IV — What is Cluster Analysis?

Reference:
B. Le Roux, *L'analyse géométrique des données multidimensionnelles*, Dunod 2014, Chapters 10 & 11.

IV.1. The Aim of Cluster Analysis

Construct homogeneous clusters of objects (in GDA subclouds of points) so that:

- *compactness* criterion: objects within a same cluster are as much similar as possible;
- *separability* criterion: objects belonging to different clusters are as little similar as possible.

The greater the similarity (or homogeneity) within a cluster and the greater the difference between clusters the better the clustering.

heterogeneity between clusters — homogeneity within clusters

Types of Clustering

1. algorithms leading to partitions.
   Partitional clustering decomposes a data set into a set of disjoint clusters.
   two following requirements:
   1) each group contains at least one point,
   2) each point belongs to exactly one group.
   clustering around moving centers or *K*-means cluster analysis.

2. algorithms leading to hierarchical clustering (the paradigm of natural sciences): system of nested clusters represented by a hierarchical tree or *dendrogram*.
   - ascending algorithms (AHC)
   - descending algorithms (segmentation methods):
     problems of discrimination and regression by gradual segmentation of the set of objects $\rightarrow$ binary decision tree
     (methods AID, CART, etc.).

The methods of type 1 are *geometric* methods.

The method of type AHC is *geometric* if the distance is Euclidean and the aggregation index is the variance index.

The methods of type "segmentation" are not geometric.

The number of partitions into k clusters of n objects

n		k		
5 objects	into	2 clusters	=	15
10 objects	into	2 clusters	=	511
10 objects	into	5 clusters	=	42 525

etc.

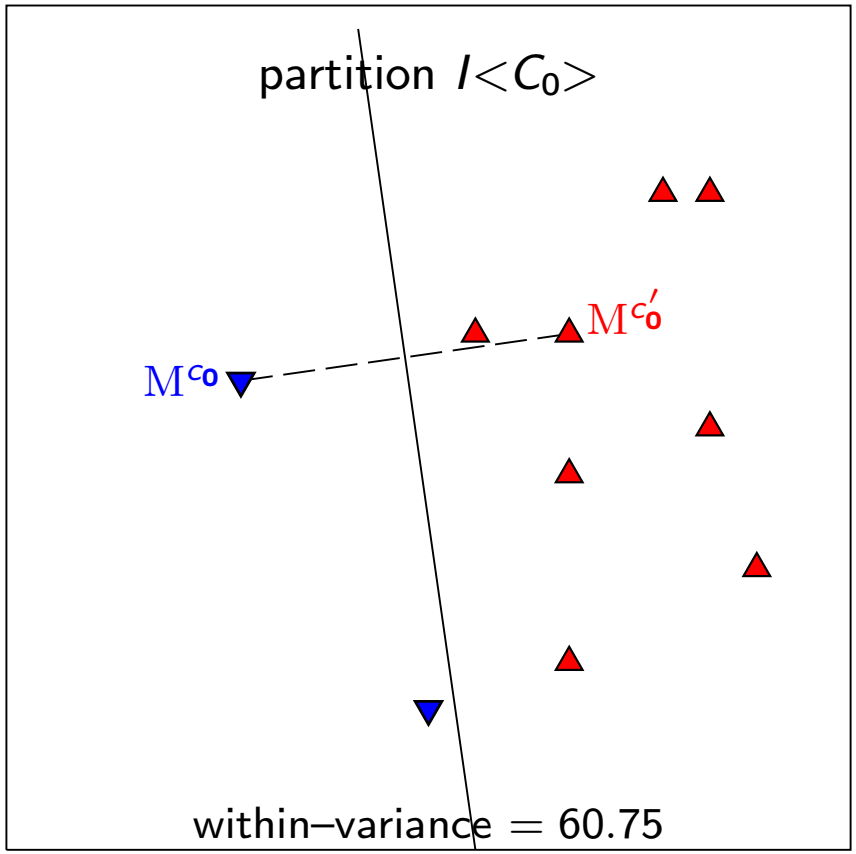
Except for small n, it is impossible to enumerate all the partitions of n individuals into k clusters

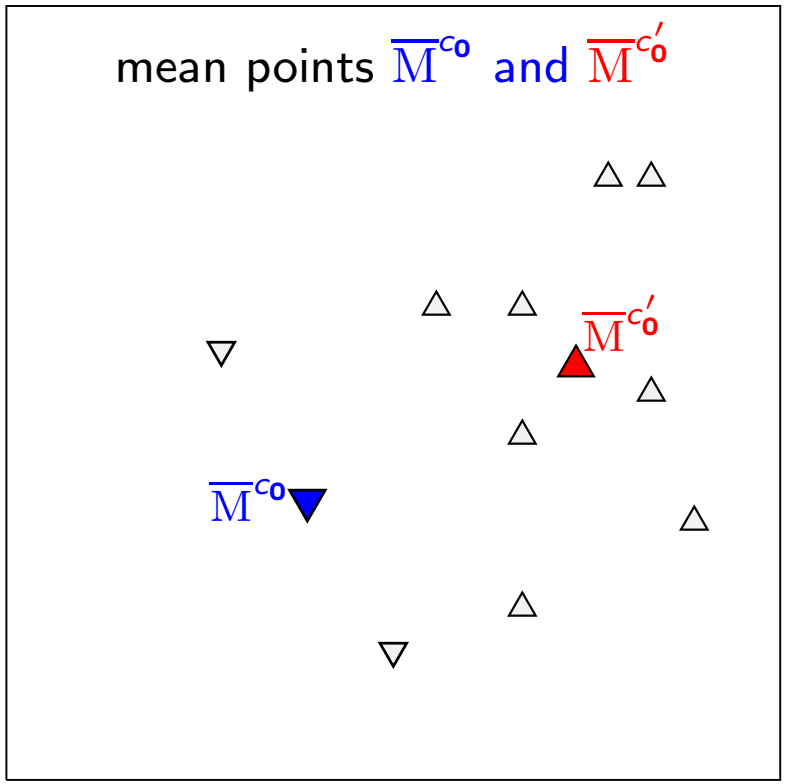
IV.2. K–means Clustering

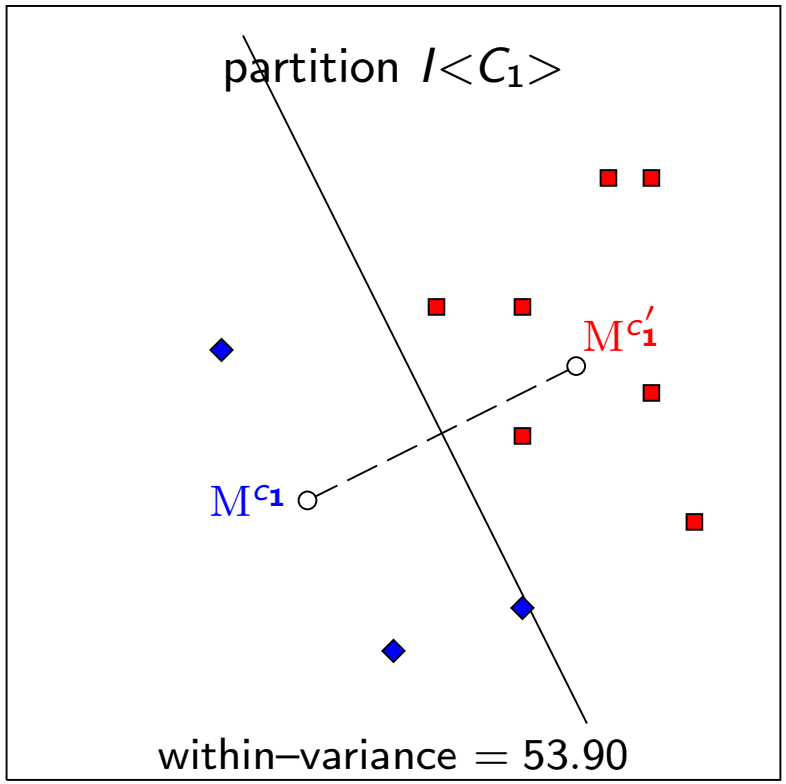
or aggregation around *moving centers*

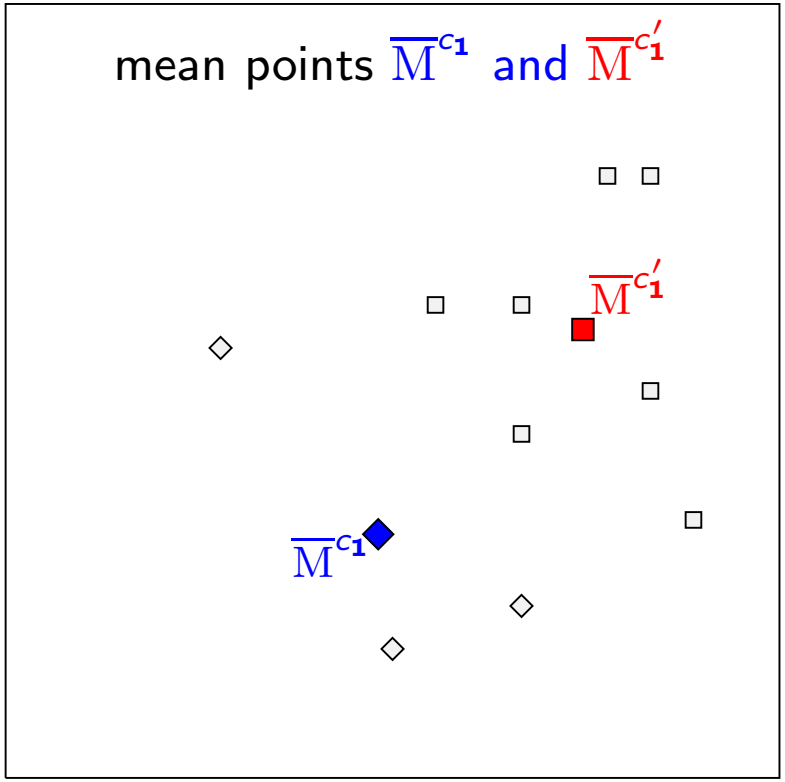
1. Fix the number of clusters, say C;
2. Choose (randomly or not) C initial class centers;
3. Assign each object to the closest center $\rightarrow$ new clusters;
4. Determine the centers of the new clusters;
5. Repeat the assignment;
6. Stop the algorithm when 2 successive iterations provide the same clusters.

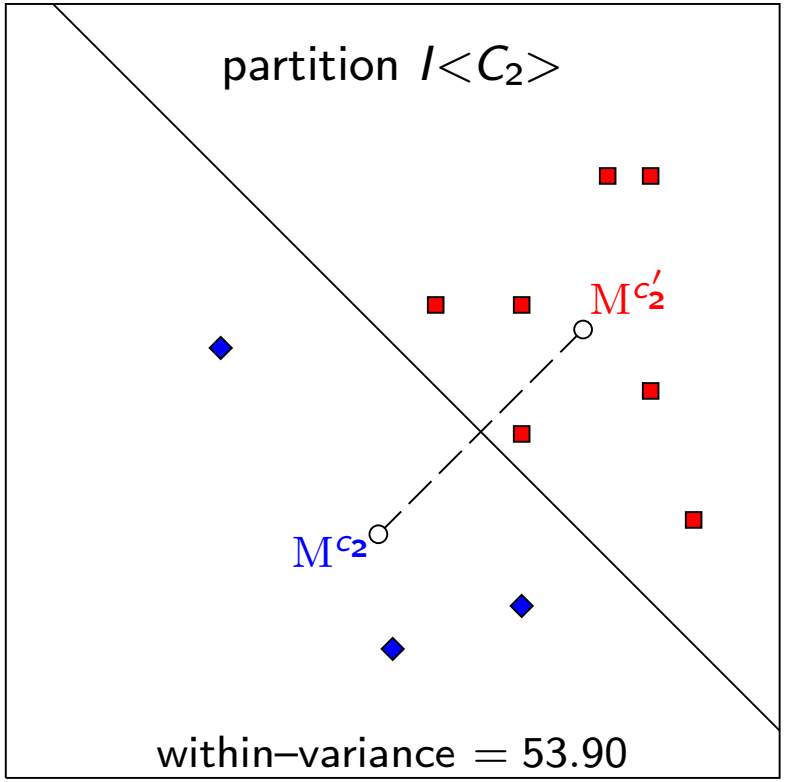
Choose 2 initial centers: M^{c_0} and $M^{c'_0}$




mean points $\overline{M}^{c_0}$ and $\overline{M}^{c'_0}$
$\overline{M}^{c'_0}$
$\overline{M}^{c_0}$


partition $I<C_1>$
$M^{c'_1}$
M^{c_1}
within–variance = 53.90





- Advantage: method is fast
- Disavantadge: The solution depends on the choice of initial centers.

IV.3. Ascending Hierarchical Clustering (AHC)

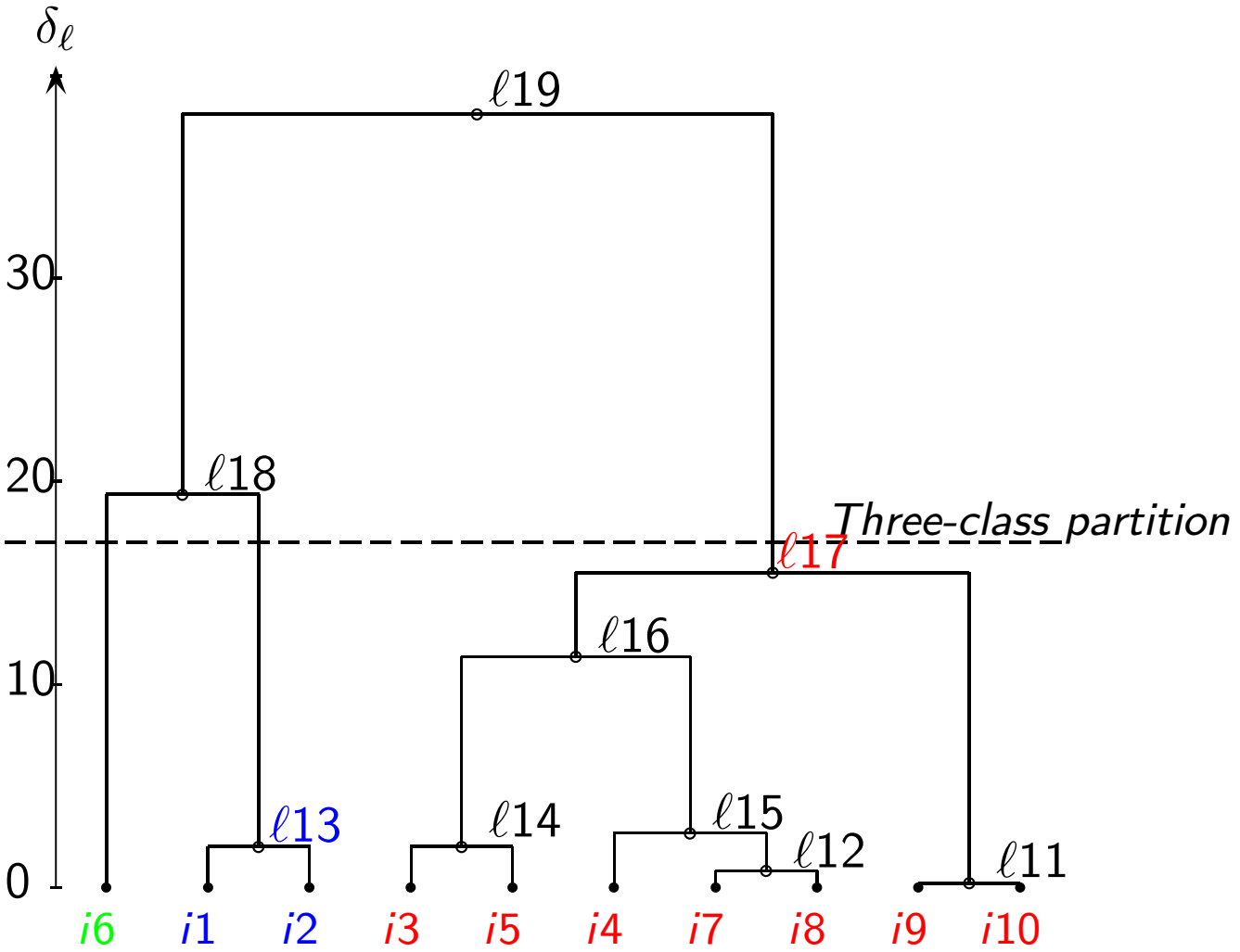
Clusters =

either the objects to be clustered (one–element class),
or the clusters of objects generated by the algorithm.

At each step, one groups the two elements which are the closest, hence the representation by a *hierarchical tree* or dendrogram.

We have to define the notion of "close", that is, the aggregation index.

Target example: hierarchical tree



Ascending/agglomerative Hierarchical Clustering

Start with the basic objects (one–element clusters)
proceed to successive aggregations
until all objects are grouped in a single class.

AHC works "bottom–up".

IV.4. Euclidean Clustering

1. Objects = *points of Euclidean cloud*.
2. *Aggregation index* (variance index) is the contribution of the two centers of the classes to be grouped (Ward's index).

Grouping property

If 2 clusters are *grouped*, the variance *decreases* from an amount equal to the contribution of the two centers of the clusters that are grouped.

Basic Algorithm

- **Step 1**. Calculate the contributions of the $9 \times 10/2 = 45$ pairs of points:

δ	$i1$	$i2$	$i3$	$i4$	$i5$	$i6$	$i7$	$i8$	$i9$
$i2$	2								
$i3$	11.6	4							
$i4$	6.8	3.2	4						
$i5$	14.4	6.8	2	2					
$i6$	13	17	27.4	10.6	20.2				
$i7$	13	10.6	12.2	2.6	5.8	5.2			
$i8$	14.6	9.8	8.2	1.8	2.6	10	0.8		
$i9$	29.2	20.8	13.6	8	5.2	19.4	5	2.6	
$i10$	31.4	21.8	13	9	5	23.2	6.8	3.6	0.2

Minimum index 0.2 for the pair of points $\{i9, i10\}$ which are aggregated (fig. 1), hence the mean point $\ell 11$ and a derived *cloud of 9 points* (fig. 2).

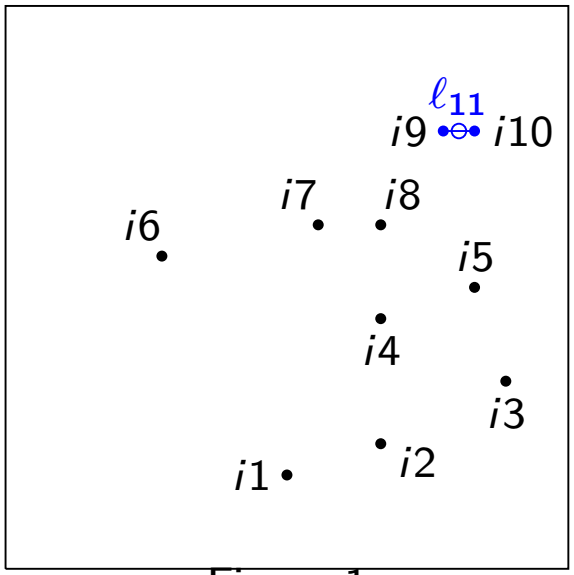
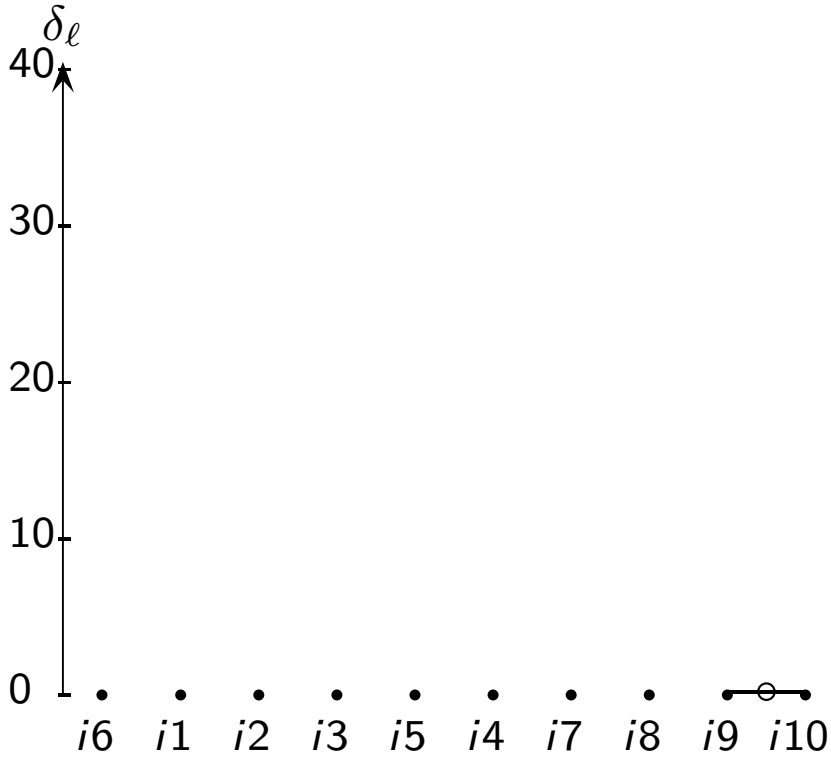


Figure 1



• **Step 2.** Calculate the aggregation index between the new point ℓ_{11} and the 8 other points.
New minimum 0.8 for $\{i7, i8\}$ which aggregated (fig. 2), hence the new point $\ell 12$ and a derived *cloud of 8 points* (fig. 3).

	$i1$	$i2$	$i3$	$i4$	$i5$	$i6$	$i7$	$i8$
ℓ_{11}	40.33	28.33	17.67	11.27	6.73	28.33	7.8	4.07

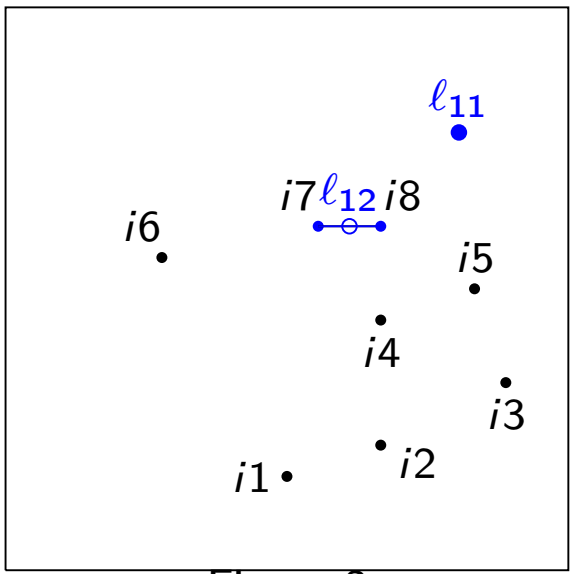
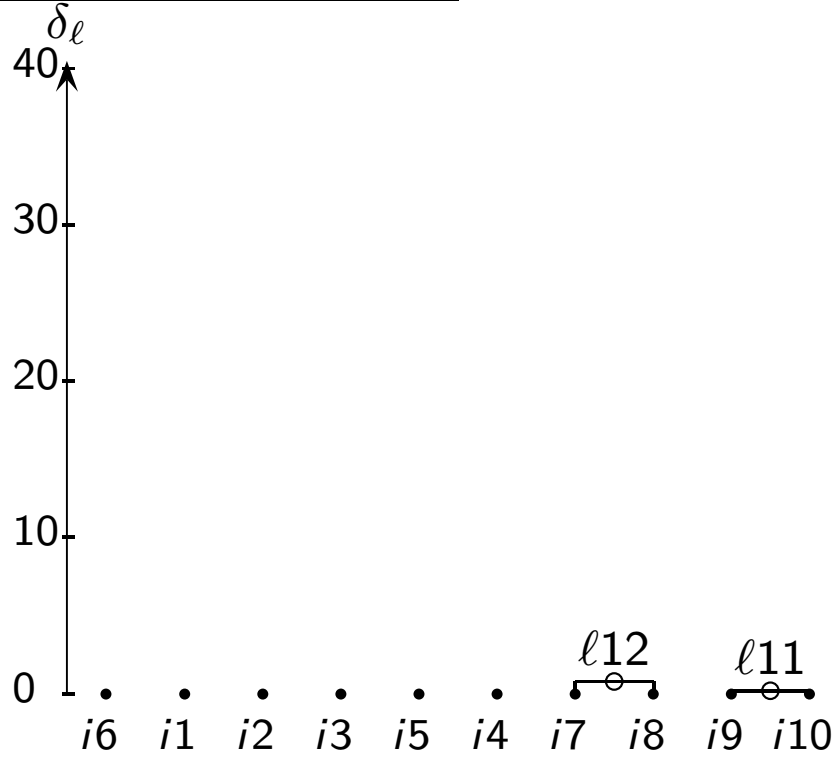


Figure 2



• **Step 3.** Iterate the procedure

Aggregation index between $\ell 12$ and the 7 other points

	$i1$	$i2$	$i3$	$i4$	$i5$	$i6$	$\ell 11$
$\ell 12$	18.13	13.33	13.33	2.67	5.33	9.87	8.2

Minimum = 2 for $\{i1, i2\}$, $\{i3, i5\}$ and $\{i4, i5\}$, aggregation of $i1$ and $i2$ (fig. 3), hence the point $\ell 13$ and a *cloud of 7 points* (fig. 4).

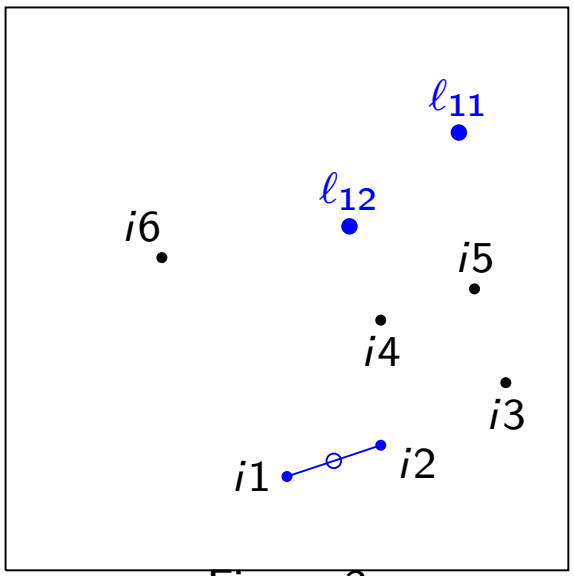
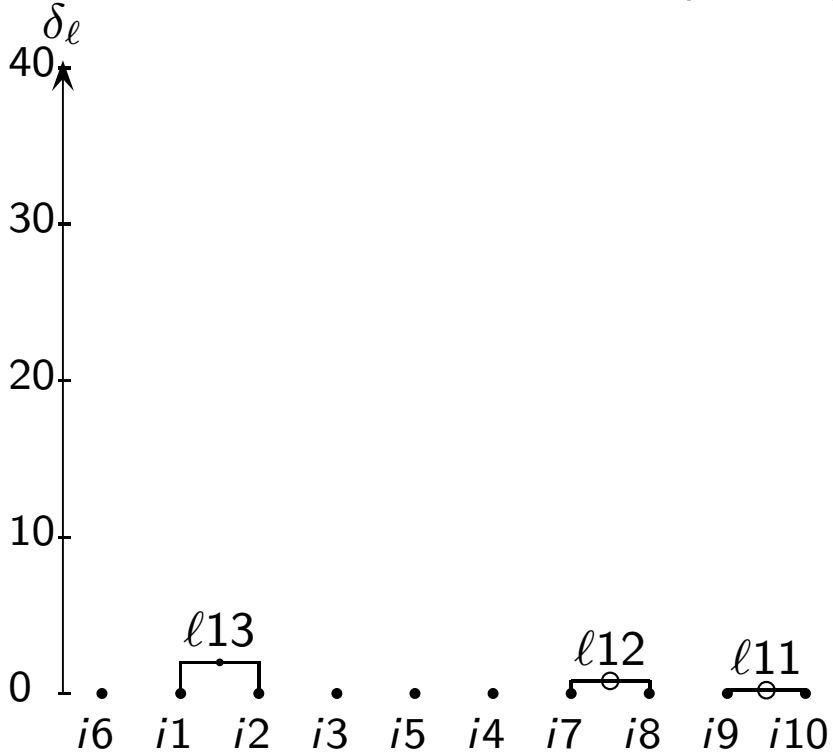


Figure 3



• **Step 4.** Iterate the procedure

Aggregation index between $\ell 13$ and the 6 other points

	$i3$	$i4$	$i5$	$i6$	$\ell 11$	$\ell 12$
$\ell 13$	9.73	6.00	13.47	19.33	50.5	22.6

Minimum of index = 2 for the two pairs $\{i3, i5\}$ and $\{i4, i5\}$. Aggregation of $i3$ and $i5$ (fig. 4), hence the point $\ell 14$ and the *cloud of 6 points* (fig. 5).

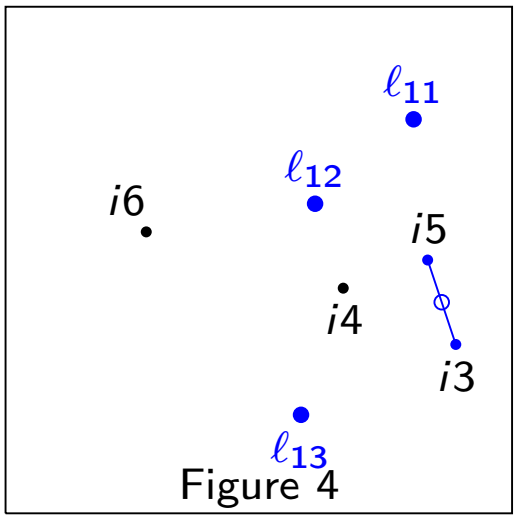
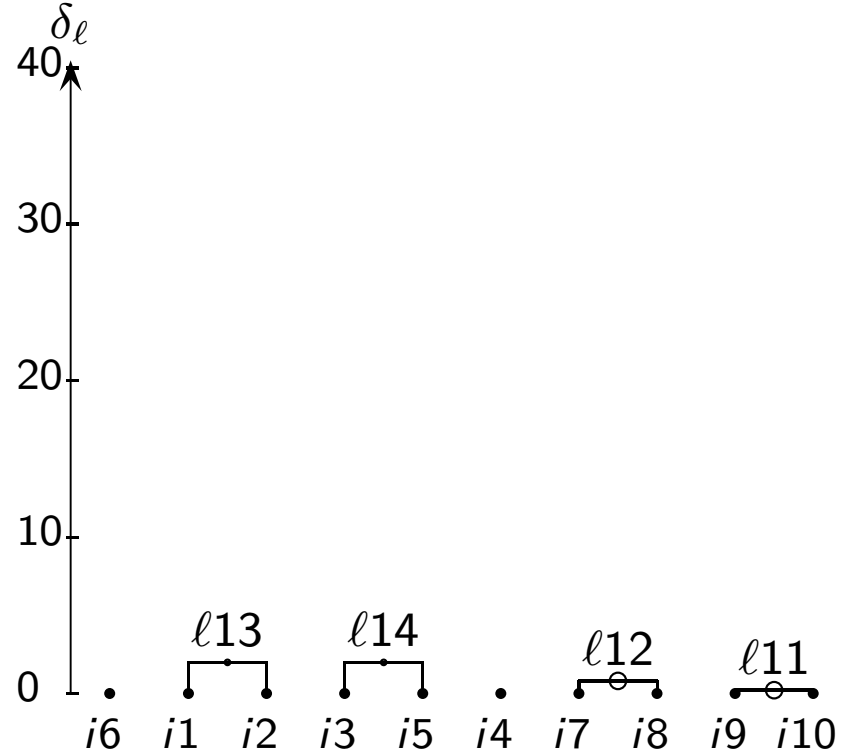


Figure 4



• **Step 5.** Aggregation index between $\ell 14$ and the 5 other points

	$i4$	$i6$	$\ell 11$	$\ell 12$	$\ell 13$
$\ell 14$	3.33	31.07	17.33	13.00	16.4

$\rightarrow$ aggregation of $\ell 12$ and $i4$ at level 2.67 (fig. 5), hence the point $\ell 15$ and the *cloud of 5 points* (fig. 6).

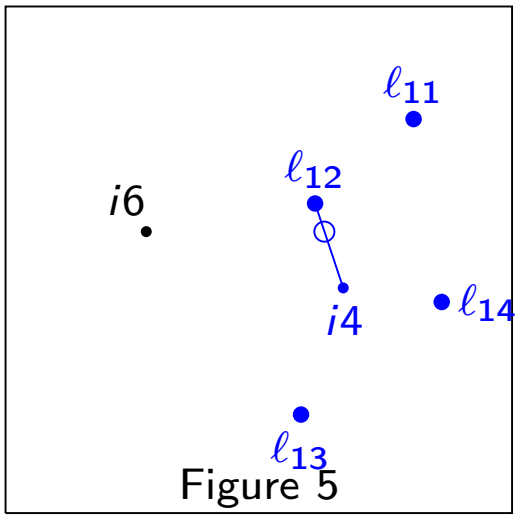
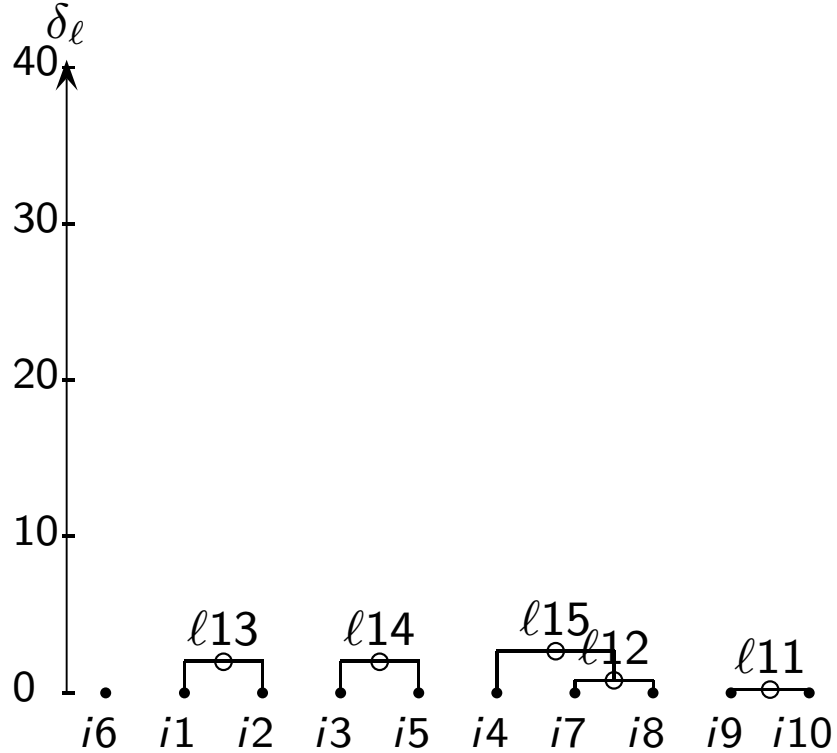


Figure 5



- **Step 6.** Aggregation index between $\ell 15$ and the 4 other points

	$i6$	$\ell 11$	$\ell 13$	$\ell 14$
$\ell 15$	12.03	12.49	20.61	11.33

$\rightarrow$ aggregation of $\ell 15$ and $\ell 14$ at level 11.33 (fig. 6), hence the point $\ell 16$ and the *cloud of 4 points* (fig. 7).

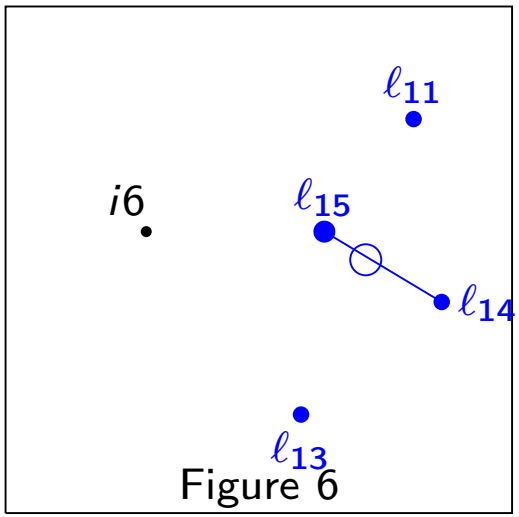
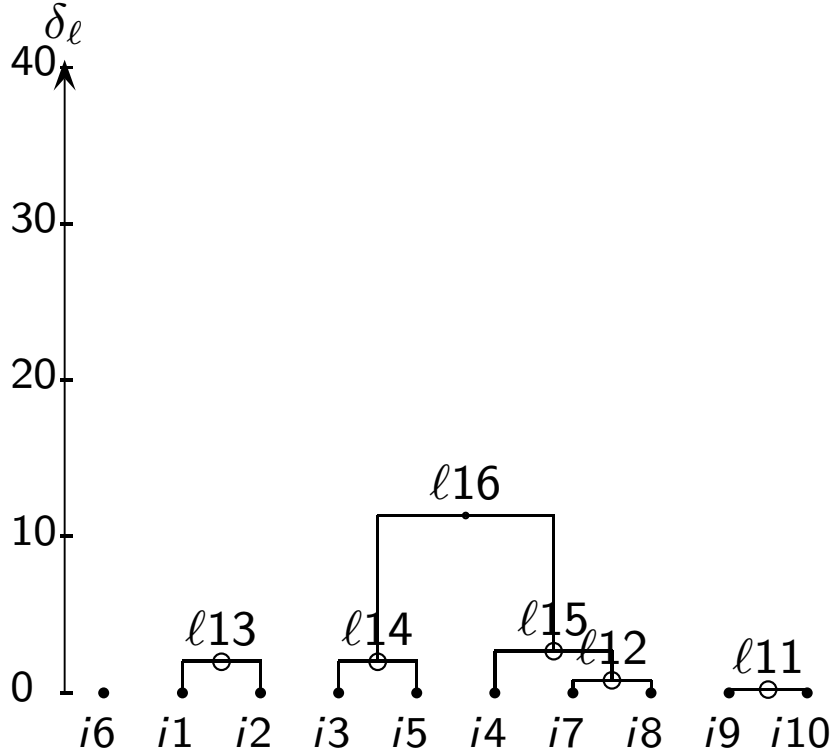


Figure 6



• **Step 7.** Aggregation index between $\ell 16$ and the 3 other points

	$i6$	$\ell 11$	$\ell 13$
$\ell 16$	21.67	15.57	20.86

$\rightarrow$ aggregation of $\ell 16$ and $\ell 11$ at level 15.57 (fig. 7), hence the point $\ell 17$ and the *cloud of 3 points* (fig. 8).

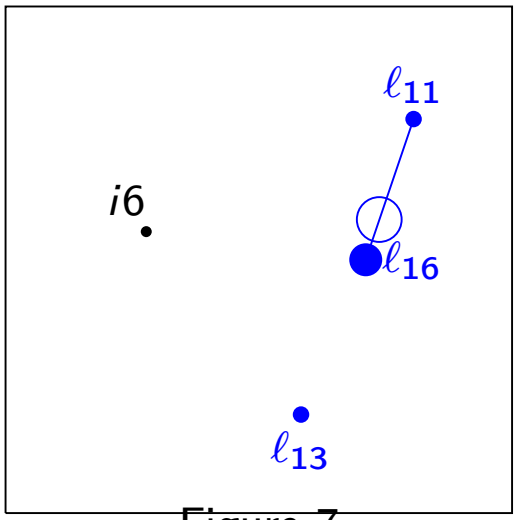
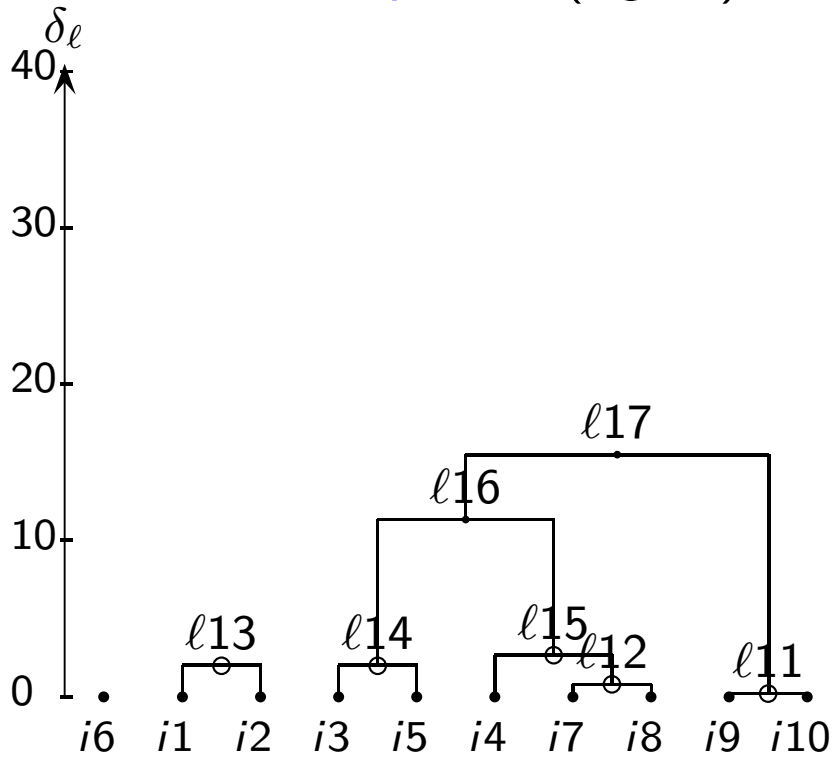


Figure 7



- **Step 8.**

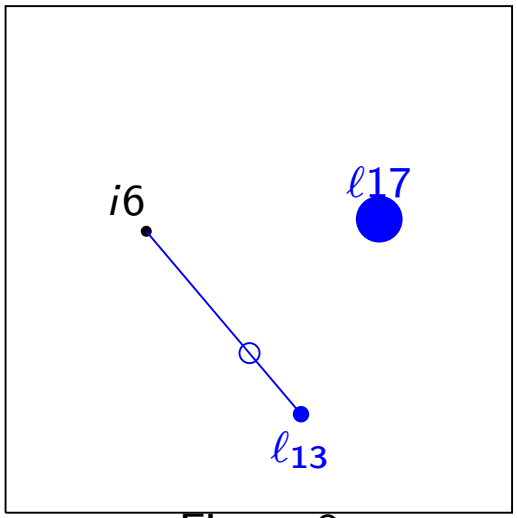
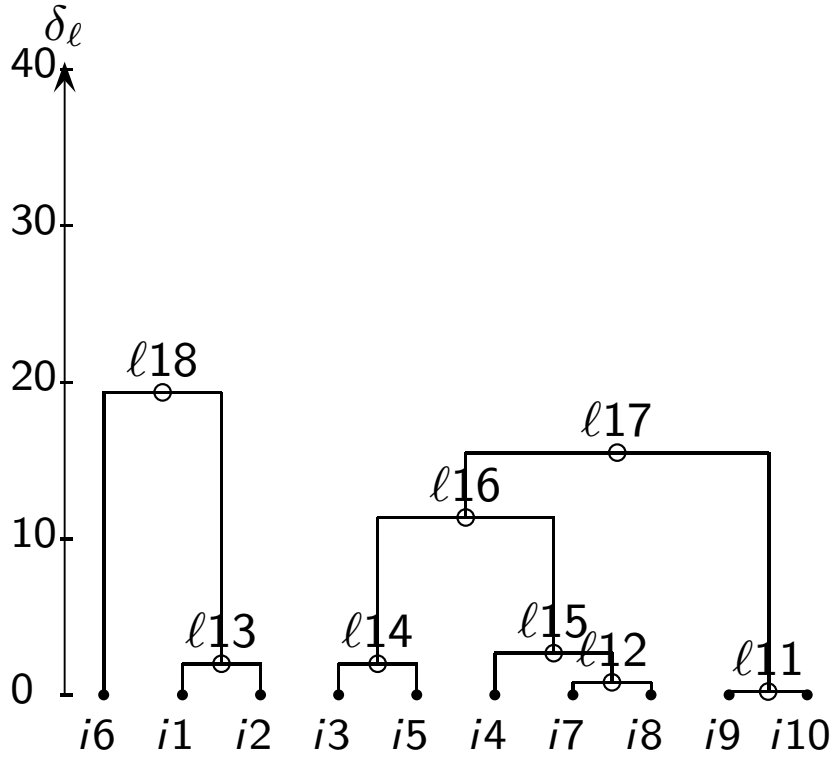


Figure 8



The three-class partition $\mathcal{A}$ ($\ell 14$), $\mathcal{B}$ ($i6$), $\mathcal{C}$ ($\ell 17$) (already studied) with mean points A ($\ell 13$), B ($i6$), C ($\ell 17$) (fig. 8).

- **Step 9.**

Table of the contributions of the 3 pairs of points

	$\ell 13$	$i6$	$\ell 17$
$\ell 13$	—		
$i6$	19.33	—	
$\ell 17$	35.21	24.93	—

$\Rightarrow$ grouping of $i6$ and $\ell 13$ at level 19.33 (fig. 9).

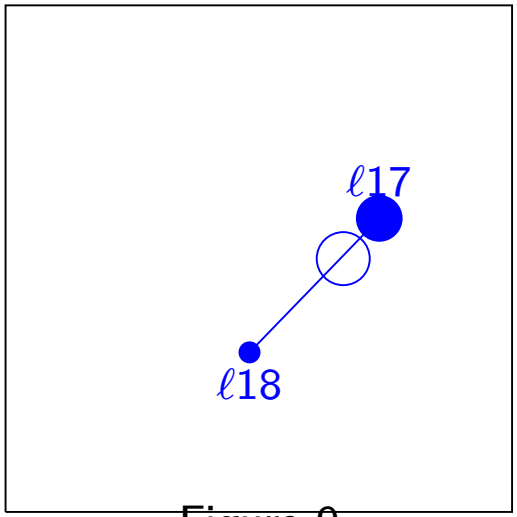
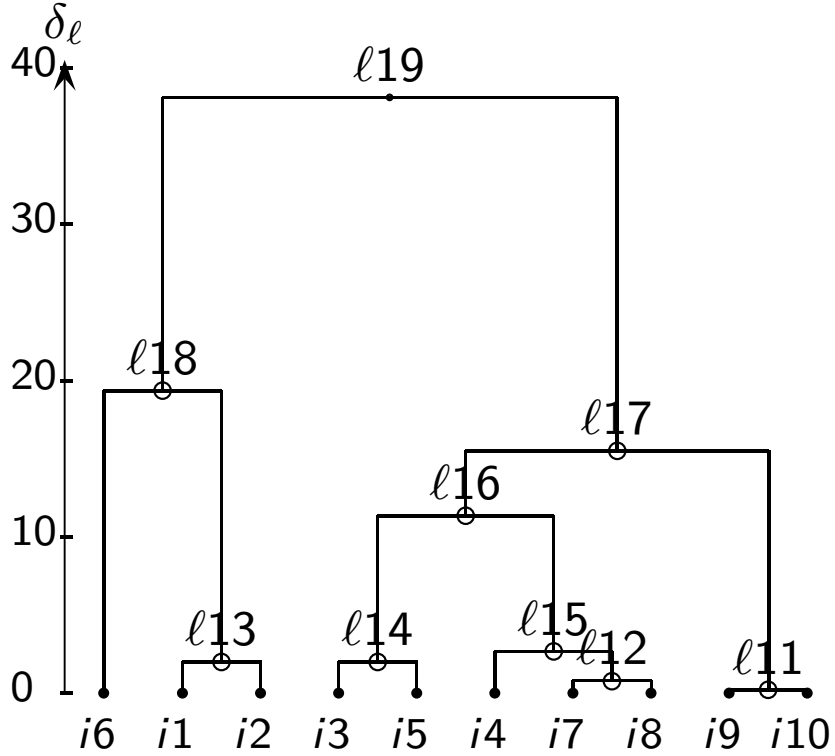
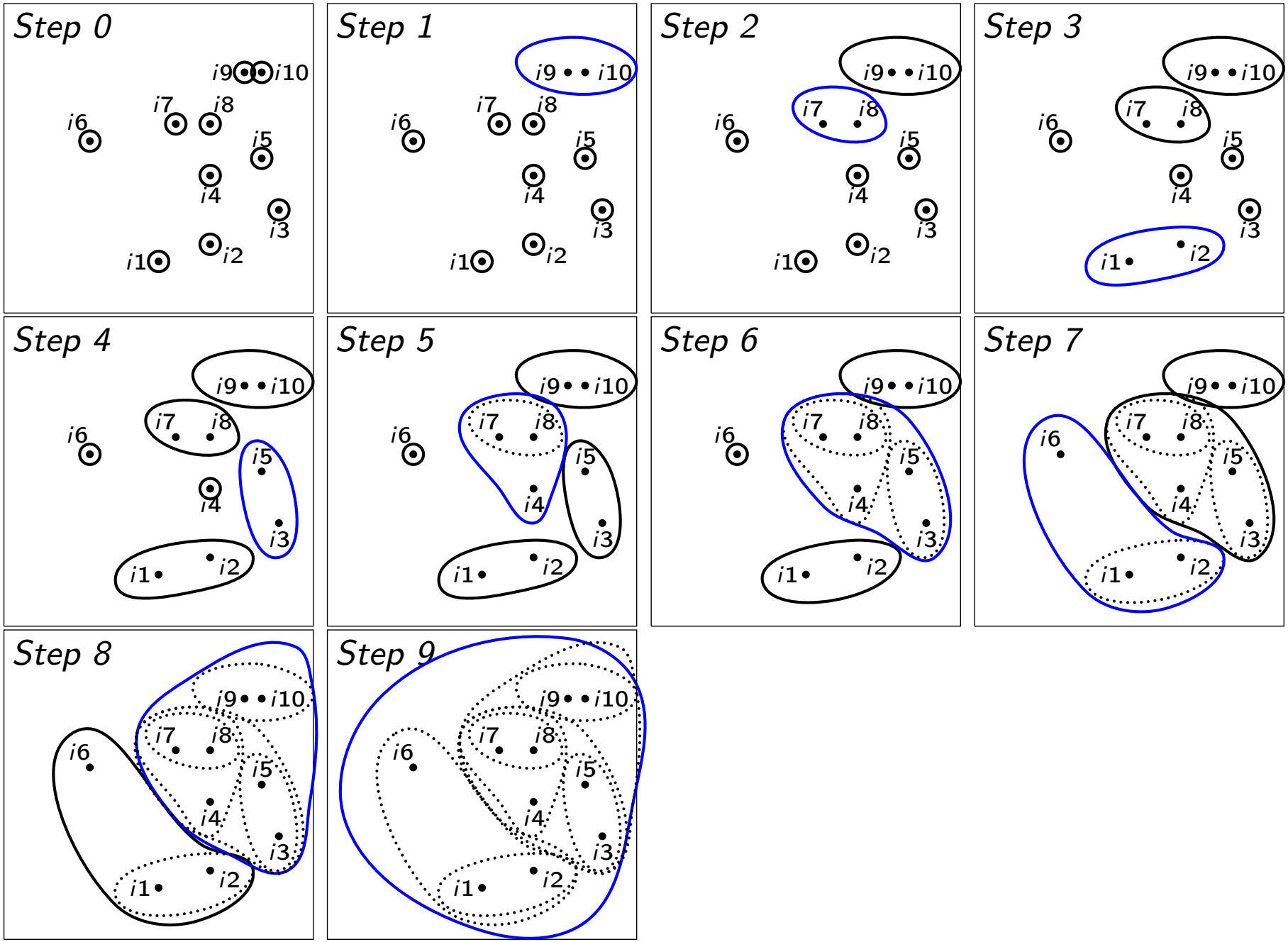


Figure 9




Step 0
Step 1
Step 2
Step 3
Step 4
Step 5
Step 6
Step 7
Step 8
Step 9
i1
i2
i3
i4
i5
i6
i7
i8
i9
i10

Successive Steps of the AHC

ℓ	δ_ℓ	clusters		n	class description
$\ell 19$	38.095	$\ell 18$	$\ell 17$	10	$i9\ i10\ i3\ i5\ i4\ i7\ i8\ i6\ i1\ i2$
$\ell 18$	19.333	$\ell 13$	$\ell 6$	3	$i6\ i1\ i2$
$\ell 17$	15.571	$\ell 16$	$\ell 11$	7	$i9\ i10\ i3\ i5\ i4\ i7\ i8$
$\ell 16$	11.333	$\ell 15$	$\ell 14$	5	$i3\ i5\ i4\ i7\ i8$
$\ell 15$	2.667	$\ell 12$	$\ell 4$	3	$i4\ i7\ i8$
$\ell 14$	2.	$\ell 5$	$\ell 3$	2	$i3\ i5$
$\ell 13$	2.	$\ell 2$	$\ell 1$	2	$i1\ i2$
$\ell 12$	0.8	$\ell 8$	$\ell 7$	2	$i7\ i8$
$\ell 11$	0.2	$\ell 10$	$\ell 9$	2	$i9\ i10$

	Between Var	η^2_ℓ
$\ell 19$		
$\ell 18$	38.10	.414
$\ell 17$	57.43	.624
$\ell 16$	73.00	.793
$\ell 15$	84.33	.917
$\ell 14$	87.00	.957
$\ell 13$	89.00	.967
$\ell 12$	91.00	.989
$\ell 11$	91.80	.998
	92.00	1

Sum of the 9 level indices = 92 (variance of the cloud).

Between-variance of the 2-class partition = 38.095.

Between-variance of the 3-class partition = 38.095 + 19.333 = 57.43, etc.

IV.5. Interpretation of clusters

Interpretation is based on active variables then supplementary variables

Categorical variables

1. descriptive criterion:

Categories over-represented:

The relative frequency of the category in the cluster (f_c)

is 5% higher than the frequency in the whole set (f)

or is twice the one in the whole set.

$$f_c - f > 0.05 \qquad f_c/f > 2$$

Categories under-represented: $f_c - f < -0.05 \qquad f_c/f < 2$

2. inductive criterion:

The hypergeometric test of comparison of the frequency in the cluster to the reference frequency is significant.

Numerical variables

Variables retained for the interpretation:

1. descriptive criterion:

$$\frac{\text{mean for the cluster} - \text{mean for the overall set}}{\text{standard deviation for the whole set}} \geq 0.5$$

or

$$\frac{\text{mean for the cluster} - \text{mean for the overall set}}{\text{standard deviation for the whole set}} \leq -0.5$$

2. inductive criterion:

The combinatorial test of comparison of the mean in the cluster to the overall mean is significant.

Interpretation of the Hierarchy

The hierarchical tree is constructed in ascending direction.

- Reading a clustering (ascending and descending reading)
- Choice of the number of clusters:
  from the diagram of level indexes.
- study of the successive dichotomies

Assignment of Supplementary Objects to Clusters

Mixed Clustering

IV.6. Other Aggregation Indices

- *Minimal jump.* the smallest distance between the elements of the 2 clusters = *single linkage clustering.*
- *Maximal jump.* The largest distance between elements of the two clusters= *diameter index*, or *complete linkage clustering.*
- *Mean distance .* Weighted mean of distances between the points of 2 clusters = *average linkage clustering*.

IV.7. Divisive Hierarchical Clustering

Start with one cluster and, at each step, split a cluster until only one–element clusters remain.
In this case, we need to decide which cluster will be split at each step and how to do the splitting.
Methods: CHAID and CART