641  2.485  2.418  2.147  0.000  1.746  2.396  0.609
(6,1)  1.260  0.800  0.769  1.735  1.746  0.000  2.486  1.911
(7,1)  1.936  3.148  2.459  0.831  2.396  2.486  0.000  2.995
(8,1)  1.131  2.536  2.658  2.683  0.609  1.911  2.995  0.000
component: classes      Same as class table
(1,1)  1.000  1.000  1.000  1.000  1.000  1.000  1.000
(2,1)  1.000  3.000  3.000  3.000  3.000  3.000  3.000
(3,1)  1.000  3.000  3.000  3.000  6.000  6.000  6.000
(4,1)  2.000  2.000  2.000  2.000  2.000  2.000  2.000
(5,1)  1.000  1.000  4.000  4.000  4.000  4.000  4.000
(6,1)  1.000  3.000  3.000  3.000  6.000  7.000  7.000
(7,1)  2.000  2.000  2.000  5.000  5.000  5.000  5.000
(8,1)  1.000  1.000  4.000  4.000  4.000  4.000  8.000
component: criterion    in reverse order of computation
(1)  2.344  2.145  0.920  0.831  0.804  0.769  0.609
```

If you don't want everything, the value of `keep` can be `"classes"`, `"criterion"`, `"distances"`, `vector("classes", "criterion")`, `vector("classes", "distances")` or `vector("criterion", "distances")`

The class table table has m-1 columns, where m is the value of keyword `nclust` (default 9). The column labeled j summarizes the allocation into j clusters.

Using `keep` usually suppresses printing, but `tree:T` or `classes:T` force printing the dendrogram or the class table. `print:T` prints both.

Check one of the distances:

Macro `euclid(x,y)` computes Euclidean distance $\|\mathbf{x} - \mathbf{y}\|$ and `standardize(x)` standardizes the columns of `x`.

```
Cmd> euclid <- macro("sqrt(sum(vector(($1)-($2))^2))")

Cmd> xs <- standardize(x) # standardize data

Cmd> euclid(xs[1,],xs[2,])#row 1 - row 2  standardized distance
(1)      2.0519
```

Compare 2.0519 with the value in row 1, column 2 of the distance table above.