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Pattern recognition on spatial data

Finding structures : numerical classification

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Introduction

- Introduction
- Example data

Introduction

Objective

- divide n individuals into k groups, based on their similarities on the values of p variables

Introduction

Data

- Raw data : matrix of numerical data
  - n rows $\equiv$ individuals
  - p columns $\equiv$ variables
- Standardized data : for each variable j
  - $x_{ij} = (y_{ij} - \bar{y}_j)/\hat{\sigma}_j$
  - $\bar{x}_j = 0$
  - $\hat{\sigma}_{x_j} = 1$

Introduction

- Introduction
- Example data

Example

Raw data : Cations and anions in mineral waters

HCO_3^-	Ca^{2+}
SO_4^{2-}	Mg^{2+}
Cl^-	Na^+

Example

```
# set working directory
setwd("....")
# source supplementary function
source("hclust.info.R")

# read data file
waters <- read.csv2("ClassEaux.csv", row.names=7)

# select 7 mineral waters
waters7 <- subset(waters, rownames(waters) %in%
 c("G", "L", "O", "S", "T", "c", "o"))
```

Raw data

	HCO3	SO4	CL	CA	MG	NA	NOM
G	357	10	2	78	24	5	EVIAN (F)
L	398	218	15	157	35	8	ONDINE (F)
O	11	65	5	4	1	3	SPA (B)
S	402	306	15	202	36	3	VITTEL (F)
T	64	7	8	10	6	8	VOLVIC (F)
c	1580	112	137	89	104	425	APOLLINARIS (D)
o	251	32	14	81	11	6	SPONTIN (B)

Scale variables

Important Unlike most of PCA tools, clustering methods don't standardize the data internally. It has to be done manually using them for clustering.

```
# scale variables (mean=0 and SD=1)
waters7std <- scale(waters7[1:6])
```

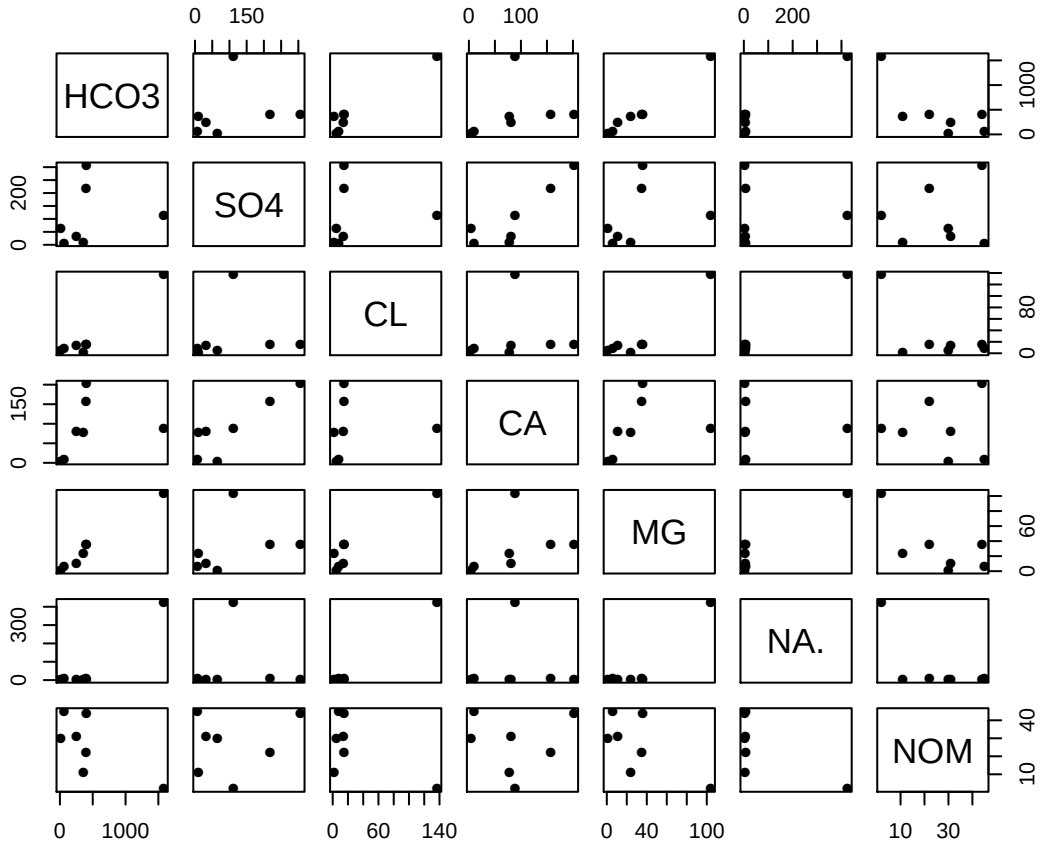
Standardized data

	HCO3	SO4	CL	CA	MG	NA	NOM
G	-0.1527	-0.8480	-0.5379	-0.1490	-0.2001	-0.3811	EVIAN (F)
L	-0.0750	0.9677	-0.2689	0.9493	0.1143	-0.3622	ONDINE (F)
O	-0.8084	-0.3679	-0.4758	-1.1777	-0.8575	-0.3937	SPA (B)
S	-0.0674	1.7358	-0.2689	1.5749	0.1429	-0.3937	VITTEL (F)
T	-0.7079	-0.8741	-0.4137	-1.0943	-0.7146	-0.3622	VOLVIC (F)
c	2.1649	0.0424	2.2549	0.0040	2.0866	2.2676	APOLLINARIS (D)
o	-0.3536	-0.6559	-0.2896	-0.1072	-0.5717	-0.3748	SPONTIN (B)

Matrix plot

```
# Matrix plot
plot(waters7, pch=16)
```

Waters = Matrix Plot



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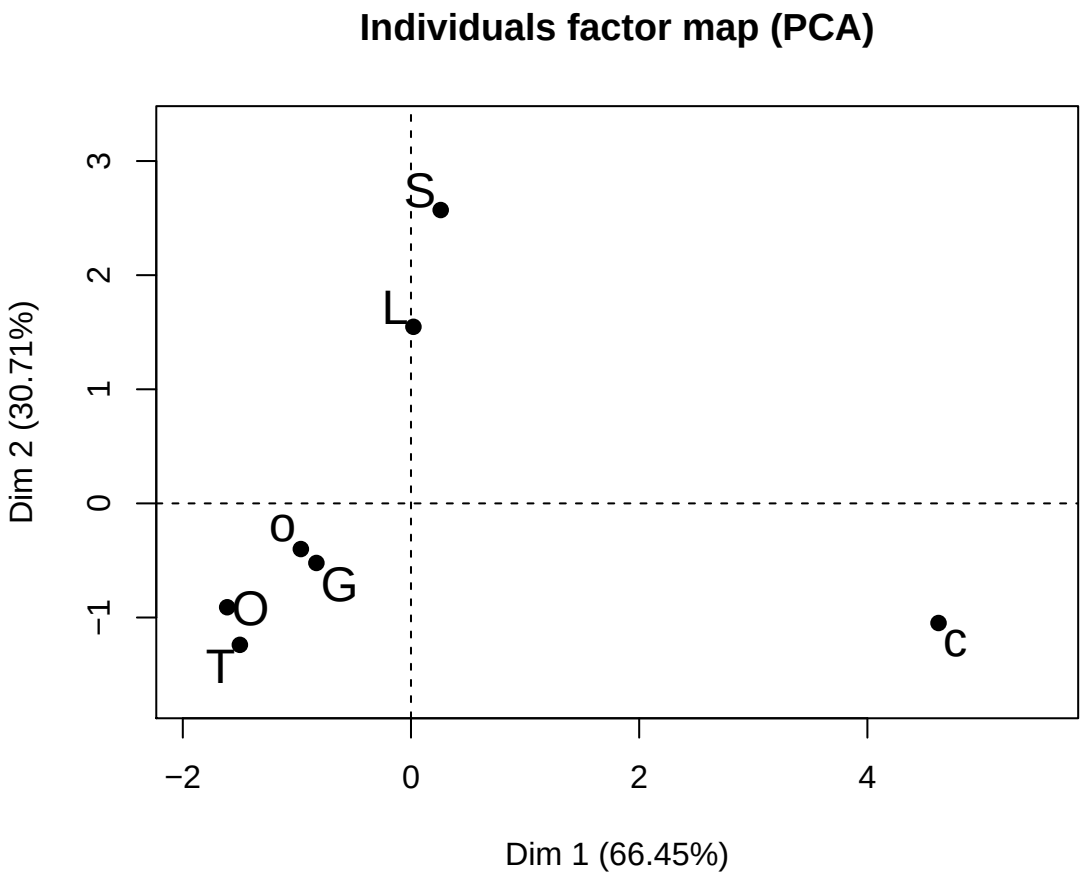
Example - PCA

```
# ACP
library(FactoMineR)
cluster.pca <- PCA(waters7std)
```

Example - PCA


Individuals factor map (PCA)
Dim 2 (30.71%)
Dim 1 (66.45%)
S
L
o
G
O
T
c
3
2
1
0
−1
−2
0
2
4

Contents

Distance

- Between observations
- Between groups

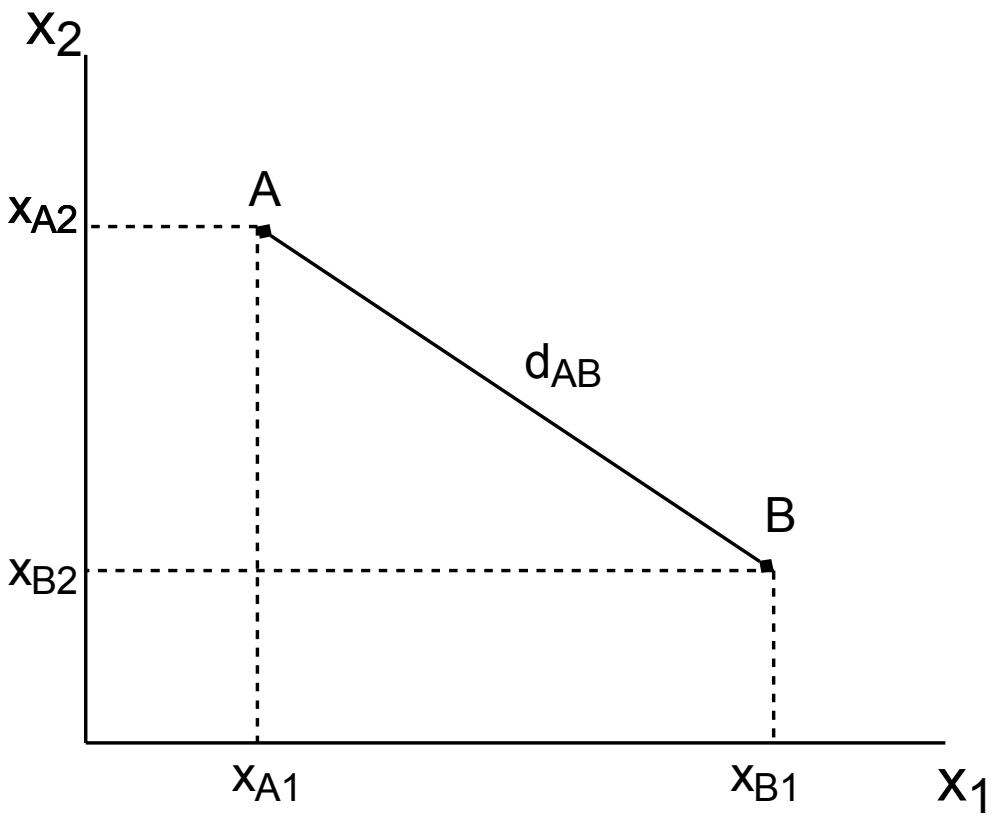
Distance space

Clustering methods heavily rely on (dis)similarity measures.

Euclidian distance is one of the most often used dissimilarity measures. But this distance is calculated into the **data space**, not the **coordinates space**.

Euclidian distance

$$
\begin{aligned}
d^2_{ii'} &= (x_{i1} - x_{i'1})^2 \\
&+ \dots \\
&+ (x_{ip} - x_{i'p})^2 \\
&= \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2
\end{aligned}
$$



Distance matrix

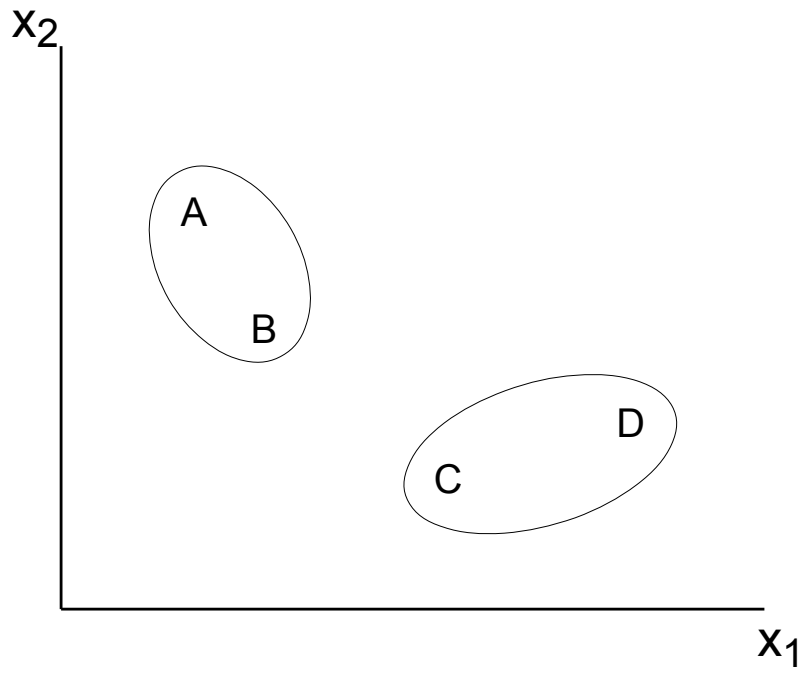
```
# Euclidean distance matrix
waters7.d <- dist(waters7std)
```

Distance

- Between observations
- Between groups

Distances between two clusters

- Nearest neighbour distance : d_{BC}
- Furthest neighbour distance : d_{AD}
- Average distance : $d^2 = (d^2_{AC} + d^2_{AD} + d^2_{BC} + d^2_{BD})/4$
- etc.



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Example

Euclidian distances between waters

Distance	G	L	O	S	T	c	o
G	0	2.16	1.47	3.14	1.22	5.12	0.53
L	2.16	0	2.80	0.99	2.95	4.89	2.07
O	1.47	2.80	0	3.69	0.55	5.80	1.25
S	3.14	0.99	3.69	0	3.89	5.25	3.02
T	1.22	2.95	0.55	3.89	0	5.67	1.09
c	5.12	4.89	5.80	5.25	5.67	0	5.23
o	0.53	2.07	1.25	3.02	1.09	5.23	0

Example

Euclidian distances between clusters

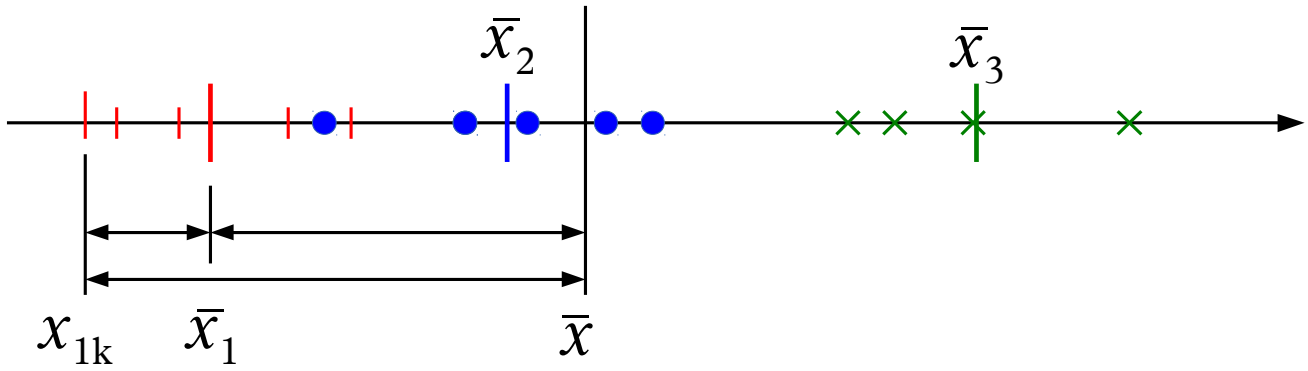
Distance	L	S
G	2.16	3.14
O	2.80	3.69
T	2.95	3.89
o	2.07	3.02

Nearest neighbour distance :
$2.07 = d_{oL}$

Furthest neighbour distance :
$3.89 = d_{TS}$

Average distance :
3.02

Ward's distance



$$\text{TOTAL SS} = \sum_{i=1}^{g} \sum_{j=1}^{n_i} (x_{ij} - \bar{x})^2$$

$$\text{WITHIN SS} = \sum_{i=1}^{g} \left[\sum_{j=1}^{n_i} (x_{ij} - \bar{x}_i)^2 \right]$$

$$\text{BETWEEN SS} = \sum_{i=1}^{g} n_i (\bar{x}_i - \bar{x})^2$$

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Ward's distance

$$
\begin{aligned}
(\text{TOTAL})_1 &= (\text{BETWEEN})_1 + (\text{WITHIN})_1 \text{ for variable 1} \\
&\dots \\
(\text{TOTAL})_j &= (\text{BETWEEN})_j + (\text{WITHIN})_j \text{ for variable } j \\
&\dots \\
(\text{TOTAL})_p &= (\text{BETWEEN})_p + (\text{WITHIN})_p \text{ for variable } p
\end{aligned}
$$

$$
\sum_{j=1}^{p}(\text{TOTAL})j = \sum_{j=1}^{p}(\text{BETWEEN})_j + \sum_{j=1}^{p}(\text{WITHIN})_j
$$

$$
R^2 = \frac{\sum_{j=1}^{p}(\text{BETWEEN})_j}{\sum_{j=1}^{p}(\text{TOTAL})_j}
$$

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Example

Analysis of variance

4 clusters : (G, o), (O, T), (L, S), (c)

Sources	df	HCO3	SO4	Cl	Ca	Mg	Na	Total
Between	3	5.97	5.56	5.97	5.80	5.92	6.00	35.22
Within	3	0.03	0.44	0.03	0.20	0.08	0.00	0.78
Total	6	6.00	6.00	6.00	6.00	6.00	6.00	36.00

R-squared $= 35.22 \ / \ 36 = 0.978$

Example

Analysis of variance

3 clusters : (G, o, O, T), (L, S), (c)

Sources	df	HCO3	SO4	Cl	Ca	Mg	Na	Total
Between	2	5.72	5.54	5.97	4.78	5.76	6.00	33.77
Within	4	0.28	0.46	0.03	1.22	0.24	0.00	2.23
Total	6	6.00	6.00	6.00	6.00	6.00	6.00	36.00

R-squared $= 33.77 \ / \ 36 = 0.938$

$\Delta R^2 = 0.978 - 0.938 = 0.04$

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Hierarchical clustering techniques

- number of clusters not fixed
- **divisive methods** : from 1 to n clusters
- **agglomerative methods** : from n to 1 cluster
- results presented in the form of a dendrogram

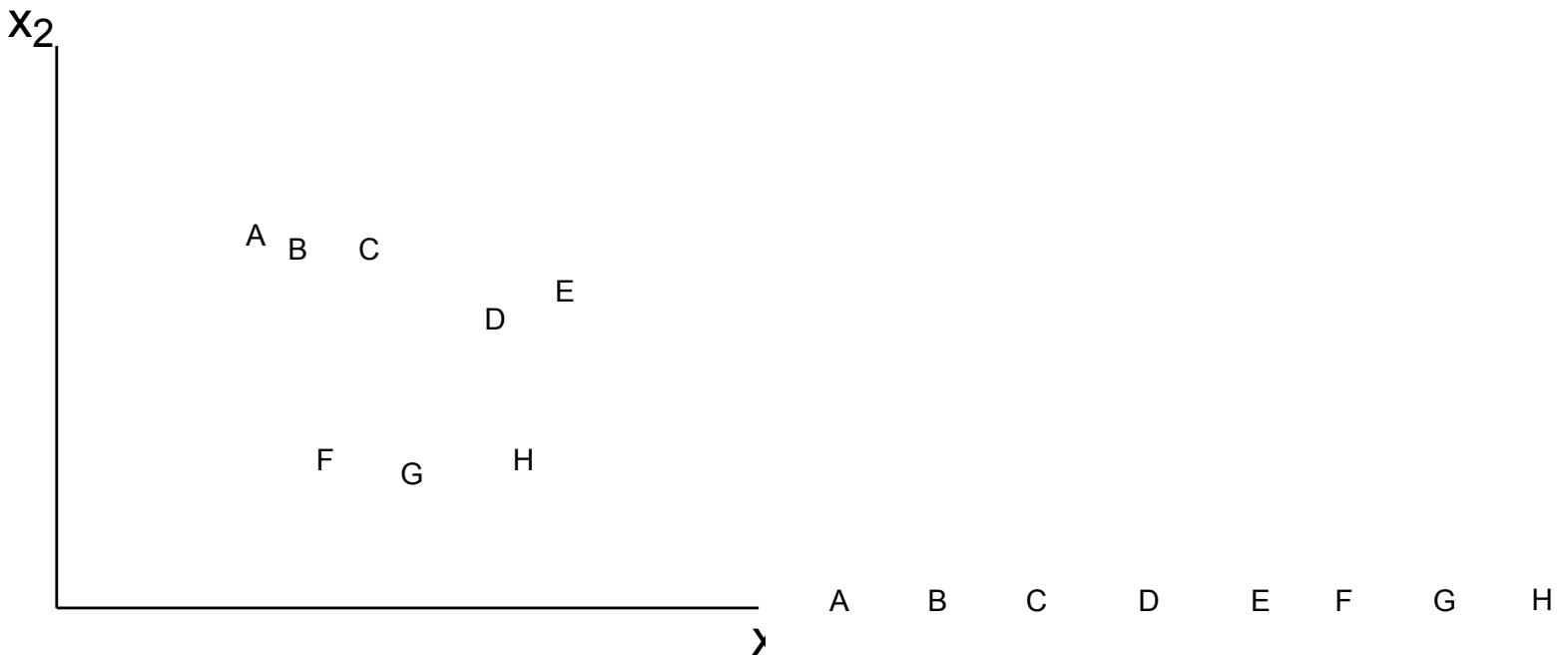
Hierarchical Clustering techniques

- Agglomerative methods
- Example

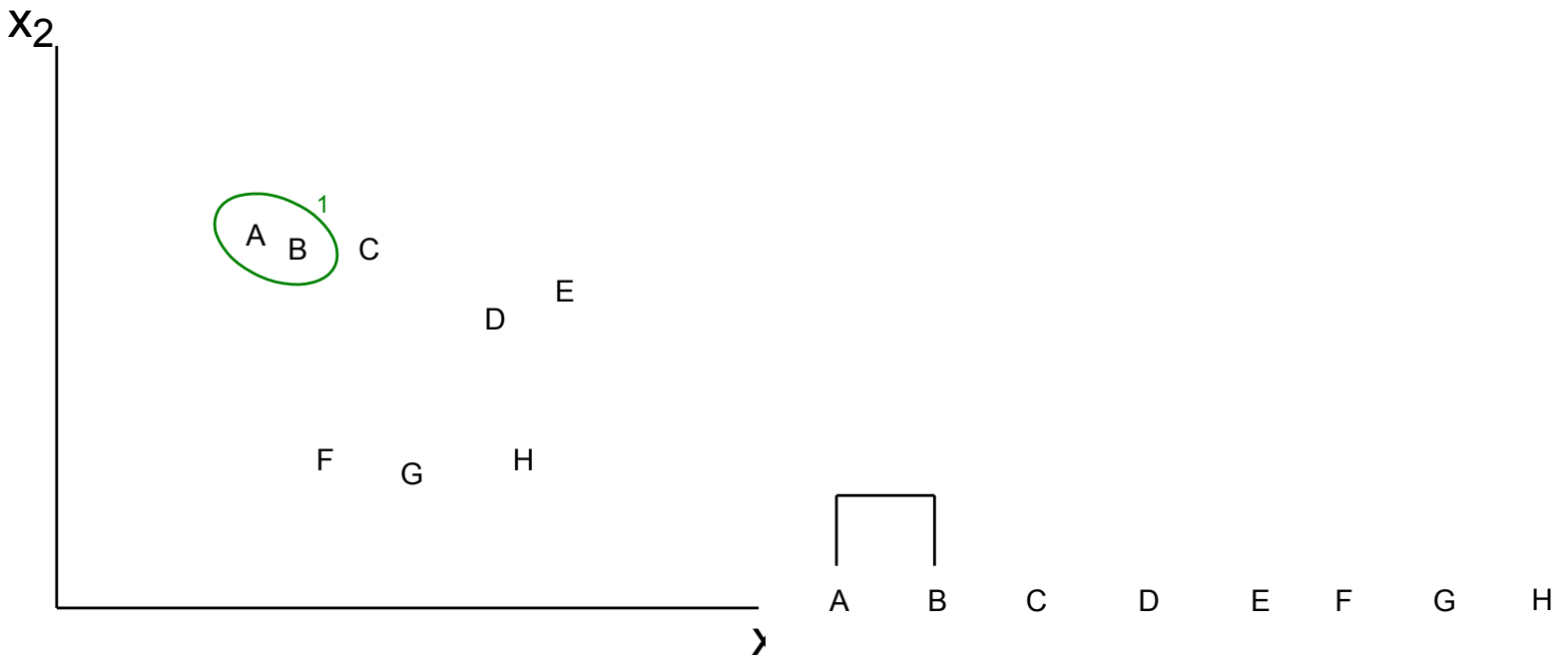
Agglomerative methods

- **WARD'S method**
  fusion of the two groups for which ΔR^2 is minimum
- **Single linkage**
  fusion of the two groups for which the nearest neighbour distance is minimum
- **Complete linkage**
  fusion of the two groups for which the furthest neighbour distance is minimum
- **Average linkage**
  fusion of the two groups for which the average distance is minimum

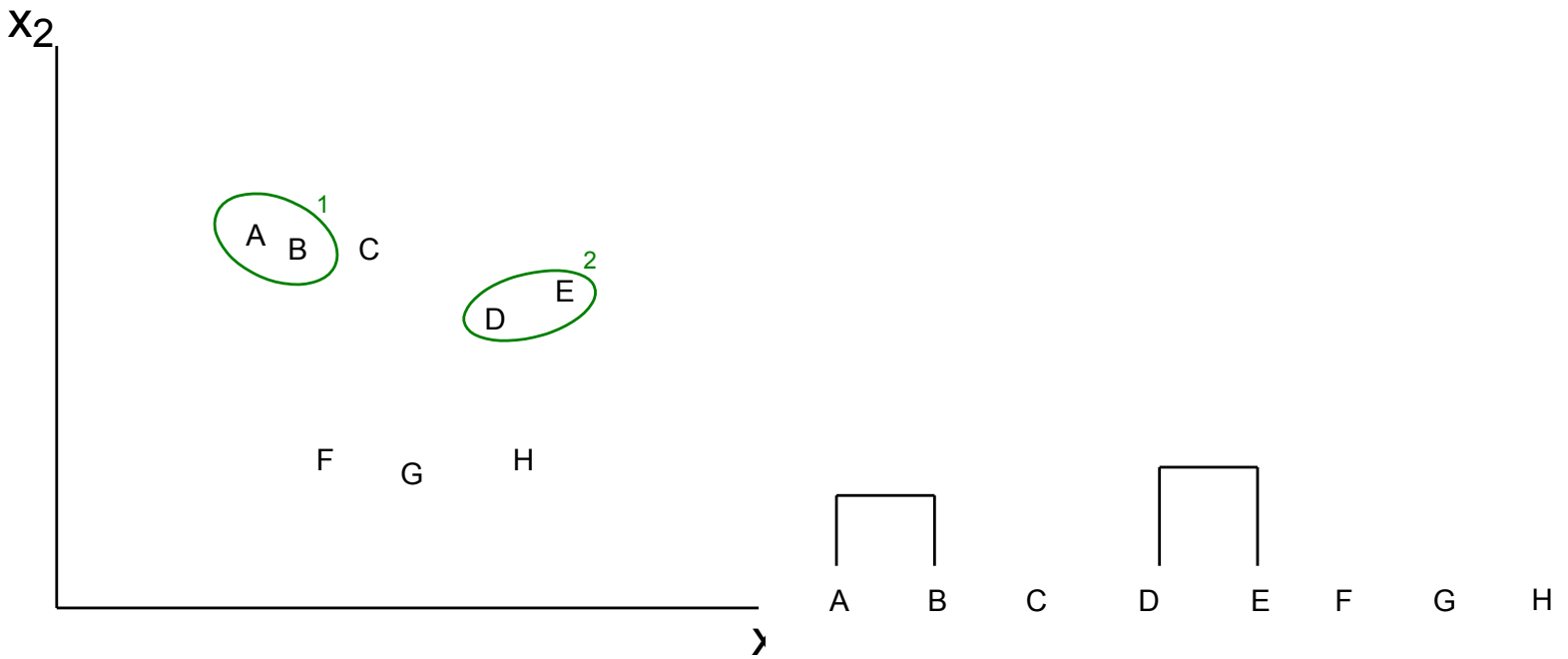
Agglomerative methods



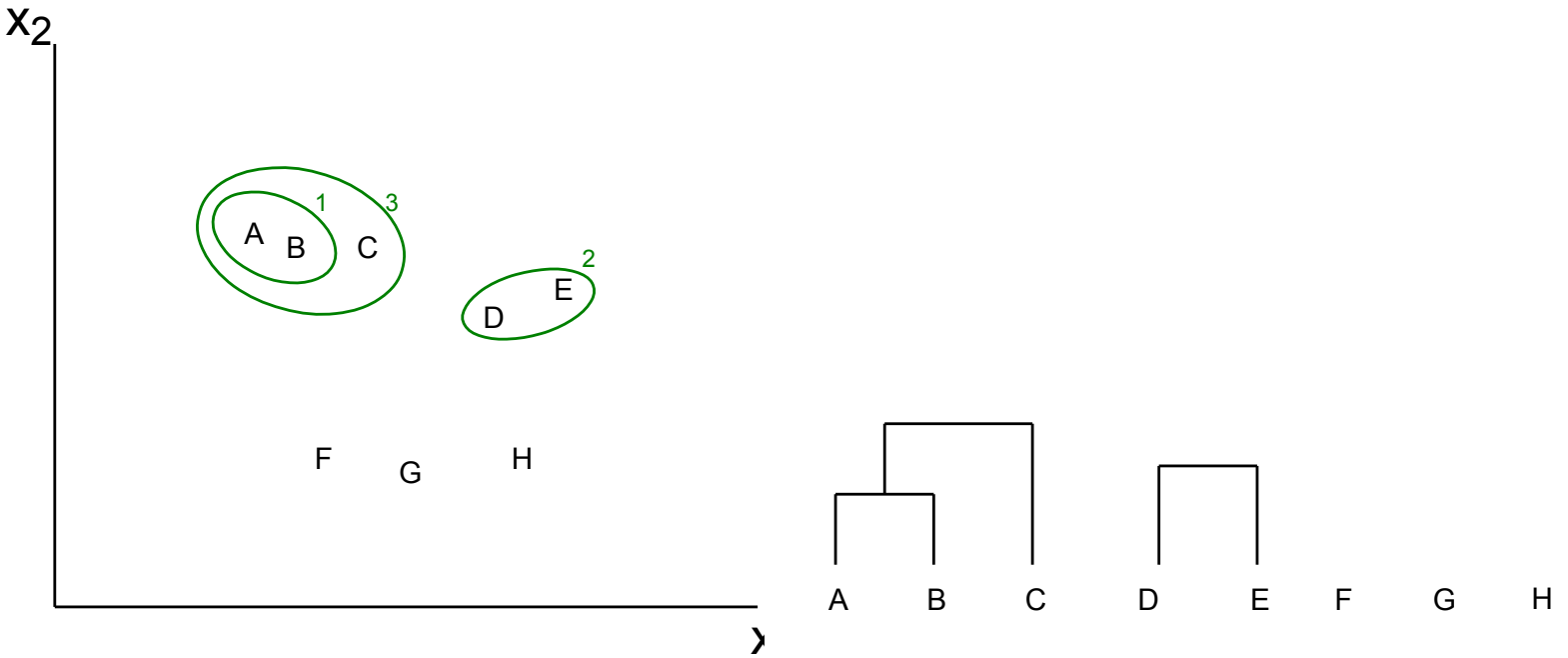
Agglomerative methods



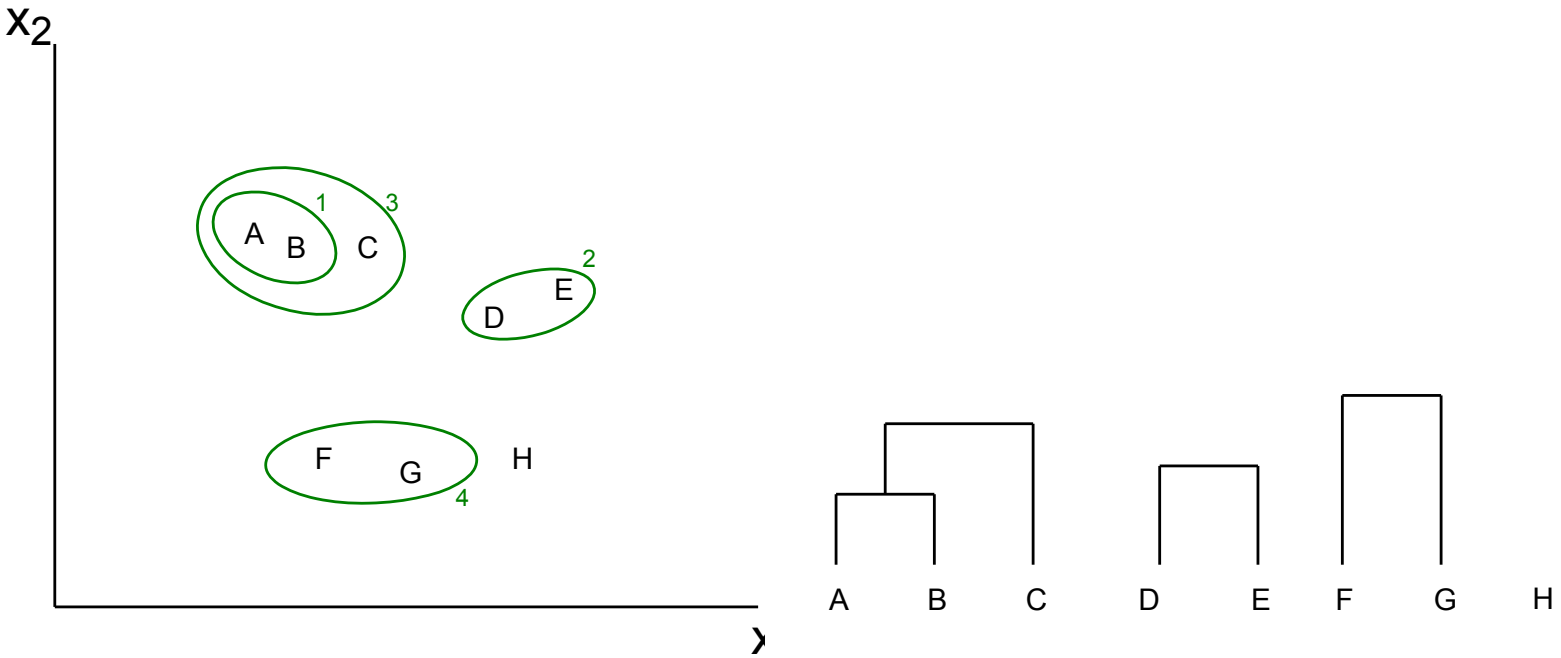
Agglomerative methods



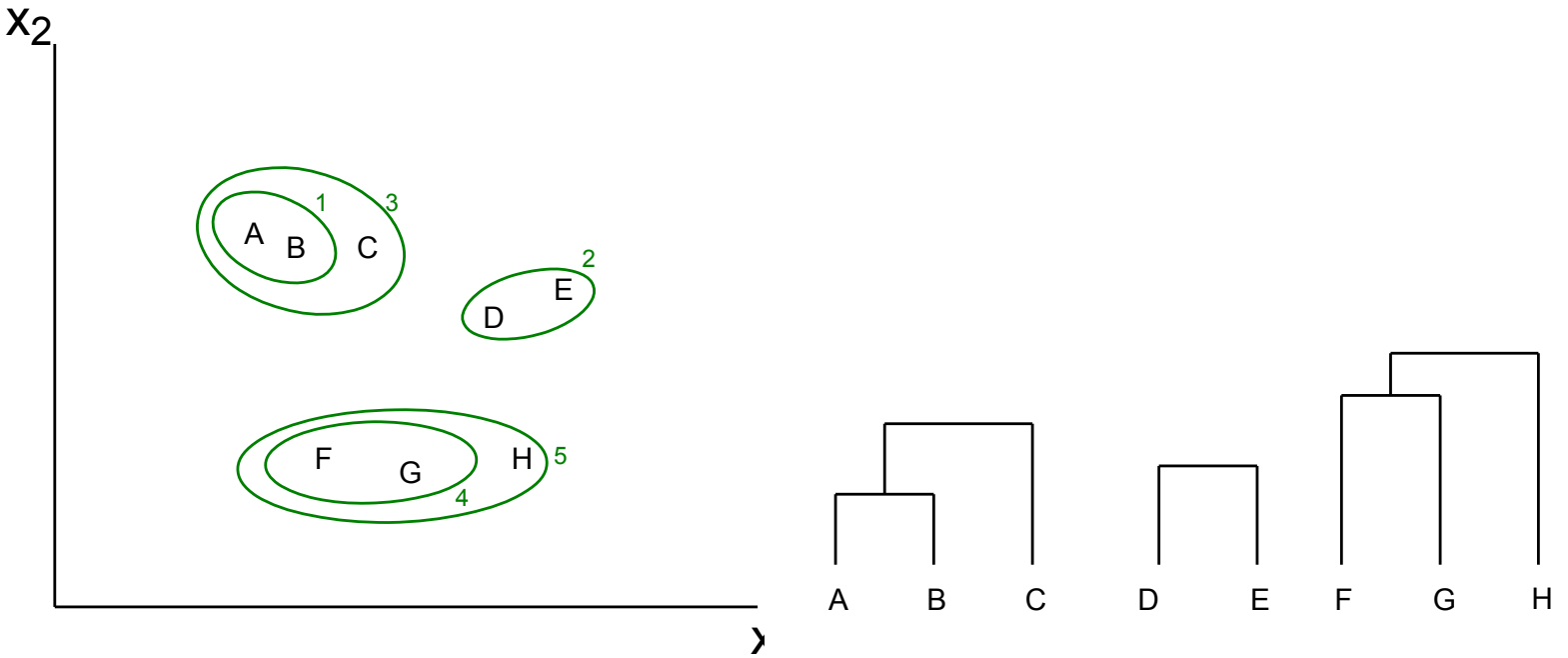
Agglomerative methods



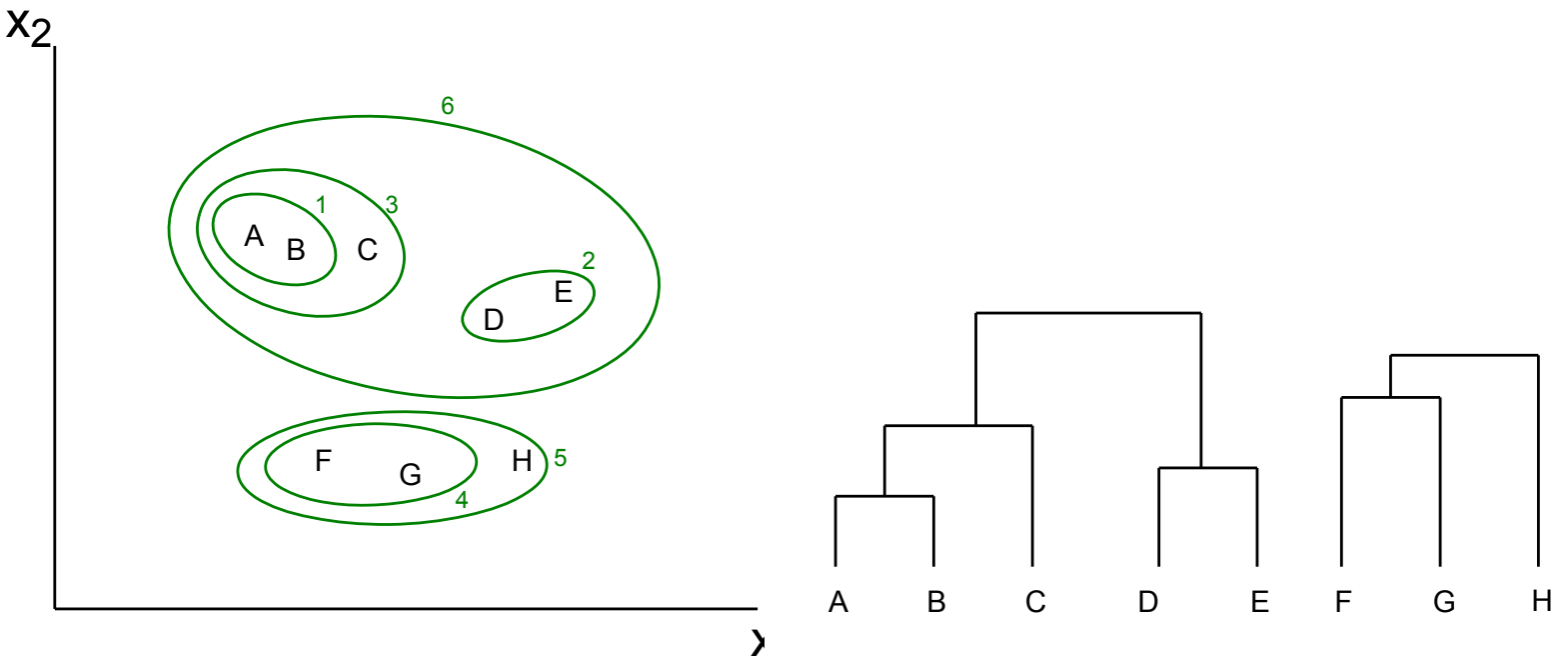
Agglomerative methods



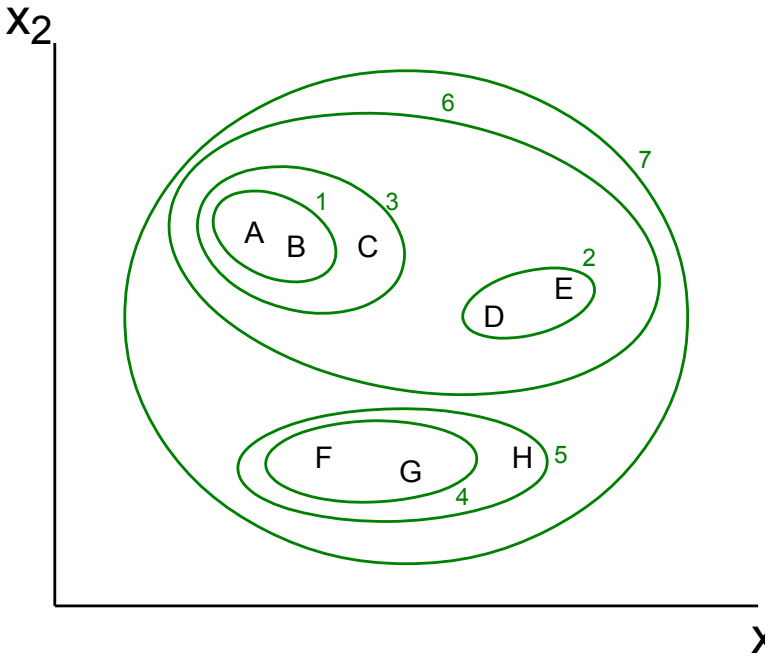
Agglomerative methods

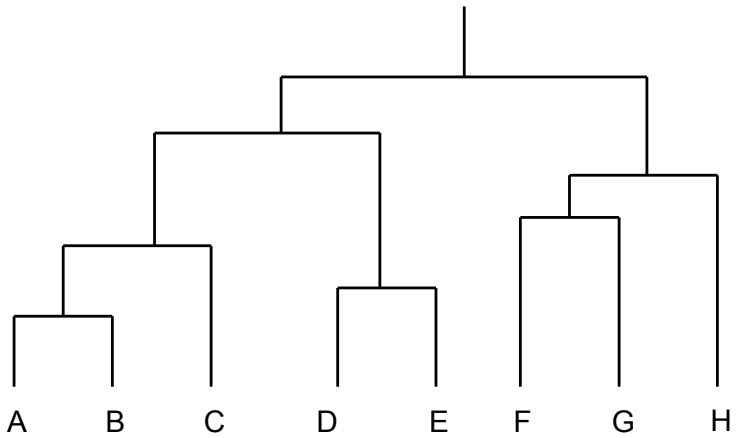


Agglomerative methods



Agglomerative methods





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Hierarchical Clustering techniques

- Agglomerative methods
- Example

Example: complete linkage clustering I

Distance	L	O	S	T	c	o
G	2.16	1.47	3.14	1.22	5.12	0.53
L	0	2.80	0.99	2.95	4.89	2.07
O		0	3.69	0.55	5.80	1.25
S			0	3.89	5.25	3.02
T				0	5.67	1.09
c					0	5.23

Example: complete linkage clustering II

Distance	L	O	S	T	c
(G,o)	2.16	1.47	3.14	1.22	5.23
L	0	2.80	0.99	2.95	4.89
O		0	3.69	0.55	5.80
S			0	3.89	5.25
T				0	5.67

Distance	L	(O,T)	S	c
(G,o)	2.16	1.47	3.14	5.23
L	0	2.95	0.99	4.89
(O,T)		0	3.89	5.80
S			0	5.25

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Example: complete linkage clustering III

Distance	(L,S)	(O,T)	c
(G,o)	3.14	1.47	5.23
(L,S)	0	3.89	5.25
(O,T)		0	5.80

Distance	(L,S)	c
(G,o,O,T))	3.89	5.80
(L,S)	0	5.25

Distance	c
(G,o,O,T,L,S))	5.80

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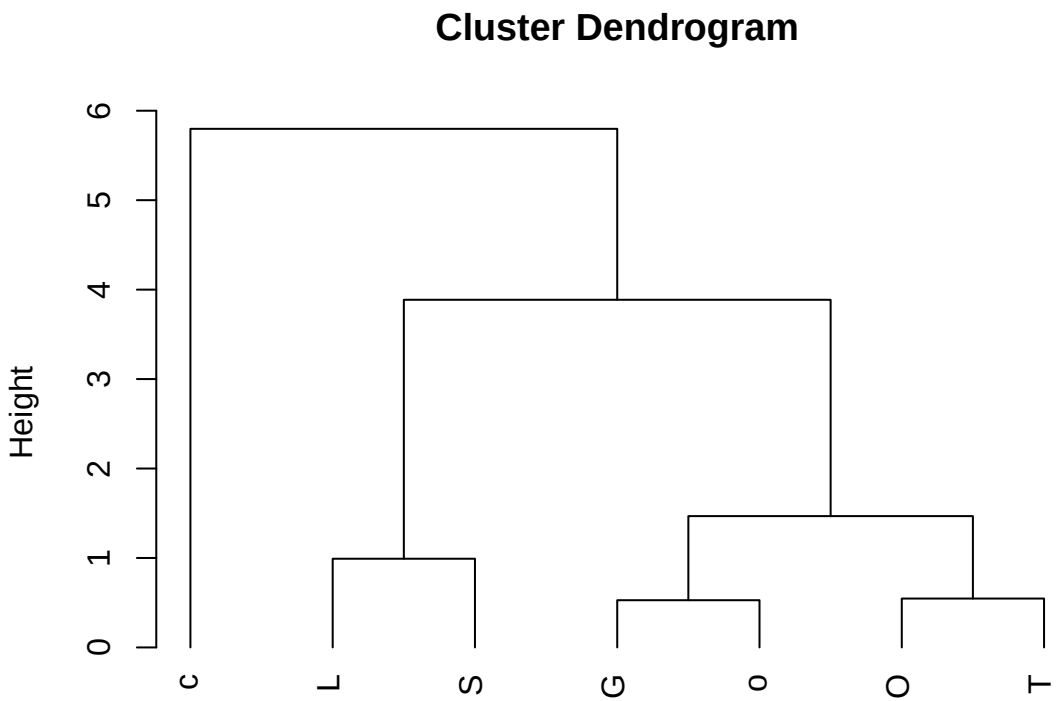
Example - waters



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Classification

```
# hierarchical clustering (default to complete link)
waters7.hc <- hclust(waters7.d)

# dendrogram
plot(waters7.hc, hang=-1)
```

Contents

Steps in clustering

1. Data collection
2. Measurement of proximity
3. Choice of a clustering algorithm
4. Number of clusters
5. Interpretation of the results

Steps in clustering

- Data collection
- Measurement of proximity
- Choice of a clustering algorithm
- Number of clusters
- Interpretation of the results

Steps in clustering

- Data collection
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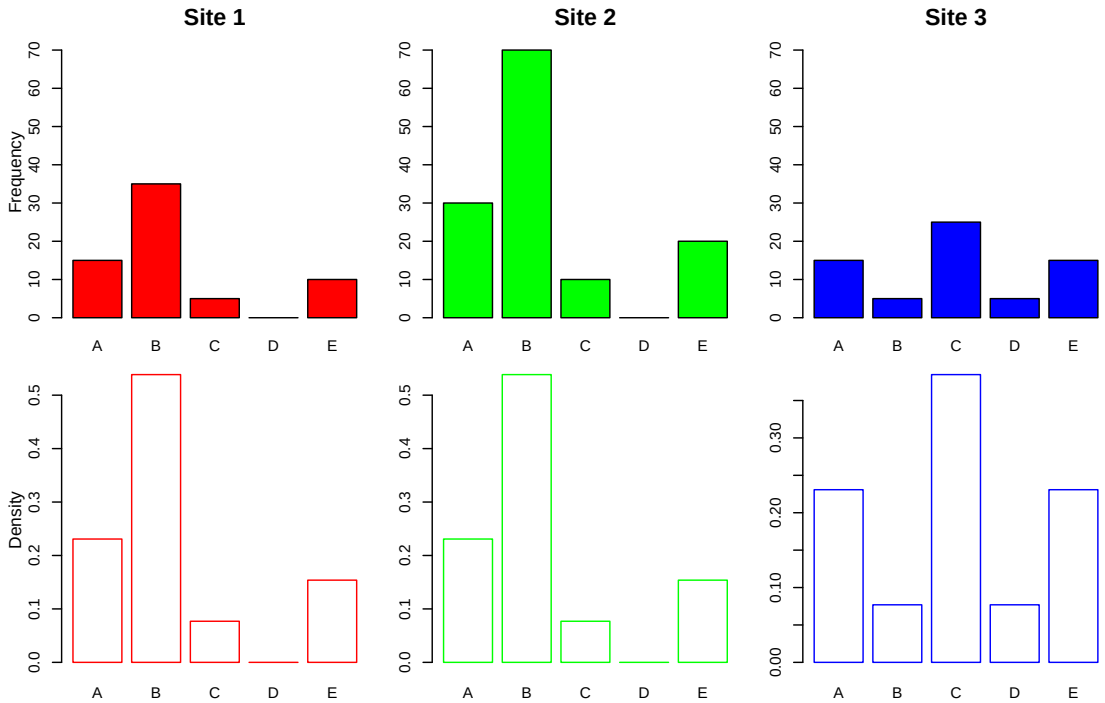
Measurement of proximity

- Euclidean distance
- other distances
  - χ^2
  - correlation
  - similarity/dissimilarity coefficients
  - ...
- transformation of coefficients :

$$d_{ii'} = 1 - s_{ii'} \quad d_{ii'} = 1 - r_{ii'} \quad d_{ii'} = 1 - r_{ii'}^2$$

χ^2 distance

- for (relative) frequencies distribution comparison (ecology)
- linked to χ^2 independance test



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Correlation

- to cluster **variables** instead of **individuals**
- importance of the choice of the transformation (relation between anticorrelated variables)

$$d_{ii'} = 1 - r_{ii'} \quad d_{ii'} = 1 - r_{ii'}^2$$

Similarity coefficients for binary data

		individual i		
		1	0	
individual i'	1	a	b	a+b
	0	c	d	c+d
		a+c	b+d	a+b+c+d

a co-presences

d co-abscences

b, c mismatches

$$s_{ii'} = \frac{a+d}{a+b+c+d}$$ SOKAL & MICHENER

$$s_{ii'} = \frac{a}{a+b+c+d}$$ RUSSEL & RAO

$$s_{ii'} = \frac{a}{a+b+c}$$ JACCARD

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Steps in clustering

- Data collection
- Measurement of proximity
- Choice of a clustering algorithm
- Number of clusters
- Interpretation of the results

Hierarchical clustering

- **Distances between observations**
  - cf. Measurement of proximity
- **Distances between groups**
  - WARD'S method
  - single linkage
  - complete linkage
  - average linkage
  - centroïd linkage
  - median linkage

Non hierarchical clustering

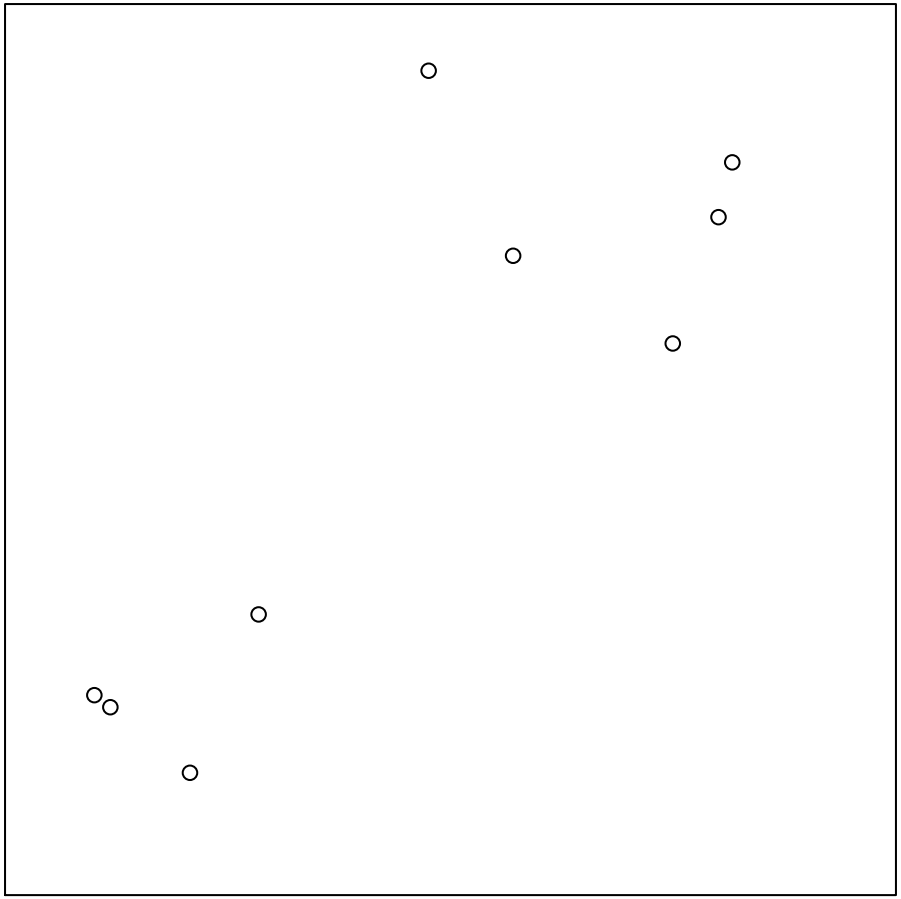
- fixed number of clusters
- methods based on the SS decompositon : $T = H + E$ (minimum of the trace of $E^{-1}H$)
- relocation methods (k-means)

K-means clustering

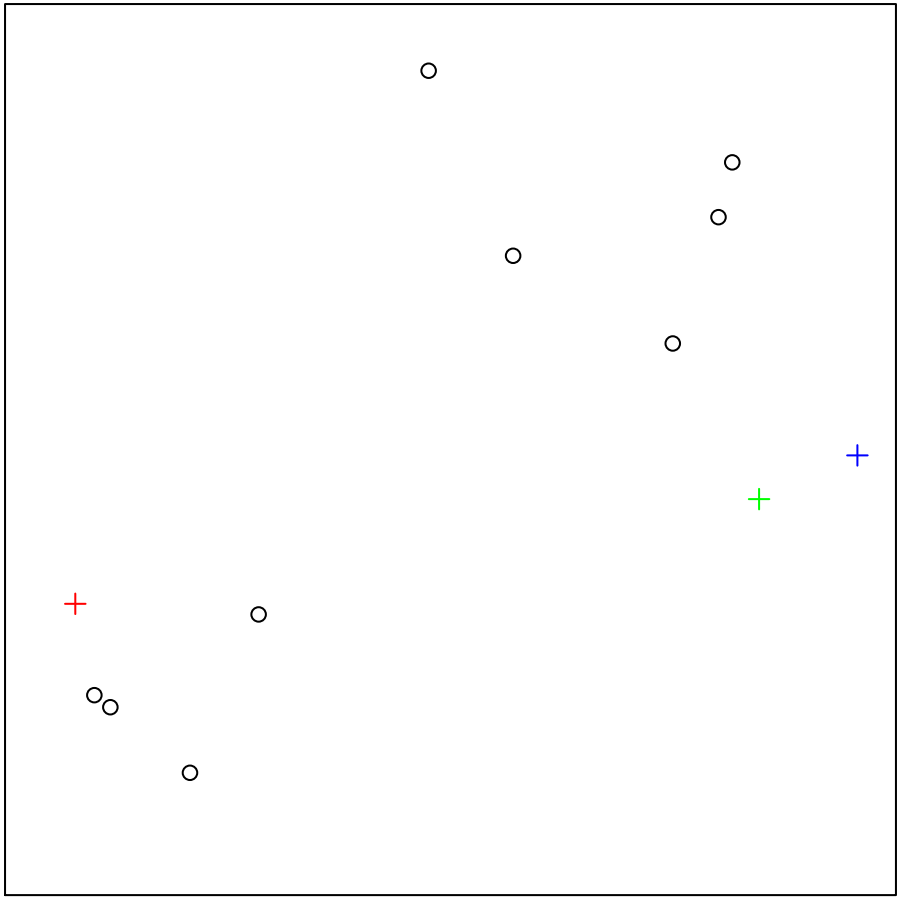
Algorithm

- generate k random centroids
- repeat until no more modifications
  - calculate distance between each points and each centroids
  - assign points to the nearest centroid group
  - recalculate centroids coordinates of the new groups

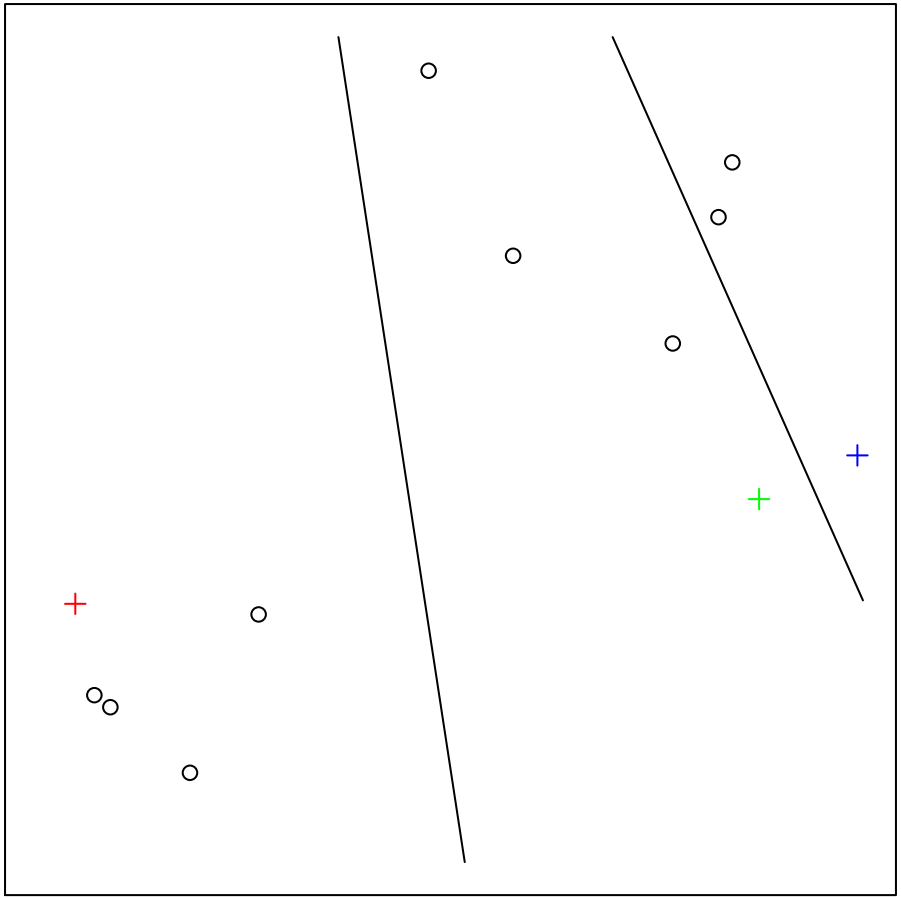
Example - K-means



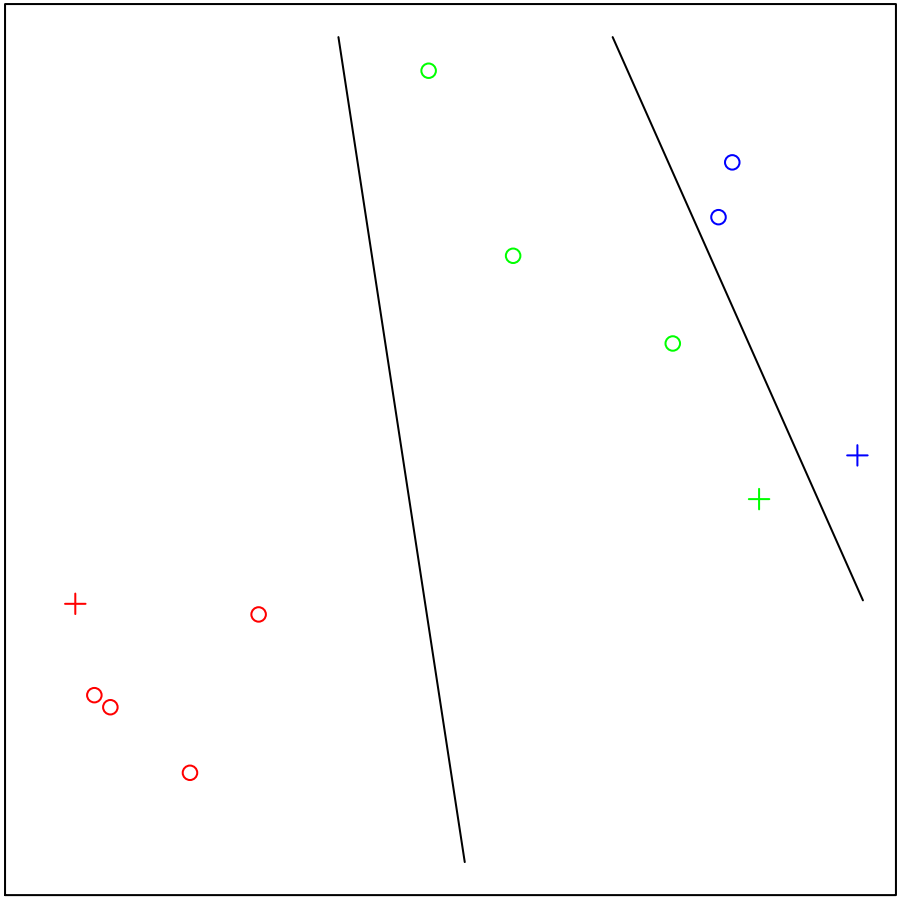
Example - K-means



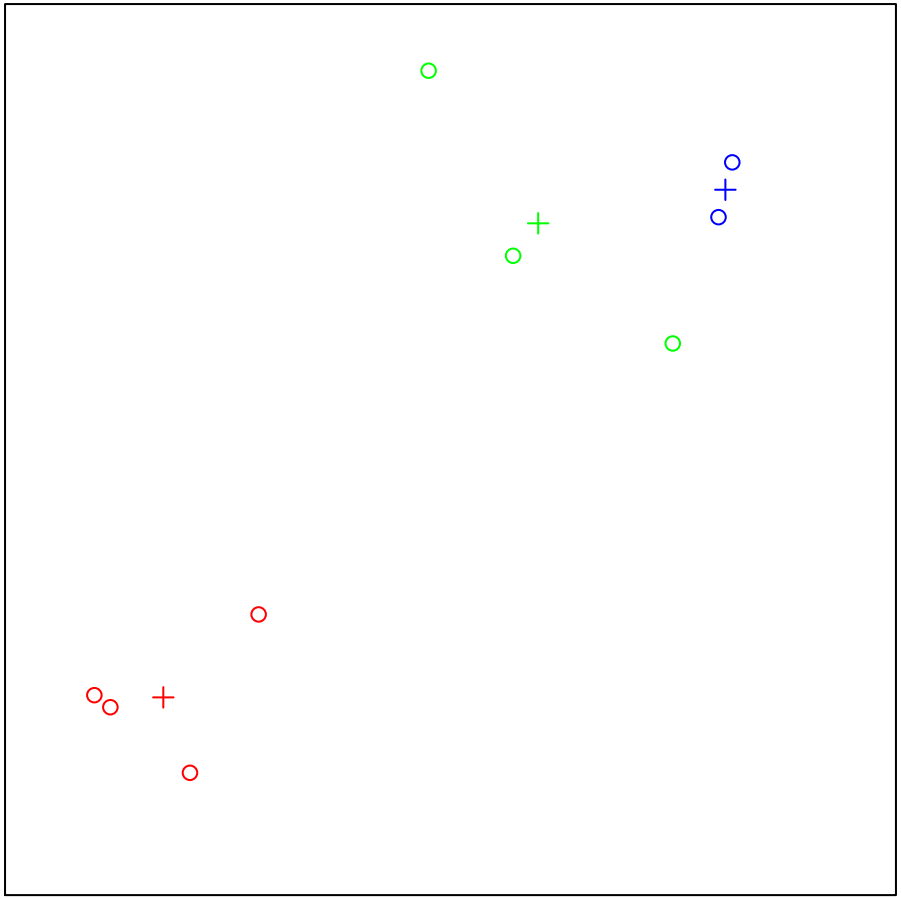
Example - K-means



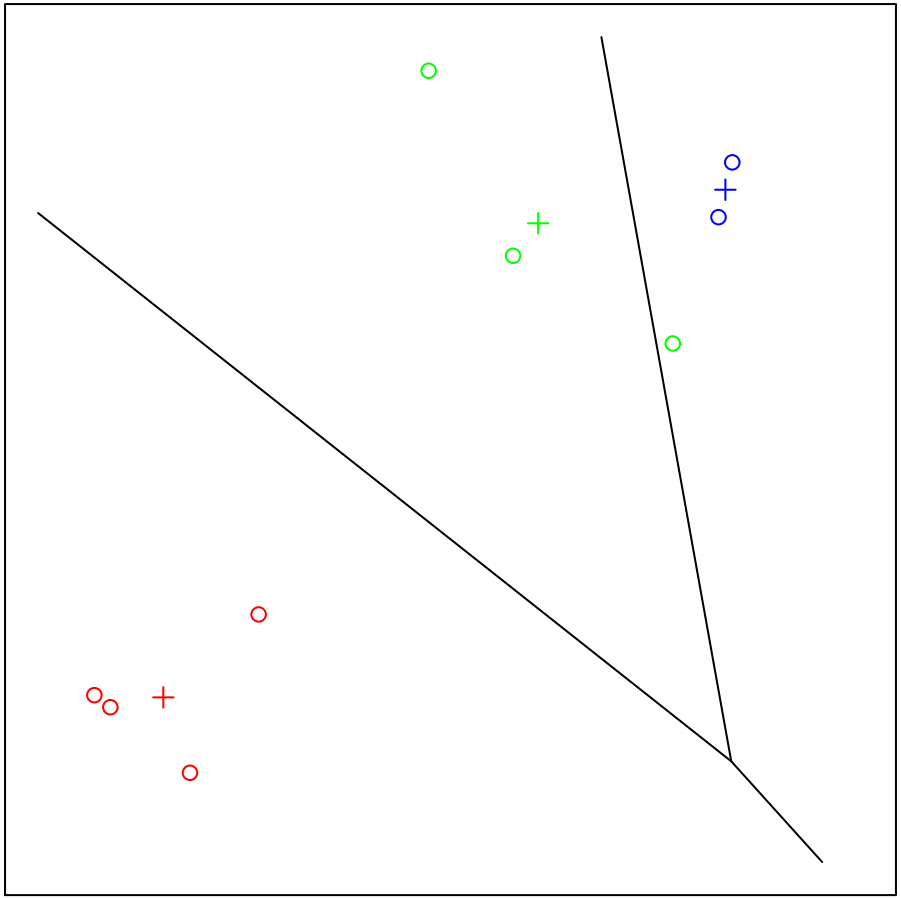
Example - K-means



Example - K-means



Example - K-means



```
waters7.km <- kmeans (waters7std, centers=3)

waters7.km
```

K-means clustering

Pros/cons

- Simple, quick and easy
- Fixed number of clusters
- Sensitive to initial conditions
  - multiple runs with random initial centroids
- Sensitive to outliers
- works best with linearly separable clusters

Combination of methods

- k-means $\rightarrow$ hierarchical clustering
  - reduce the number of initial observations
  - used when initials steps are not important to speed up process
- hierarchical clustering $\rightarrow$ k-means
  - test robustness of partition
  - fix initial centroids as centers of the hierarchical clusters

```
# calculate groups centroïds
init <- aggregate(.~groups, data=as.data.frame(data.std), FUN=mean)
# generate kmeans partition based on previous centroïds
kmean.res <- kmeans(data.std, centers=init[-1])
# compare groupings
table(groups, kmean.res$cluster)
```

Steps in clustering

- Data collection
- Measurement of proximity
- Choice of a clustering algorithm
- Number of clusters
- Interpretation of the results

Number of clusters

- plot of R^2 as a function of the number of clusters
- pseudo $F = \frac{tr(H)/(g-1)}{tr(E)/(n-g)}$
- etc.

More generally, look for discontinuities in the clustering process (sudden raise of the height of merging)

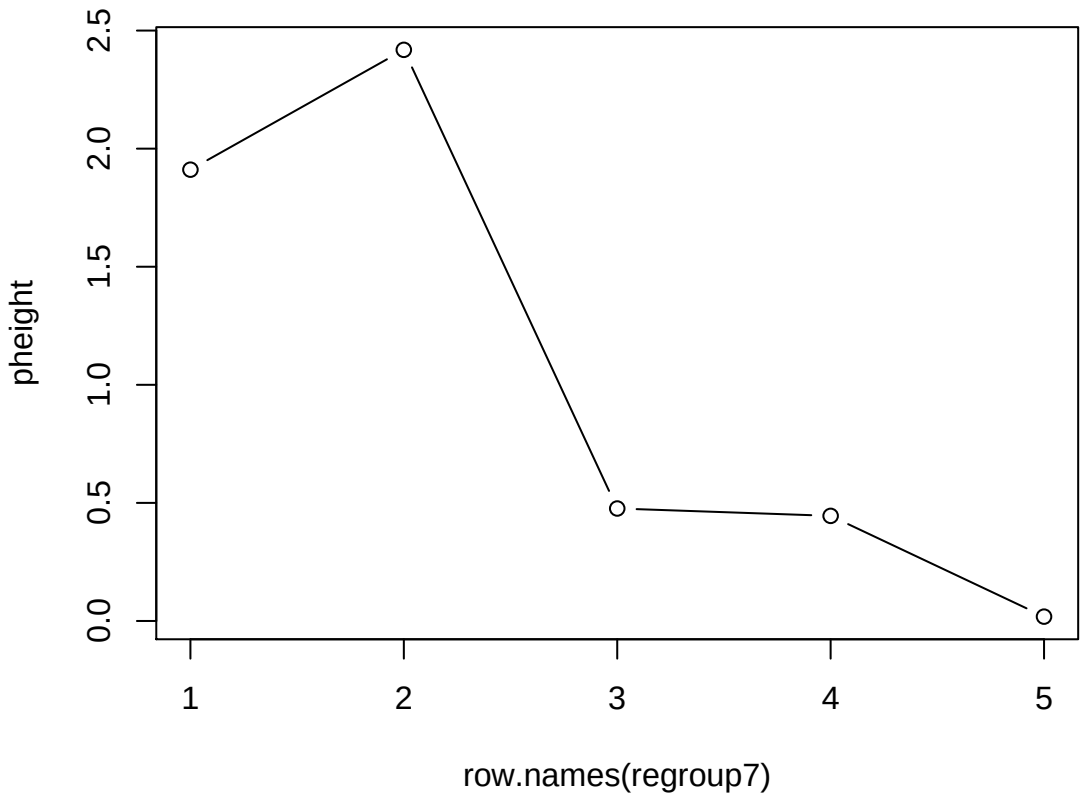
Successive merging steps

```
# informations on successive merging steps

regroup7 <- hclust.info(waters7.hc)

plot(height~row.names(regroup7), data=regroup7,
type="b")

plot(height~row.names(regroup7), data=regroup7,
type="b")
```

Example - waters

	height	pheight
1	5.798	1.911
2	3.886	2.418
3	1.468	0.476
4	0.992	0.445
5	0.546	0.019

Example - waters



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Steps in clustering

- Data collection
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Interpretation of the results

- univariate descriptive techniques
  - mean and standard deviation of each variable for each group
- multivariate descriptive techniques
  - distances between centroids of groups
  - principal components analysis

Group partition

```
# Group partition
gr3 <- cutree(waters7.hc, 3)
sort(gr3)
# Frequencies
table(gr3)
# Means
aggregate(.~gr3, data=waters7[1:6], FUN=mean)
# Standard diviations
aggregate(.~gr3, data=waters7[1:6], FUN=sd)
```

Example - waters

3 groups: $(G,O,T,o)_1$, $(L,S)_2$, $(c)_3$

Group means

Groups	HCO3	SO4	Cl	Ca	Mg	Na
1	170.75	28.5	7.25	43.25	10.5	5.5
2	400	262	15	179.5	35.5	5.5
3	1580	112	137	89	104	425
Total	437.57	107.14	28.00	88.71	31.00	65.43

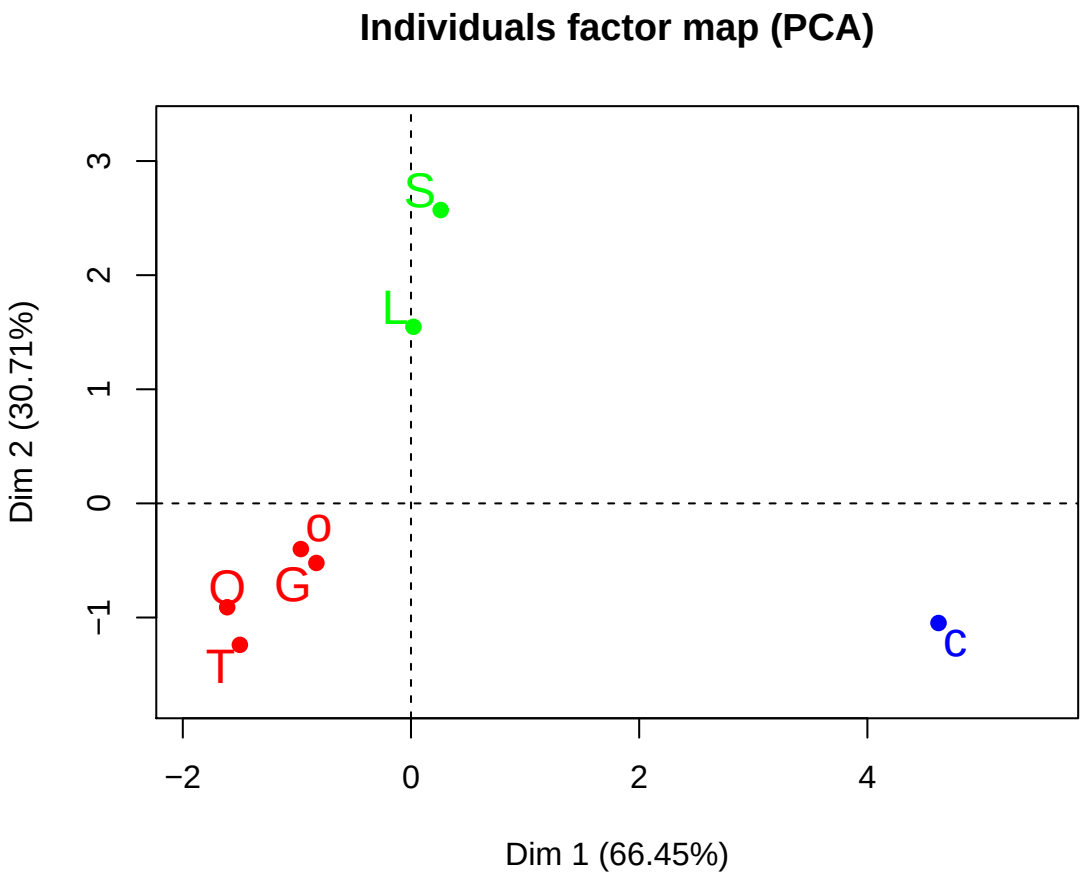
ACP

```
# ACP
library(FactoMineR)
cluster.pca <- PCA(waters7std)

# generate colors vector according to groups
col.gr <- rainbow(length(unique(gr3)))[gr3]

# plot groups
plot(cluster.pca, col.ind=col.gr, cex=1.5)
```

Example - waters



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