Multivariate Data Analysis

Special focus on Clustering and Multiway Methods

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Why a tutorial on Multivariate Data Analysis?

- Our research focus is principal component methods
- We teach multivariate data analysis
- We have developed R packages:
    - **FactoMineR** to perform principal component methods
        - PCA, correspondence analysis (CA), multiple correspondence analysis (MCA), multiple factor analysis (MFA)
        - complementarity between clustering and principal component methods
    - **missMDA** to handle missing values in and with multivariate data analysis
        - perform principal component methods (PCA, MCA) with missing values
        - simple and multiple imputation based on principal component models for continuous and categorical data

Outline

Multivariate data analysis with a special focus on clustering and multiway methods

1. Principal Component Analysis (PCA)
2. Multiple Factor Analysis (MFA)
3. Complementarity between Clustering and Principal Component methods

⇒ Multidimensional descriptive methods
⇒ Graphical representations

Principal Component Analysis

1. Data - Issues - Preprocessing
2. Individuals Study
3. Variables Study
4. Helps to Interpret

Principal Component Analysis

Dimensionality reduction $\Rightarrow$ describes the dataset with a smaller number of variables

Technique widely used for applications such as: data compression, data reconstruction, preprocessing before clustering, and ...

Descriptive methods

PCA deals with which kind of data?

PCA deals with continuous variables, but categorical variables can also be included in the analysis

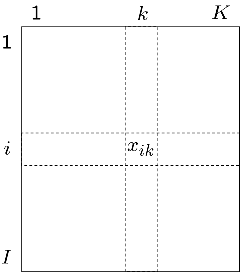


Figure: Data table in PCA

Many examples:

- Sensory analysis: products - descriptors
- Ecology: plants - measurements; waters - physico-chemical analyses
- Economy: countries - economic indicators
- Microbiology: cheeses - microbiological analyses
- etc.

Wine data

- 10 individuals (rows): white wines from Val de Loire
- 30 variables (columns):
    - 27 continuous variables: sensory descriptors
    - 2 continuous variables: odour and overall preferences
    - 1 categorical variable: label of the wines (Vouvray - Sauvignon)

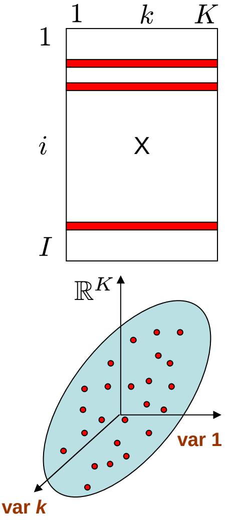
	O.fruity	O.passion	O.citrus	...	Sweetness	Acidity	Bitterness	Astringency	Aroma.intensity	Aroma.persistency	Visual.intensity	Odor.preferene	Overall.preference	Label
S Michaud	4.3	2.4	5.7	...	3.5	5.9	4.1	1.4	7.1	6.7	5.0	6.0	5.0	Sauvignon
S Renaudie	4.4	3.1	5.3	...	3.3	6.8	3.8	2.3	7.2	6.6	3.4	5.4	5.5	Sauvignon
S Trotignon	5.1	4.0	5.3	...	3.0	6.1	4.1	2.4	6.1	6.1	3.0	5.0	5.5	Sauvignon
S Buisse Domaine	4.3	2.4	3.6	...	3.9	5.6	2.5	3.0	4.9	5.1	4.1	5.3	4.6	Sauvignon
S Buisse Cristal	5.6	3.1	3.5	...	3.4	6.6	5.0	3.1	6.1	5.1	3.6	6.1	5.0	Sauvignon
V Aub Silex	3.9	0.7	3.3	...	7.9	4.4	3.0	2.4	5.9	5.6	4.0	5.0	5.5	Vouvray
V Aub Marigny	2.1	0.7	1.0	...	3.5	6.4	5.0	4.0	6.3	6.7	6.0	5.1	4.1	Vouvray
V Font Domaine	5.1	0.5	2.5	...	3.0	5.7	4.0	2.5	6.7	6.3	6.4	4.4	5.1	Vouvray
V Font Brûlés	5.1	0.8	3.8	...	3.9	5.4	4.0	3.1	7.0	6.1	7.4	4.4	6.4	Vouvray
V Font Coteaux	4.1	0.9	2.7	...	3.8	5.1	4.3	4.3	7.3	6.6	6.3	6.0	5.7	Vouvray

Problems - objectives

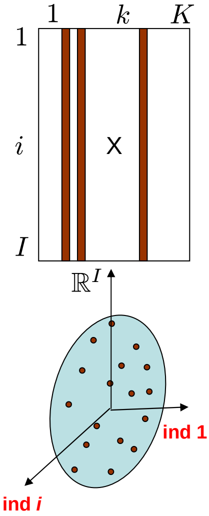
- Individuals study:
  similarity between individuals with respect to all the variables
  $\Rightarrow$ partition between individuals
- Variables study:
  linear relationships between variables $\Rightarrow$ visualization of the correlation matrix (denoted S); find synthetic variables
- Link between the two studies:
  characterization of the groups of individuals by the variables; specific individuals to better understand links between variables

Two clouds of points

Individuals study



Variables study



Preprocessing

⇒ Similarity between individuals: Euclidean distance

- Choosing active variables

$$d^2(i,i') = \sum_{k=1}^{K}(x_{ik} - x_{i'k})^2$$

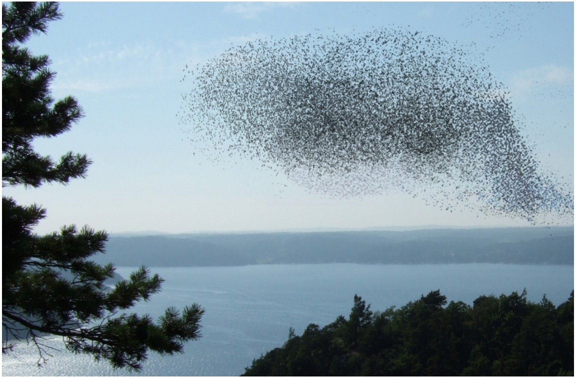
- Variables are always centred

$$d^2(i,i') = \sum_{k=1}^{K}((x_{ik} - \bar{x}_k) - (x_{i'k} - \bar{x}_k))^2$$

- Standardizing variables or not?

$$d^2(i,i') = \sum_{k=1}^{K}\frac{1}{s_k^2}(x_{ik} - x_{i'k})^2$$

Individuals cloud



- Study the structure, *i.e.* the shape of the cloud of individuals
- Individuals are in $\mathbb{R}^K$

Fit the individuals cloud

Find the subspace which better sums up the data

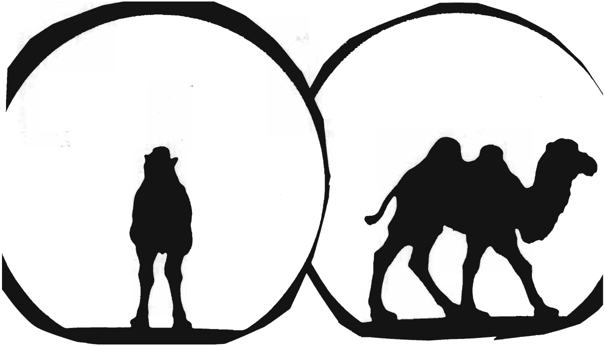
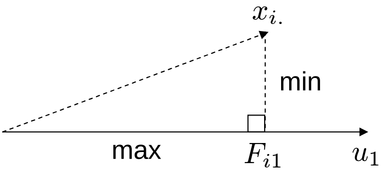


Figure: Camel vs dromedary?

⇒ Closest representation by projection

⇒ Best representation of the diversity, variability

Fit the individuals cloud



$$\begin{aligned} P_{u_1}(x_{i.}) &= u_1 (u_1' u_1)^{-1} u_1' x_{i.} \\ &= < x_{i.}, u_1 > u_1 \\ F_{i1} &= < x_{i.}, u_1 > \end{aligned}$$

- Minimize the distance between individuals and their projections
- Maximize the variance of the projected data

$$u_1 = \arg\max_{u_1 \in \mathbb{R}^K} (var(F_{.1})) = \arg\max_{u_1 \in \mathbb{R}^K} (var(Xu_1)) \text{ with } u_1' u_1 = 1$$

$\Rightarrow$ u_1 first eigenvector of the correlation matrix associated with the largest eigenvalue λ_1: $Su_1 = \lambda_1 u_1$

$$Var(F_{.1}) = var(Xu_1) = 1/I \; u_1' X' X u_1 = u_1' S u_1 = \lambda_1 u_1' u_1 = \lambda_1$$

Fit the individuals cloud

Additional axes are sequentially defined: each new direction maximizes the projected variance among all orthogonal directions
$\Rightarrow Q$ eigenvectors $u_1,\ldots,u_Q$ associated to $\lambda_1,\ldots,\lambda_Q$

Representation quality: dimensionality reduction $\Rightarrow$ loosing information

- Total variance of the initial individuals cloud (total inertia):

$$\frac{1}{I}\|x_{i.} - g\|^2 = tr(S) = \sum_{k=1}^{K} \lambda_k \quad (= K)$$

- Variance of the projected individuals cloud (Q-dimensional representation): $var(F_1) + var(F_2) + \ldots + var(F_Q)$

$\Rightarrow$ Percentage of variance explained: $\frac{\sum_{k=1}^{Q} \lambda_k}{\sum_{k=1}^{K} \lambda_k}$

Example: wine data

- Sensory descriptors are used as active variables: only these variables are used to construct the axes
- Variables are (centred and) standardized

	O.fruity	O.passion	O.citrus	...	Sweetness	Acidity	Bitterness	Astringency	Aroma.intensity	Aroma.persistency	Visual.intensity	Odor.preferene	Overall.preference	Label
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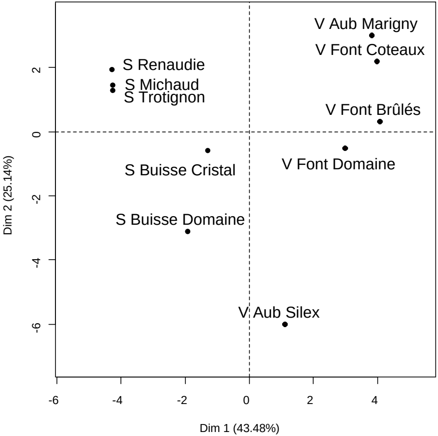
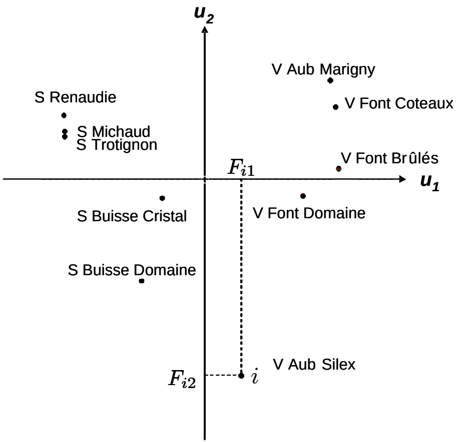
V Font Coteaux	4.1	0.9	2.7	...	3.8	5.1	4.3	4.3	7.3	6.6	6.3	6.0	5.7	Vouvray

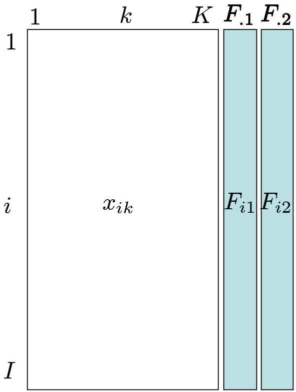
Example: graph of the individuals



⇒ Need variables to interpret the dimensions of variability

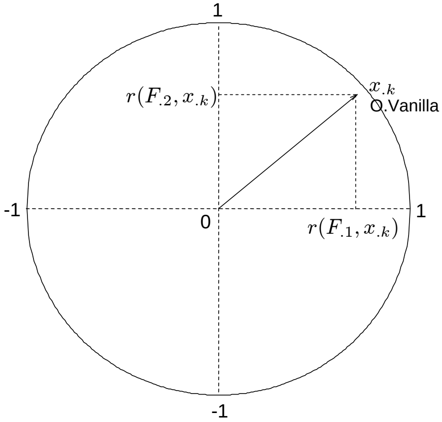
Individuals coordinates considered as variables





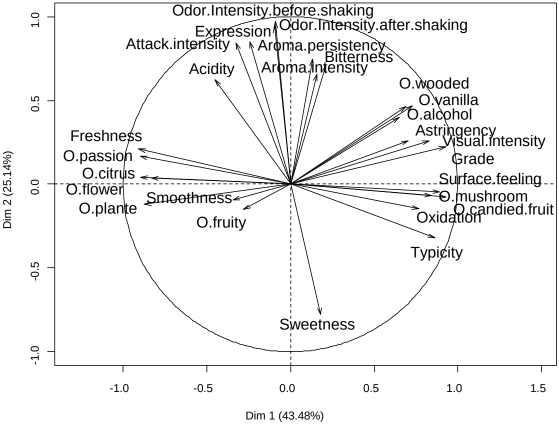
Interpretation of the individuals graph with the variables

- Correlation between variable $x_{.k}$ and $F_{.1}$ (and $F_{.2}$)

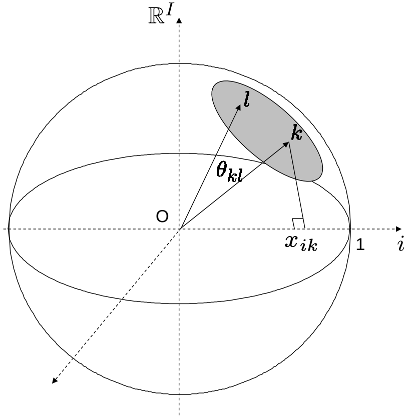


$\Rightarrow$ Correlation circle

Interpretation of the individuals graph with the variables



Cloud of variables

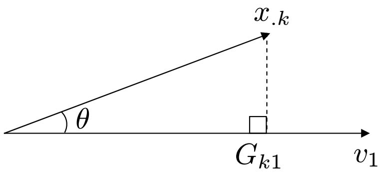


Since variables are centred:

$$cos(\theta_{kl}) = \frac{< x_{.k}, x_{.l} >}{\|x_{.k}\| \; \|x_{.l}\|} = \frac{\sum_{i=1}^{I} x_{ik} x_{il}}{\sqrt{(\sum_{i=1}^{I} x_{ik}^2)(\sum_{i=1}^{I} x_{il}^2)}} = r(x_{.k}, x_{.l})$$

Fit the variables cloud

Find v_1 (in $\mathbb{R}^I$, with $v_1'v_1 = 1$) which best fits the cloud



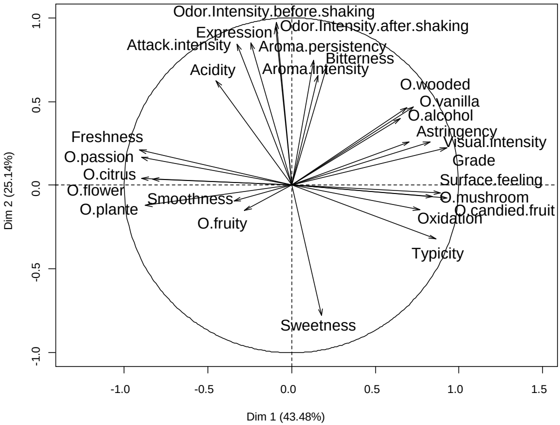
$$
\begin{aligned}
P_{v_1}(x_{.k}) &= v_1(v_1'v_1)^{-1}v_1'x_{.k} \\
G_{k1} &= 1/I \;\; < v_1, x.k > \\
G_{k1} &= 1/I \; \frac{< v_1, x.k >}{\|v_1\| \; \|x_{.k}\|}
\end{aligned}
$$

$$
\arg\max_{v_1 \in \mathbb{R}^I} \sum_{i=k}^{K} G_{k1}^2 = \arg\max_{v_1 \in \mathbb{R}^I} \sum_{i=k}^{K} r(v_1, x_{.k})^2
$$

$\Rightarrow$ v_1 is the best synthetic variable

$\Rightarrow$ $v_1, \ldots, v_Q$ are the eigenvectors of $W = XX'$ the inner product matrix associated with the largest eigenvalues: $Wv_q = \lambda_q v_q$

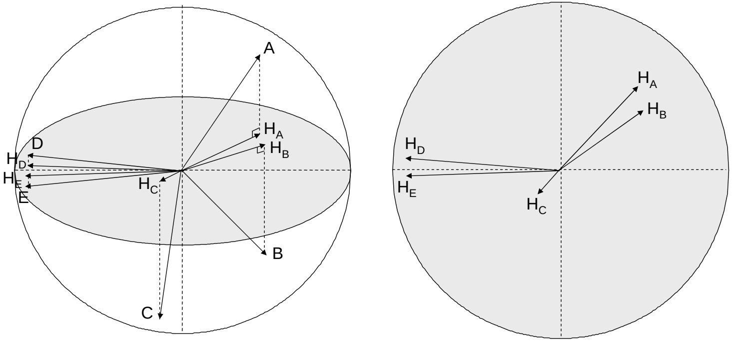
Fit the variables cloud



⇒ Same representation! What a wonderful result!

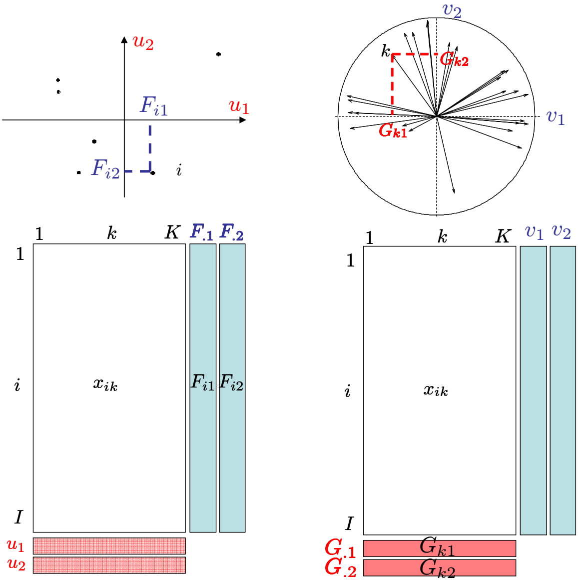
Projections...

$r(A, B) = cos(\theta_{A,B})$
$cos(\theta_{A,B}) \approx cos(\theta_{H_A,H_B})$ if variables are well projected



Only well projected variables can be interpreted!

Link between the two representations: transition formulae



Link between the two representations: transition formulae

- $Su = X'Xu = \lambda u$
- $XX'Xu = X\lambda u \rightarrow W(Xu) = \lambda(Xu)$
- $WF = \lambda F$ and since $Wv = \lambda v$ then F and v are collinear
- Since, $||F|| = \lambda$ and $||v|| = 1$ we have:

$$v = \frac{1}{\sqrt{\lambda}}F \quad \Rightarrow G = X'v = \frac{1}{\sqrt{\lambda}}X'F$$
$$u = \frac{1}{\sqrt{\lambda}}G \quad \Rightarrow F = Xu = \frac{1}{\sqrt{\lambda}}XG$$

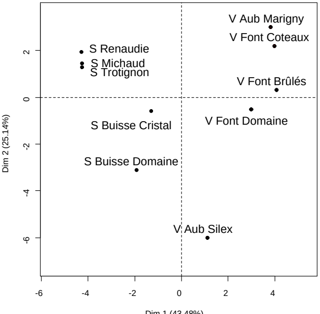
$$\boxed{F_{iq} = \frac{1}{\sqrt{\lambda_q}}\sum_{k=1}^{K} x_{ik}\,G_{kq}} \qquad \boxed{G_{kq} = \frac{1}{\sqrt{\lambda_q}}\sum_{i=1}^{I} x_{ik}\,F_{iq}}$$

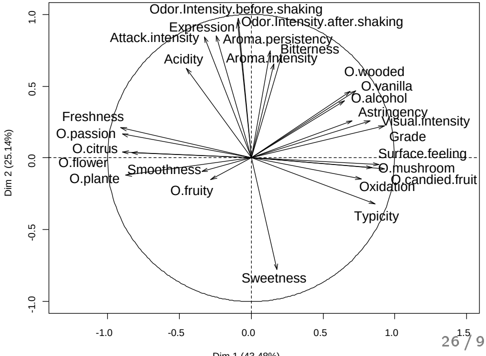
$F_{.q}$: principal components, scores
$G_{.q}$: correlations between variables and principal components

Link between the two representations: transition formulae

$$F_{iq} = \frac{1}{\sqrt{\lambda_q}} \sum_{k=1}^{K} x_{ik}\, G_{kq} \qquad G_{kq} = \frac{1}{\sqrt{\lambda_q}} \sum_{i=1}^{I} x_{ik}\, F_{iq}$$

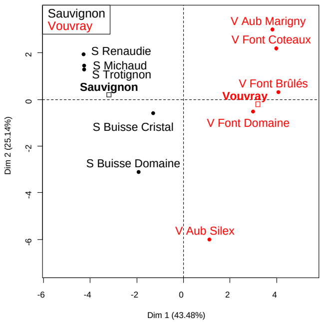
What does it mean? An individual is at the same side as the variables for which it takes high values

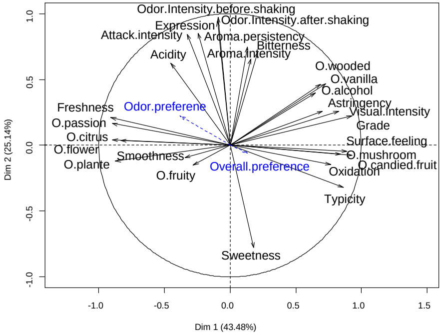




Supplementary information

- For the continuous variables: projection of supplementary variables on the dimensions
- For the individuals: projection
- For the categories: projection at the barycentre of the individuals who take the categories

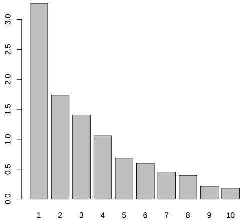




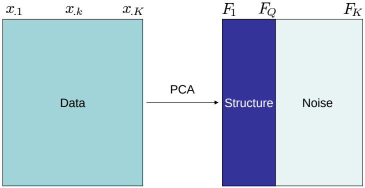
⇒ Supplementary information do not create the dimensions

Choosing the number of components

Bar plot, test on eigenvalues, confidence interval, cross-validation (functions `estim_ncpPCA` and `estim_ncp`), etc.



Two objectives:
⇒ Interpretation
⇒ Separate structure and noise



Percentage of variance obtained under independence

⇒ Is there a structure on my data?

	Number of variables												
nbind	4	5	6	7	8	9	10	11	12	13	14	15	16
5	96.5	93.1	90.2	87.6	85.5	83.4	81.9	80.7	79.4	78.1	77.4	76.6	75.5
6	93.3	88.6	84.8	81.5	79.1	76.9	75.1	73.2	72.2	70.8	69.8	68.7	68.0
7	90.5	84.9	80.9	77.4	74.4	72.0	70.1	68.3	67.0	65.3	64.3	63.2	62.2
8	88.1	82.3	77.2	73.8	70.7	68.2	66.1	64.0	62.8	61.2	60.0	59.0	58.0
9	86.1	79.5	74.8	70.7	67.4	65.1	62.9	61.1	59.4	57.9	56.5	55.4	54.3
10	84.5	77.5	72.3	68.2	65.0	62.4	60.1	58.3	56.5	55.1	53.7	52.5	51.5
11	82.8	75.7	70.3	66.3	62.9	60.1	58.0	56.0	54.4	52.7	51.3	50.1	49.2
12	81.5	74.0	68.6	64.4	61.2	58.3	55.8	54.0	52.4	50.9	49.3	48.2	47.2
13	80.0	72.5	67.2	62.9	59.4	56.7	54.4	52.2	50.5	48.9	47.7	46.6	45.4
14	79.0	71.5	65.7	61.5	58.1	55.1	52.8	50.8	49.0	47.5	46.2	45.0	44.0
15	78.1	70.3	64.6	60.3	57.0	53.9	51.5	49.4	47.8	46.1	44.9	43.6	42.5
16	77.3	69.4	63.5	59.2	55.6	52.9	50.3	48.3	46.6	45.2	43.6	42.4	41.4
17	76.5	68.4	62.6	58.2	54.7	51.8	49.3	47.1	45.5	44.0	42.6	41.4	40.3
18	75.5	67.6	61.8	57.1	53.7	50.8	48.4	46.3	44.6	43.0	41.6	40.4	39.3
19	75.1	67.0	60.9	56.5	52.8	49.9	47.4	45.5	43.7	42.1	40.7	39.6	38.4
20	74.1	66.1	60.1	55.6	52.1	49.1	46.6	44.7	42.9	41.3	39.8	38.7	37.5
25	72.0	63.3	57.1	52.5	48.9	46.0	43.4	41.4	39.6	38.1	36.7	35.5	34.5
30	69.8	61.1	55.1	50.3	46.7	43.6	41.1	39.1	37.3	35.7	34.4	33.2	32.1
35	68.5	59.6	53.3	48.6	44.9	41.9	39.5	37.4	35.6	34.0	32.7	31.6	30.4
40	67.5	58.3	52.0	47.3	43.4	40.5	38.0	36.0	34.1	32.7	31.3	30.1	29.1
45	66.4	57.1	50.8	46.1	42.4	39.3	36.9	34.8	33.1	31.5	30.2	29.0	27.9
50	65.6	56.3	49.9	45.2	41.4	38.4	35.9	33.9	32.1	30.5	29.2	28.1	27.0
100	60.9	51.4	44.9	40.0	36.3	33.3	31.0	28.9	27.2	25.8	24.5	23.3	22.3

Table: 95 % quantile inertia on the two first dimensions of 10000 PCA on data with independent variables

Percentage of variance obtained under independence

	Number of variables												
nbind	17	18	19	20	25	30	35	40	50	75	100	150	200
5	74.9	74.2	73.5	72.8	70.7	68.8	67.4	66.4	64.7	62.0	60.5	58.5	57.4
6	67.0	66.3	65.6	64.9	62.3	60.4	58.9	57.6	55.8	52.9	51.0	49.0	47.8
7	61.3	60.7	59.7	59.1	56.4	54.3	52.6	51.4	49.5	46.4	44.6	42.4	41.2
8	57.0	56.2	55.4	54.5	51.8	49.7	47.8	46.7	44.6	41.6	39.8	37.6	36.4
9	53.6	52.5	51.8	51.2	48.1	45.9	44.4	42.9	41.0	38.0	36.1	34.0	32.7
10	50.6	49.8	49.0	48.3	45.2	42.9	41.4	40.1	38.0	35.0	33.2	31.0	29.8
11	48.1	47.2	46.5	45.8	42.8	40.6	39.0	37.7	35.6	32.6	30.8	28.7	27.5
12	46.2	45.2	44.4	43.8	40.7	38.5	36.9	35.5	33.5	30.5	28.8	26.7	25.5
13	44.4	43.4	42.8	41.9	39.0	36.8	35.1	33.9	31.8	28.8	27.1	25.0	23.9
14	42.9	42.0	41.3	40.4	37.4	35.2	33.6	32.3	30.4	27.4	25.7	23.6	22.4
15	41.6	40.7	39.8	39.1	36.2	34.0	32.4	31.1	29.0	26.0	24.3	22.4	21.2
16	40.4	39.5	38.7	37.9	35.0	32.8	31.1	29.8	27.9	24.9	23.2	21.2	20.1
17	39.4	38.5	37.6	36.9	33.8	31.7	30.1	28.8	26.8	23.9	22.2	20.3	19.2
18	38.3	37.4	36.7	35.8	32.9	30.7	29.1	27.8	25.9	22.9	21.3	19.4	18.3
19	37.4	36.5	35.8	34.9	32.0	29.9	28.3	27.0	25.1	22.2	20.5	18.6	17.5
20	36.7	35.8	34.9	34.2	31.3	29.1	27.5	26.2	24.3	21.4	19.8	18.0	16.9
25	33.5	32.5	31.8	31.1	28.1	26.0	24.5	23.3	21.4	18.6	17.0	15.2	14.2
30	31.2	30.3	29.5	28.8	26.0	23.9	22.3	21.1	19.3	16.6	15.1	13.4	12.5
35	29.5	28.6	27.9	27.1	24.3	22.2	20.7	19.6	17.8	15.2	13.7	12.1	11.1
40	28.1	27.3	26.5	25.8	23.0	21.0	19.5	18.4	16.6	14.1	12.7	11.1	10.2
45	27.0	26.1	25.4	24.7	21.9	20.0	18.5	17.4	15.7	13.2	11.8	10.3	9.4
50	26.1	25.3	24.6	23.8	21.1	19.1	17.7	16.6	14.9	12.5	11.1	9.6	8.7
100	21.5	20.7	19.9	19.3	16.7	14.9	13.6	12.5	11.0	8.9	7.7	6.4	5.7

Table: 95 % quantile inertia on the two first dimensions of 10000 PCA on data with independent variables

Quality of the representation: $\cos^2$

- For the variables: only well projected variables (high $\cos^2$ between the variable and its projection) can be interpreted!

```
round(res.pca$var$cos2,2)
                             Dim.1 Dim.2
Odor.Intensity.before.shaking  0.01  0.94
Odor.Intensity.after.shaking   0.01  0.89
Expression                     0.11  0.71
```

- For the individuals: (same idea) distance between individuals can only be interpreted for well projected individuals

```
round(res.pca$ind$cos2,2)
              Dim.1 Dim.2
S Michaud      0.62  0.07
S Renaudie     0.73  0.15
S Trotignon    0.78  0.07
```

Contribution

$\Rightarrow$ Contribution to the construction of the dimension (percentage of variability):

- for each individual: $Ctr_q(i) = \frac{F_{iq}^2}{\sum_{i=1}^{I} F_{iq}^2} = \frac{F_{iq}^2}{\lambda_q}$

  $\Rightarrow$ Individuals with a large coordinate contribute the most

```
round(res.pca$ind$contrib,2)
                 Dim.1 Dim.2
S Michaud        15.49  3.10
S Renaudie       15.56  5.56
S Trotignon      15.46  2.43
```

- for each variable: $Ctr_q(k) = \frac{G_{kq}^2}{\lambda_q} = \frac{r(x_{.k}, v_q)^2}{\lambda_q}$

  $\Rightarrow$ Variables highly correlated with the principal component contribute the most

Description of the dimensions

By the continuous variables:

- correlation between each variable and the principal component of rank q is calculated
- correlation coefficients are sorted and significant ones are given

```
> dimdesc(res.pca)
            $Dim.1$quanti                                            $Dim.2$quanti
                 corr p.value                                              corr p.value
O.candied.fruit  0.93 9.5e-05  Odor.Intensity.before.shaking 0.97 3.1e-06
Grade            0.93 1.2e-04  Odor.Intensity.after.shaking  0.95 3.6e-05
Surface.feeling  0.89 5.5e-04  Attack.intensity              0.85 1.7e-03
Typicity         0.86 1.4e-03  Expression                    0.84 2.2e-03
O.mushroom       0.84 2.3e-03  Aroma.persistency             0.75 1.3e-02
Visual.intensity 0.83 3.1e-03  Bitterness                    0.71 2.3e-02
   ...            ...     ...  Aroma.intensity               0.66 4.0e-02
O.plante        -0.87 1.0e-03
O.flower        -0.89 4.9e-04
O.passion       -0.90 4.5e-04
Freshness       -0.91 2.9e-04  Sweetness                    -0.78 8.0e-03
```

Description of the dimensions

By the categorical variables:

- Perform a one-way analysis of variance with the coordinates of the individuals ($F_{.q}$) explained by the categorical variable
  - a F-test by variable
  - for each category, a Student's t-test to compare the average of the category with the general mean

```
> dimdesc(res.pca)
Dim.1$quali
           R2      p.value
Label    0.874    7.30e-05

Dim.1$category
          Estimate       p.value
Vouvray      3.203      7.30e-05
Sauvignon   -3.203      7.30e-05
```

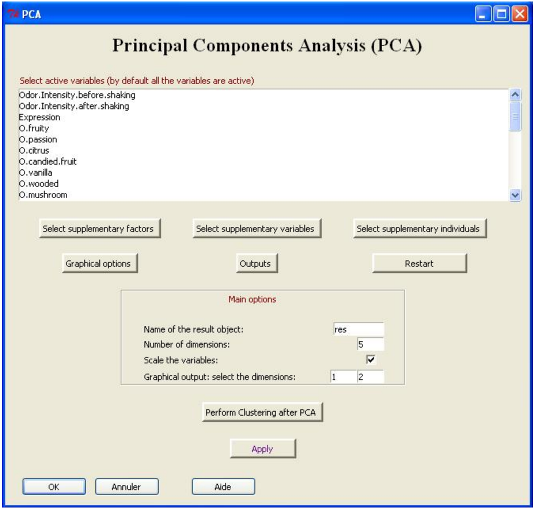
Practice with R

1. Choose active variables
2. Scale or not the variables
3. Perform PCA
4. Choose the number of dimensions to interpret
5. Simultaneously interpret the individuals and variables graphs
6. Use indicators to enrich the interpretation

```
library(FactoMineR)
Expert <- read.table("http://factominer.free.fr/useR2010/Expert_wine.csv",
   header=TRUE, sep=";",row.names=1)
res.pca <- PCA(Expert,scale=T,quanti.sup=29:30,quali.sup=1)
res.pca
x11()
barplot(res.pca$eig[,1],main="Eigenvalues",names.arg=1:nrow(res.pca$eig))
plot.PCA(res.pca,habillage=1)
res.pca$ind$coord
res.pca$ind$cos2
res.pca$ind$contrib
plot.PCA(res.pca,axes=c(3,4),habillage=1)
dimdesc(res.pca)
write.infile(res.pca,file="my_FactoMineR_results.csv") #to export a list
```

Practice with GUI

```
source("http://factominer.free.fr/install-facto.r")
```



Handling missing values: missMDA package

$\Rightarrow$ Obtain the principal components from observed data with an EM-type algorithm

- Impute missing values with PCA using `imputePCA` function (tuning parameter: number of components)
- Perform the usual PCA on the completed data set

```
library(missMDA)
data(orange)
nb.dim <- estim_ncpPCA(orange,ncp.max=5)
res.comp <- imputePCA(orange,ncp=2)
res.pca <- PCA(res.comp$completeObs)
```

MCA: problems - objectives

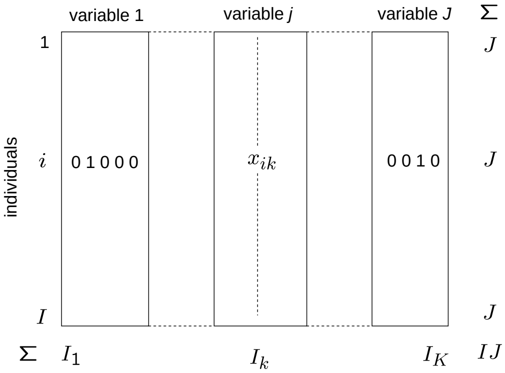
- Individuals study: similarity between individuals (for all the variables) $\rightarrow$ partition between individuals
  Individuals are different if they don't take the same levels

- Variables study: find some synthetic variables (continuous variables that sum up categorical variables); link between variables $\Rightarrow$ levels study
- Categories study:
  - two levels of different variables are similar if individuals that take these levels are the same (ex: 65 years and retired)
  - two levels are similar if individuals taking these levels behave the same way, they take the same levels for the other variables (ex: 60 years and 65 years)

- Link between these studies: characterization of the groups of individuals by the levels (ex: executive dynamic women)

MCA: a PCA on an indicator matrix

- Binary coding of the factors: a factor with K_j levels $\rightarrow$ K_j columns containing binary values, also called dummy variables



$$d^2(i,i') = \frac{I}{J}\sum_{j=1}^{J}\sum_{k=1}^{K_j}\frac{1}{I_k}(x_{ik} - x_{i'k})^2$$

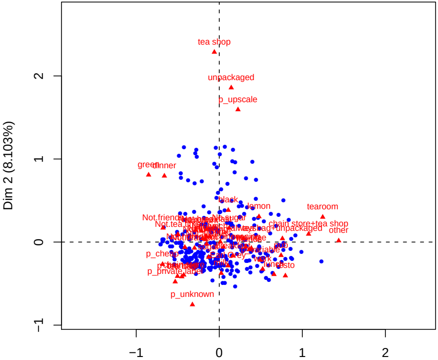
MCA: the superimposed representation

$$F_{iq} = \frac{1}{\sqrt{\lambda_q}} \sum_{k=1} K \frac{x_{ik}}{J} G_{kq}$$

$\Rightarrow$ Individual i at the barycenter of its levels

$$G_{kq} = \frac{1}{\sqrt{\lambda_q}} \sum_{i=1}^{I} \frac{x_{ik}}{I_k} F_{iq}$$

$\Rightarrow$ Level k at the barycenter of the individuals who take this level



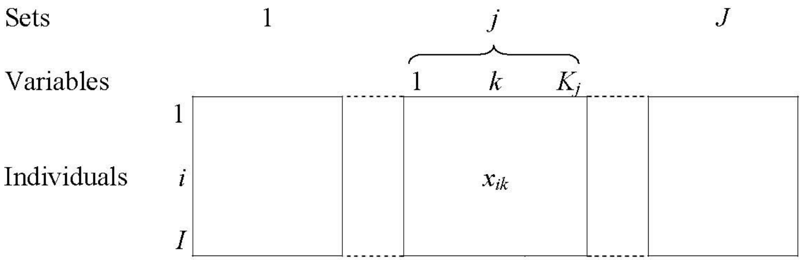
Multiple Factor Analysis

1. Data - Issues
2. Common Structure
3. Groups Study
4. Partial Analyses
5. Example

"Doing a data analysis, in good mathematics, is simply searching eigenvectors, all the science of it (the art) is just to find the right matrix to diagonalize"

Benzécri

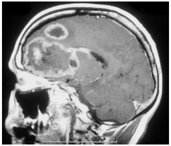
Multiway data set



Examples with **continuous and/or categorical** sets of variables:

- genomic: DNA, protein
- sensory analysis: sensorial, physico-chemical
- survey: student health (addicted consumptions, psychological conditions, sleep, identification, etc.)
- economy: economic indicators for countries by year

Example: gliomas brain tumors



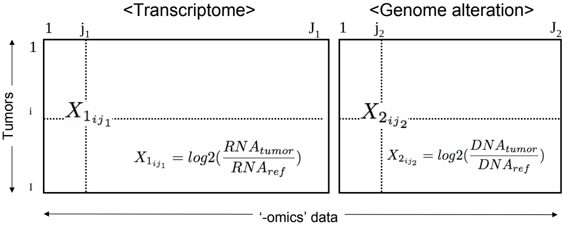
Gliomas: Brain tumors, WHO classification

- astrocytoma (A) x5
- oligodendroglioma (O) x8
- oligo-astrocytoma (OA) x6
- glioblastoma (GBM) x24

43 tumor samples

(Bredel *et al.*,2005)

- Transcriptional modification (RNA), microarrays: 489 variables
- Damage to DNA (CGH array): 113 variables



Objectives

- Study the similarities between individuals with respect to all the variables
- Study the linear relationships between variables

$\Rightarrow$ taking into account the structure on the data (balancing the influence of each group)

- Find the common structure with respect to all the groups - highlight the specificities of each group
- Compare the typologies obtained from each group of variables (separate analyses)

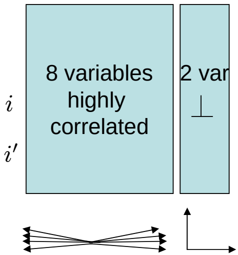
Balancing the groups of variables

MFA is a weighted PCA:

- compute the first eigenvalue λ_1^j of each group of variables
- perform a global PCA on the weighted data table:

$$\left[\frac{X_1}{\sqrt{\lambda_1^1}}; \frac{X_2}{\sqrt{\lambda_1^2}}; \ldots; \frac{X_J}{\sqrt{\lambda_1^J}}\right]$$

$\Rightarrow$ Same idea as in PCA when variables are standardized: variables are weighted to compute distances between individuals i and i'

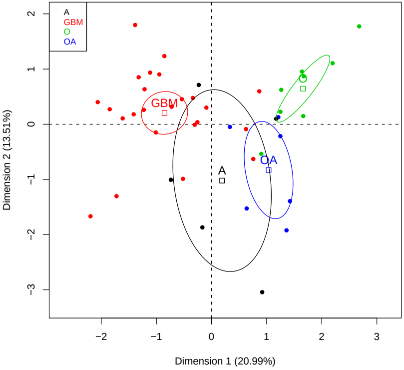


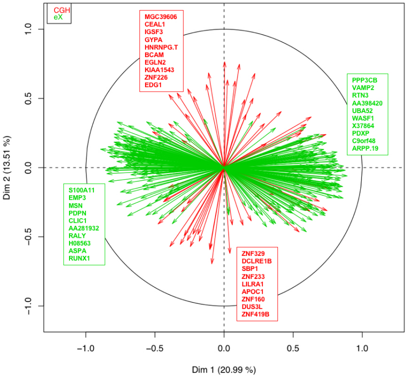
Balancing the groups of variables

This weighting allows that:

- same weight for all the variables of one group: the structure of the group is preserved
- for each group the variance of the main dimension of variability (first eigenvalue) is equal to 1
- no group can generate by itself the first global dimension
- a multidimensional group will contribute to the construction of more dimensions than a one-dimensional group

Individuals and variables representations





Same representations and same interpretation as in PCA

Groups study

$\Rightarrow$ Synthetic comparison of the groups

$\Rightarrow$ Are the relative positions of individuals globally similar from one group to another? Are the partial clouds similar?

$\Rightarrow$ Do the groups bring the same information?

Similarity between two groups

Measure of similarity between groups K_j and K_m:

$$\mathcal{L}_g(K_j, K_m) = \sum_{k \in K_j} \sum_{l \in K_m} cov^2\left(\frac{x_{.k}}{\sqrt{\lambda_1^k}}, \frac{x_{.l}}{\sqrt{\lambda_1^l}}\right)$$

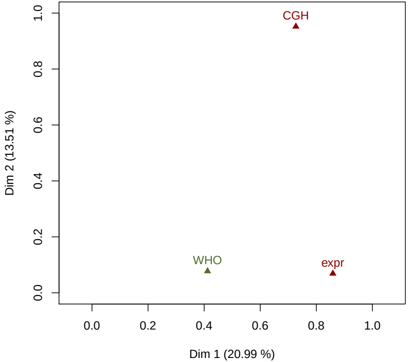
MFA = weighted PCA $\Rightarrow$ first principal component of MFA maximizes

$$\sum_{j=1}^{J} \mathcal{L}_g(v_1, K_j) = \sum_{j=1}^{J} \sum_{k \in K_j} cov^2\left(\frac{x_{.k}}{\sqrt{\lambda_1^j}}, v_1\right)$$

Inertia of K_j projected on v_1

Representation of the groups

Group j has the coordinates $(\mathcal{L}_g(v_1, K_j), \mathcal{L}_g(v_2, K_j))$



- 2 groups are all the more close that they induce the same structure
- The 1st dimension is common to all the groups
- 2nd dimension mainly due to CGH

$$0 \leq \mathcal{L}_g(v_1, K_j) = \frac{1}{\lambda_1^j} \underbrace{\sum_{k \in K_j} cov^2(x_{.k}, v_1)}_{\leq \lambda_1^j} \leq 1$$

Numeric indicators

```
> res.mfa$group$Lg
      CGH expr  WHO  MFA
CGH  2.51 0.60 0.46 1.96
expr 0.60 1.10 0.36 1.07
WHO  0.46 0.36 0.50 0.51
MFA  1.96 1.07 0.51 1.91
```

$$\mathcal{L}_g(K_j, K_j) = \frac{\sum_{k=1}^{K_j}(\lambda_k^j)^2}{(\lambda_1^j)^2} = 1 + \frac{\sum_{k=2}^{K_j}(\lambda_k^j)^2}{(\lambda_1^j)^2}$$

```
> res.mfa$group$RV
      CGH expr  WHO  MFA
CGH  1.00 0.36 0.41 0.90
expr 0.36 1.00 0.48 0.74
WHO  0.41 0.48 1.00 0.53
MFA  0.90 0.74 0.53 1.00
```

- CGH gives richer description ($\mathcal{L}_g$ greater)
- RV: a standardized $\mathcal{L}_g$
- CGH and expr are not linked (RV=0.36)
- CGH closest to the overall (RV=0.90)

Contribution of each group to each component of the MFA

```
> res.mfa$group$contrib
     Dim.1 Dim.2 Dim.3
CGH   45.8  93.3  78.1
expr  54.2   6.7  21.9
```

- Similar contribution of the 2 groups to the first dimension
- Second dimension only due to CGH

The RV coefficient

$X_{j_{(I \times K_j)}}$ and $X_{m_{(I \times K_m)}}$ not directly comparable
$W_{j_{(I \times I)}} = X_j X_j'$ and $W_{m_{(I \times I)}} = X_m X_m'$ can be compared
Inner product matrices = relative position of the individuals

Covariance between two groups:

$$< W_j, W_m >= \sum_{k \in K_j} \sum_{l \in K_m} cov^2(x_{.k}, x_{.l})$$

Correlation between two groups:

$$RV(K_j, K_m) = \frac{< W_j, W_m >}{\|W_j\| \; \|W_m\|} \qquad 0 \leq RV \leq 1$$

$RV = 0$: variables of K_j are uncorrelated with variables of K_m
$RV = 1$: the two clouds of points are homothetic

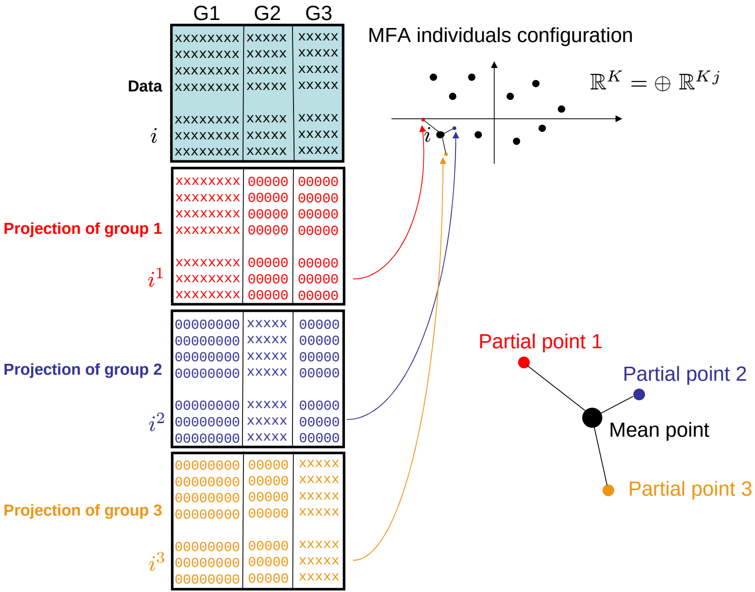
Partial analyses

- Comparison of the groups through the individuals

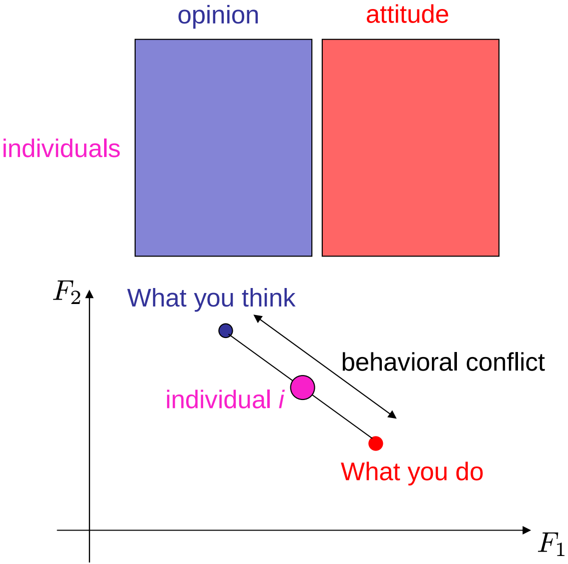
⇒ Comparison of the typologies provided by each group in a common space
⇒ Are there individuals very particular with respect to one group?

- Comparison of the separate PCA

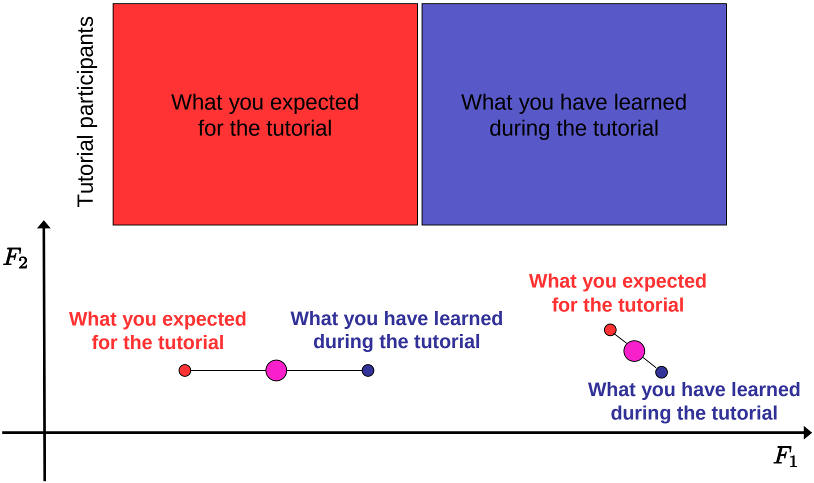
Projection of partial points



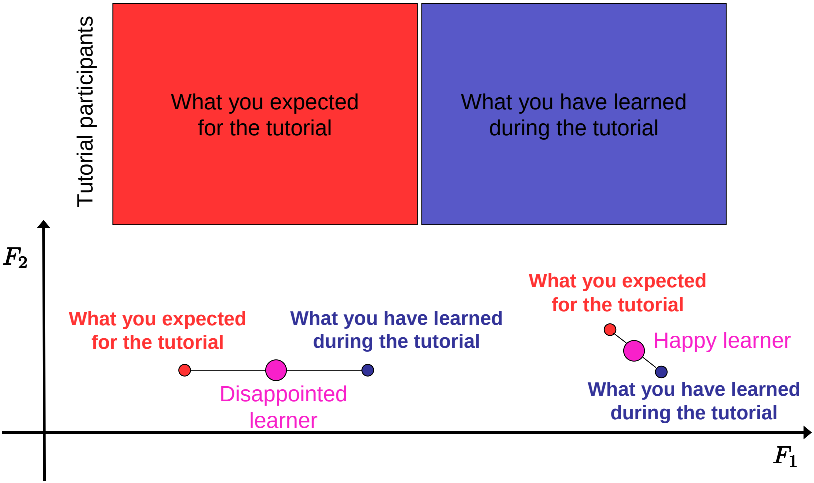
Partial points



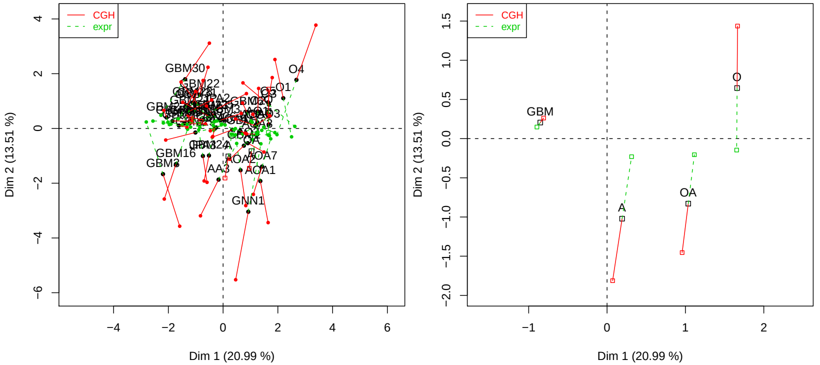
Partial points



Partial points



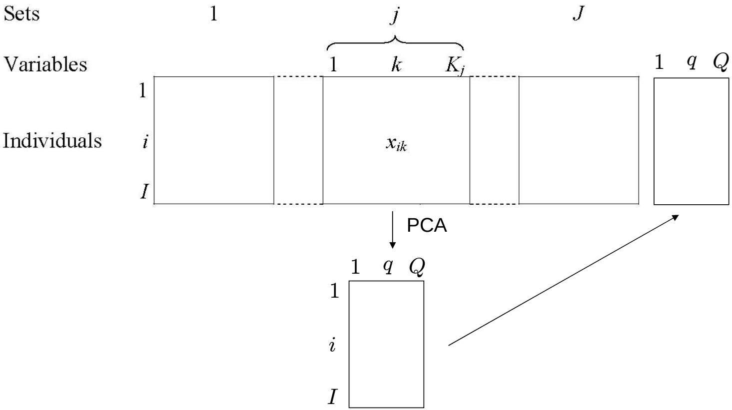
Representation of the partial points



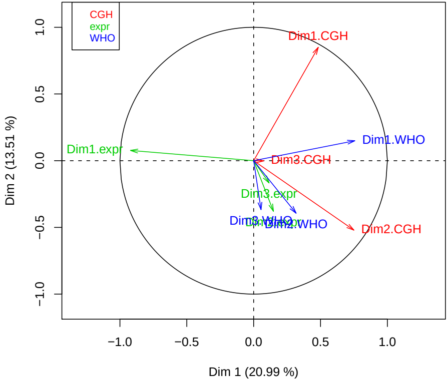
- an individual is at the barycentre of its partial points
- an individual is all the more "homogeneous" that its superposed representations are close (`res.mfa$ind$within.inertia`)

Representation of the partial components

Do the separate analyses give similar dimensions as MFA?

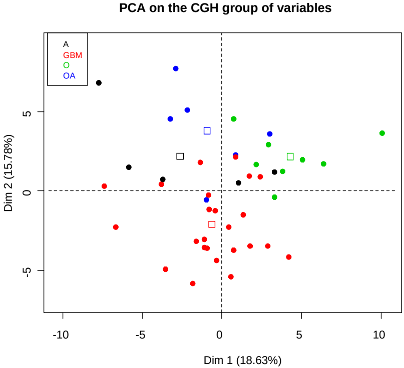


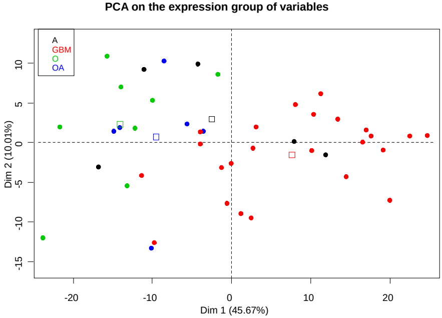
Representation of the partial components



- The first dimension of each group is well projected
- CGH has same dimensions as MFA

Representation of the partial components





Separate PCA maps that can be compared to the MFA map slide 7

Use of biological knowledge

Genes can be grouped by gene ontology (GO) biological process

GO:0006928
cell motility

- ANXA1
- CALD1
- EGFR
- ENPP2
- FN1
- FPRL2
- LSP1
- MSN
- PDPN
- PLAUR
- PRSS3
- SAA2
- SPINT2
- TNFRSF12A
- VEGF
- WASF1
- YARS

GO:0009966
regulation of signal transduction

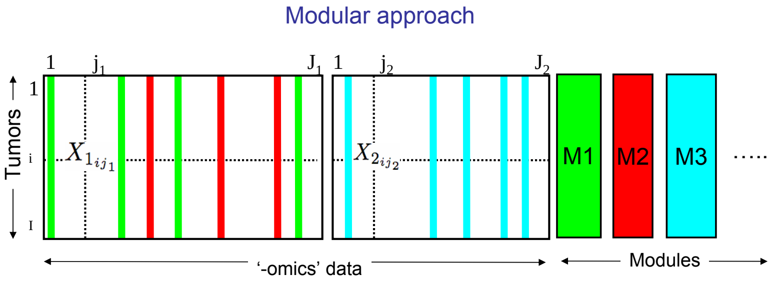
- CASP1
- EDG2
- F2R
- HCLS1
- HMOX1
- IGFBP3
- IQSEC1
- LYN
- MALT1
- TCF7L1
- TNFAIP3
- TRIO
- VEGF
- YWHAG
- YWHAH

GO:0052276
chromosome organisation and biogenesis

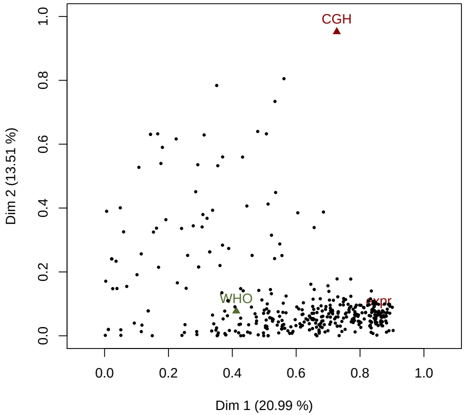
- CBX6
- NUSAP1
- PCOLN3
- PTTG1
- SUV39H1
- TCF7L1
- TSPYL1

Use of biological knowledge

- Biological processes considered as supplementary groups of variables



Use of biological knowledge



Many biological processes induce the same structure on the individuals than MFA

Back to the wine example!

	Continuous variables				Categorical
	Expert (27)	Consumer (15)	Student (15)	Preference (60)	Label (1)
wine 1					
wine 2					
…					
wine 10					

Objectives:

- How are the products described by the panels?
- Do the panels describe the products in a same way? Is there a specific description done by one panel?

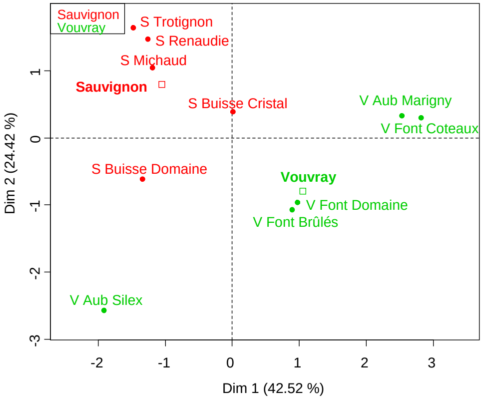
Practice with R

1. Define groups of active and supplementary variables
2. Scale or not the variables
3. Perform MFA
4. Choose the number of dimensions to interpret
5. Simultaneously interpret the individuals and variables graphs
6. Study the groups of variables
7. Study the partial representations
8. Use indicators to enrich the interpretation

Practice with R

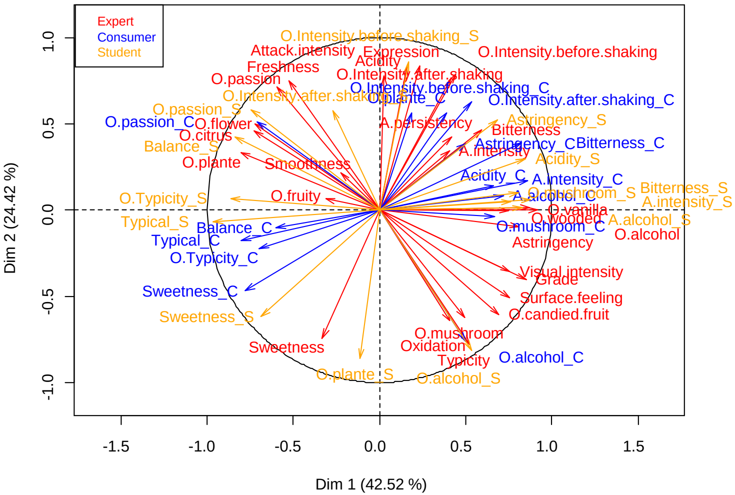
```
library(FactoMineR)
Expert <- read.table("http://factominer.free.fr/useR2010/Expert_wine.csv",
   header=TRUE, sep=";", row.names=1)
Consu <- read.table(".../Consumer_wine.csv",header=T,sep=";",row.names=1)
Stud <- read.table(".../Student_wine.csv",header=T,sep=";",row.names=1)
Pref <- read.table(".../Pref_wine.csv",header=T,sep=";",row.names=1)

palette(c("black","red","blue","orange","darkgreen","maroon","darkviolet"))
complet <- cbind.data.frame(Expert[,1:28],Consu[,2:16],Stud[,2:16],Pref)
res.mfa <- MFA(complet,group=c(1,27,15,15,60),type=c("n",rep("s",4)),
   num.group.sup=c(1,5),graph=FALSE,
   name.group=c("Label","Expert","Consumer","Student","Preference"))
plot(res.mfa,choix="group",palette=palette())
plot(res.mfa,choix="var",invisible="sup",hab="group",palette=palette())
plot(res.mfa,choix="var",invisible="actif",lab.var=FALSE,palette=palette())
plot(res.mfa,choix="ind",partial="all",habillage="group",palette=palette())
plot(res.mfa,choix="axes",habillage="group",palette=palette())
dimdesc(res.mfa)
write.infile(res.pca,file="my_FactoMineR_results.csv") #to export a list
```

Representation of the individuals

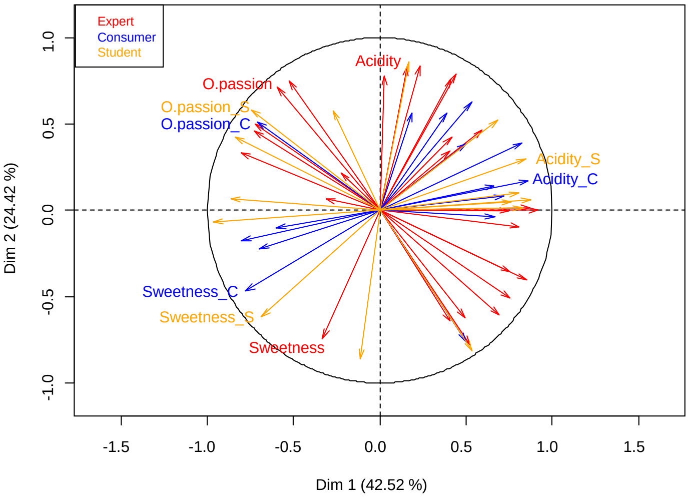


- The two labels are well separated
- Vouvray are sensorially more different
- Several groups of wines, ...

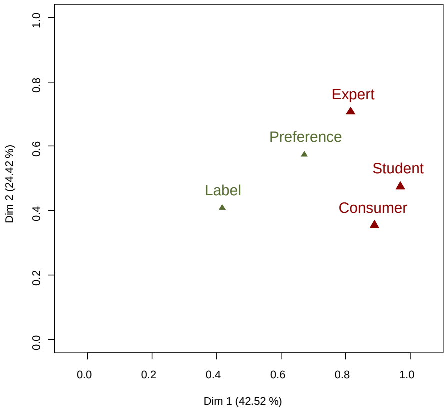
Representation of the active variables



Representation of the active variables

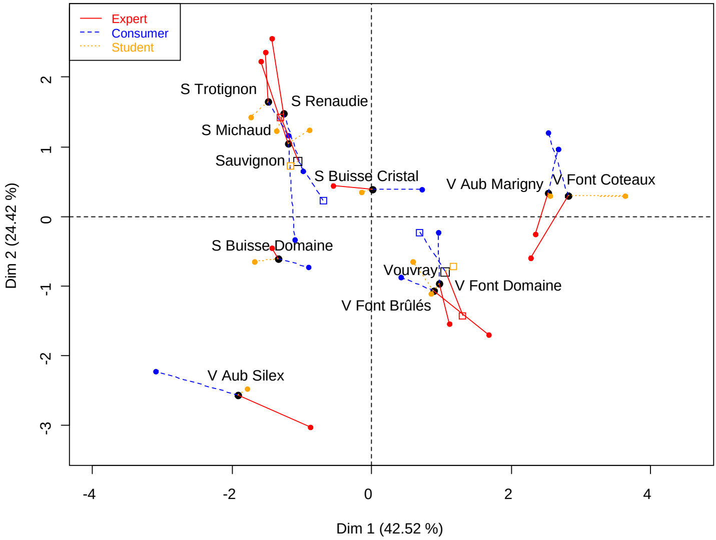


Representation of the groups

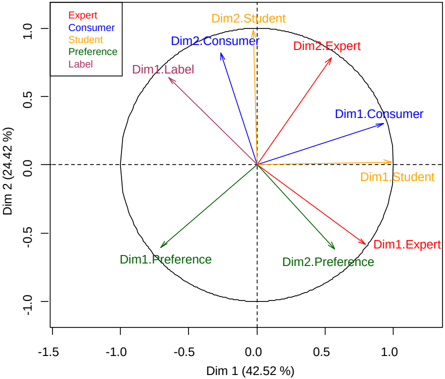


- 2 groups are all the more close that they induce the same structure
- The 1st dimension is common to all the panels
- 2nd dimension mainly due to the experts
- Preference linked to sensory description

Representation of the partial points

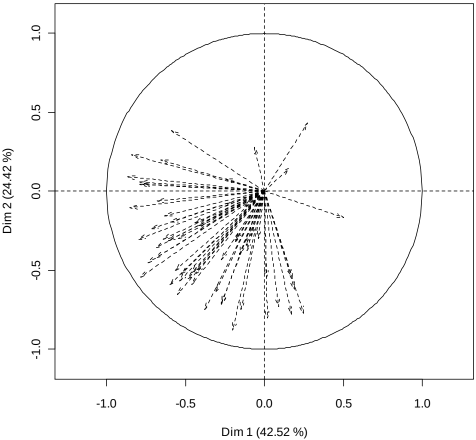


Representation of the partial dimensions



- The two first dimensions of each group are well projected
- Consumer has same dimensions as MFA

Representation of supplementary continuous variables



Preferences are linked to sensory description
The favourite wine is *Vouvray Aubussière Silex*

Helps to interpret

- Contribution of each group of variables to each component of the MFA

```
> res.mfa$group$contrib
         Dim.1 Dim.2 Dim.3
Expert    30.5  46.0  33.7
Consumer  33.2  23.1  31.2
Student   36.3  30.9  35.1
```

- Similar contribution of the 3 groups to the first dimension
- Second dimension mainly due to the expert

- Correlation between the global cloud and each partial cloud

```
> res.mfa$group$correlation
         Dim.1 Dim.2 Dim.3
Expert    0.95  0.95  0.96
Consumer  0.95  0.83  0.87
Student   0.99  0.99  0.84
```

First components are highly linked to the 3 groups: the 3 clouds of points are nearly homothetic

Similarity measures between groups

```
> res.mfa$group$Lg
           Expert Consumer Student Preference Label  MFA
Expert       1.45     0.94    1.17       1.01  0.89 1.33
Consumer     0.94     1.25    1.04       1.11  0.28 1.21
Student      1.17     1.04    1.29       1.03  0.62 1.31
Preference   1.01     1.11    1.03       1.47  0.37 1.18
Label        0.89     0.28    0.62       0.37  1.00 0.67
MFA          1.33     1.21    1.31       1.18  0.67 1.44

> res.mfa$group$RV
           Expert Consumer Student Preference Label  MFA
Expert       1.00     0.70    0.85       0.69  0.74 0.92
Consumer     0.70     1.00    0.82       0.82  0.25 0.90
Student      0.85     0.82    1.00       0.75  0.55 0.96
Preference   0.69     0.82    0.75       1.00  0.31 0.81
Label        0.74     0.25    0.55       0.31  1.00 0.56
MFA          0.92     0.90    0.96       0.81  0.56 1.00
```

- Expert gives a richer description ($\mathcal{L}_g$ greater)
- Groups Student and Expert are linked (RV = 0.85)
- Group Student is the closest to the overall (RV = 0.96)

To go further

- Mixed data: MFA with 1 group = 1 variable
  if there are only continuous variables, PCA is recovered; if there are only categorical variables, MCA is recovered
  a specific function: AFDM
- MFA used for methodological purposes:
  - comparison of coding (continuous or categorical)
  - comparison between preprocessing (standardized PCA and unstandardized PCA)
  - comparison of results from different analyses
- Hierarchical Multiple Factor Analysis
  Takes into account a hierarchy on the variables: variables are grouped and subgrouped (like in questionnaires structured in topics and subtopics)

Clustering and Principal Component Methods

1. Clustering Methods
2. Principal Components Methods as a Preprocessing Step
3. Graphical Complementarity

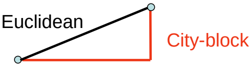
Unsupervised classification

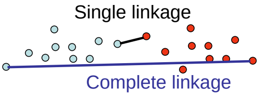
- Data set: table individuals $\times$ variables (or a distance matrix)
- Objective: to produce homogeneous groups of individuals (or groups of variables)
- Two kinds of clustering to define two structures on individuals: hierarchy or partition

Hierarchical Clustering

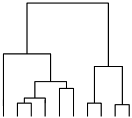
Principle: sequentially agglomerate (clusters of) individuals using

- a distance between individuals: City block, Euclidean
- an agglomerative criterion: single linkage, complete linkage, average linkage, Ward's criterion





Representation with a dendrogram



$\Rightarrow$ Eulidean distance is used in principal component methods
$\Rightarrow$ Ward's criterion is based on multidimensional variance (inertia) which is the core of principal component methods

Ascending Hierarchical Clustering

AHC algorithm:

- Compute the Euclidean distance matrix ($I \times I$)
- Consider each individual as a cluster
- Merge the two clusters A and B which are the closest with respect to the Ward's criterion:

$$\Delta_{ward}(A, B) = \frac{I_A I_B}{I_A + I_B} d^2(\mu_A, \mu_B)$$

  with d the Euclidean distance, μ_A the barycentre and I_A the cardinality of the set A
- Repeat until the number of clusters is equal to one

Ward's criterion

- Individuals can be represented by a cloud of points in $\mathbb{R}^K$
- Total inertia = multidimensional variance

With Q groups of individuals, inertia can be decomposed as:

$$\sum_{k=1}^{K}\sum_{q=1}^{Q}\sum_{i=1}^{I_q}(x_{iqk}-\bar{x}_k)^2 = \sum_{k=1}^{K}\sum_{q=1}^{Q} I_q(\bar{x}_{qk}-\bar{x}_k)^2+\sum_{k=1}^{K}\sum_{q=1}^{Q}\sum_{i=1}^{I_q}(x_{iqk}-\bar{x}_{qk})^2$$

Total inertia = Between inertia + Within inertia

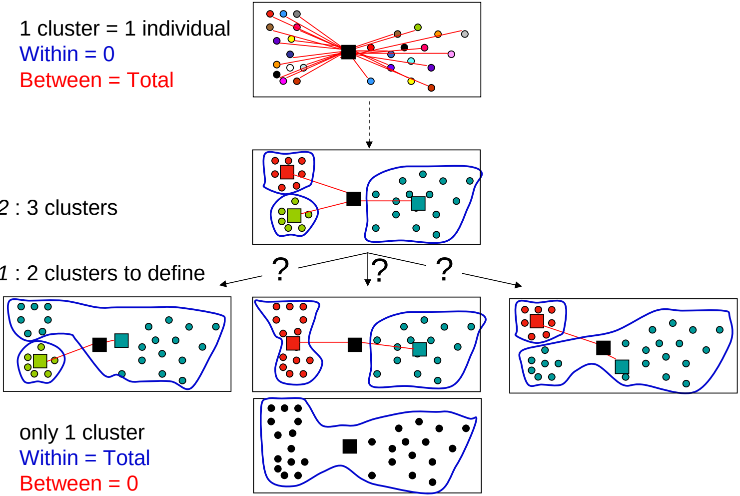
Ward's criterion

Step 1: 1 cluster = 1 individual
Within = 0
Between = Total

Step *I-2* : 3 clusters

Step *I-1* : 2 clusters to define

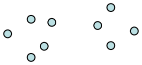
Step *I* : only 1 cluster
Within = Total
Between = 0



$\Rightarrow$ Ward minimizes the increasing of within inertia

K-means algorithm

1. Choose Q points at random (the barycentre)
2. Affect the points to the closest barycentre
3. Compute the new barycentre
4. Iterate 2 and 3 until convergence



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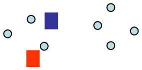

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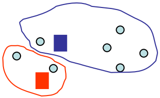

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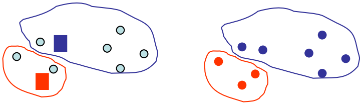

K-means algorithm

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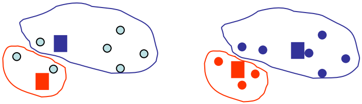

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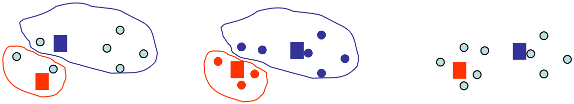

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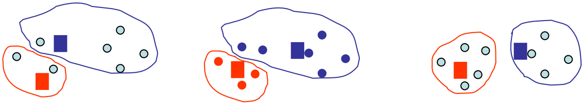

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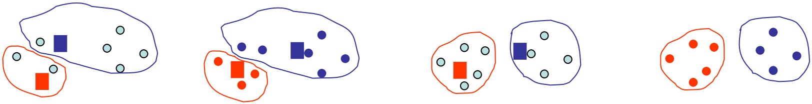

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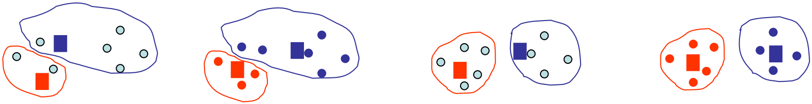
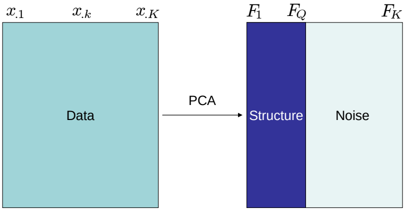


PCA as a preprocessing

With continuous variables:
$\Rightarrow$ AHC and k-means onto the raw data
$\Rightarrow$ AHC or k-means onto principal components

PCA transforms the raw variables into orthogonal principal components $F_{.1}, ..., F_{.K}$ with decreasing variance $\lambda_1 \geq \lambda_2 \geq ...\lambda_K$



$\Rightarrow$ Keeping the first components makes the clustering more robust
$\Rightarrow$ But, how many components do you keep to denoise?

MCA as a preprocessing

Clustering on categorical variables: which distance to use?

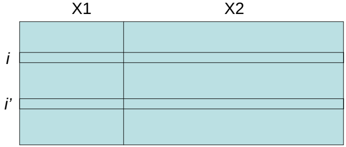
- with two categories: Jaccard index, Dice's coefficient, simple match, etc. Indices well-fitted for presence/absence data
- with more than 2 categories: use for example the χ^2-distance

Using the χ^2-distance $\Leftrightarrow$ computing distances from all the principal components obtained from MCA

In practice, MCA is used as a preprocessing in order to

- transform categorical variables in continuous ones
- delete the last dimensions to make the clustering more robust

MFA as a preprocessing



MFA balances the influence of the groups when computing distances between individuals

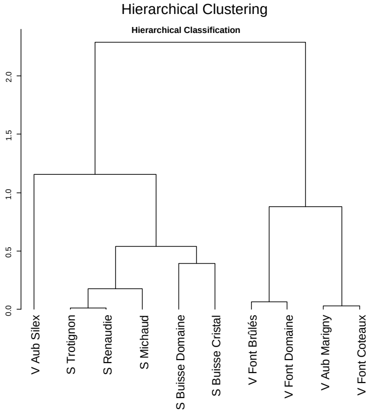
$$d^2(i,i') = \sum_{j=1}^{J} \frac{1}{\sqrt{\lambda_j}} \sum_{k=1}^{K_j} (x_{ik} - x_{i'k})^2$$

AHC or k-means onto the first principal components $(F_{.1}, ..., F_{.Q})$ obtained from MFA allows to

- take into account the groups structure in the clustering
- make the clustering more robust by deleting the last dimensions

Back to the wine data!

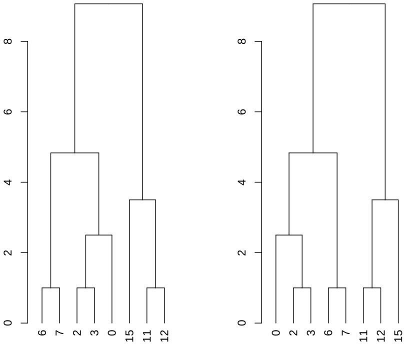
AHC onto the first 5 principal components from MFA



Individuals are sorted according to their coordinate $F_{.1}$

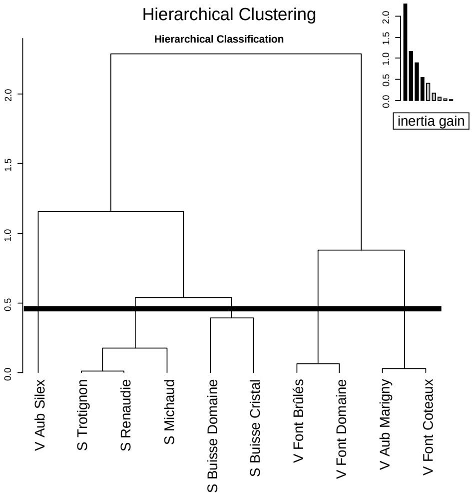
Why sorting the tree?

```
X <- c(6,7,2,0,3,15,11,12)
names(X) <- X
library(cluster)
par(mfrow=c(1,2))
plot(as.dendrogram(agnes(X)))
plot(as.dendrogram(agnes(sort(X))))
```



Partition from the tree

An empirical number of clusters is suggested $(\min_q \frac{W_q - W_{q+1}}{W_{q-1} - W_q})$



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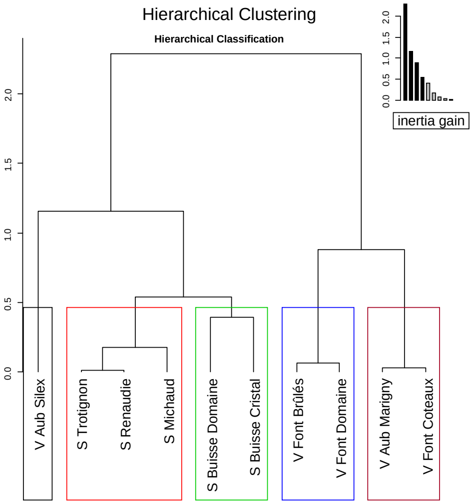
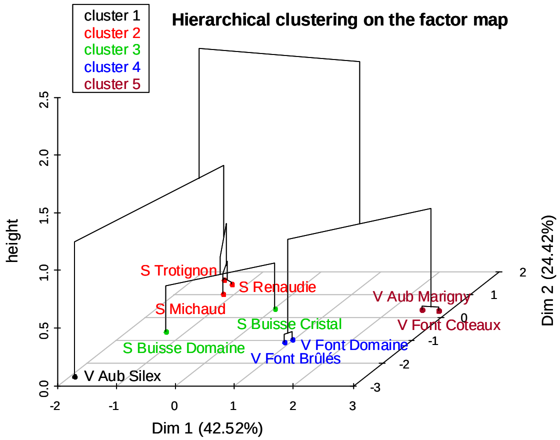
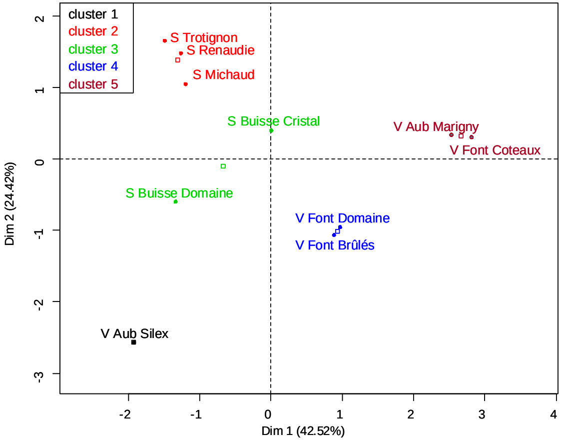


Hierarchical tree on the principal component map



Hierarchical tree gives an idea of the other dimensions

Partition on the principal component map



Continuous view (principal components) and discontinuous (clusters)

Cluster description by variables

$$\text{v.test} = \frac{\bar{x}_q - \bar{x}}{\sqrt{\frac{s^2}{I_q}\left(\frac{I-I_q}{I-1}\right)}} \sim \mathcal{N}(0,1) \qquad H_0 : \bar{x}_q = \bar{x}$$

with $\bar{x}_q$ the mean of variable x in cluster q, $\bar{x}$ (s) the mean (standard deviation) of the variable x in the data set, I_q the cardinal of cluster q

```
$desc.var$quanti$‘2‘
                 v.test  Mean in Overall     sd in   Overall p.value
                         category    mean category        sd
O.passion_C        2.58      6.17    4.61      0.79      1.18    0.01
O.citrus           2.50      5.40    3.66      0.22      1.37    0.01
O.passion_S        2.45      5.69    4.18      0.54      1.20    0.01
....
Typicity          -2.42      1.36    3.91      0.72      2.07    0.02
O.candied.fruit   -2.44      0.78    2.58      0.16      1.45    0.01
O.alcohol_S       -2.48      3.98    4.33      0.13      0.28    0.01
Surface.feeling   -2.52      2.63    3.62      0.12      0.77    0.01
```

Cluster description

- by the principal components (individuals coordinates) : same description than for continuous variables

```
$desc.axes$quanti$‘2‘
       v.test  Mean in  Overall     sd in  Overall  p.value
              category     mean  category       sd
Dim.2    2.20     1.39 7.77e-17     0.253     1.24   0.0276
```

- by categorical variables : chi-square and hypergeometric test

⇒ Active and supplementary elements are used
⇒ Only significant results are presented

Cluster description by individuals

- parangon: the closest individuals to the barycentre of the cluster

$$\min_{i \in q} d(x_{i.}, \mu_q) \text{ with } \mu_q \text{ the barycentre of cluster } q$$

- specific individuals: the furthest individuals to the barycentres of the other clusters (the individuals sorted according to their distance from the highest to the smallest to the closest barycentre)

$$\max_{i \in q} \min_{q' \neq q} d(x_{i.}, \mu_{q'})$$

```
desc.ind$para
cluster: 2
 S Renaudie   S Trotignon     S Michaud
    0.1002890     0.3101154     0.3640145
-------------------------------------------
desc.ind$dist
cluster: 2
S Trotignon    S Renaudie     S Michaud
     1.934103      1.687849      1.265386
-------------------------------------------
```

Complementarity between hierarchical clustering and partitioning

- Partitioning after AHC: the k-means algorithm is initialized from the barycentres of the partition obtained from the tree
  - consolidate the partition
  - loss of the hierarchy

- AHC with many individuals: time-consuming
  $\Rightarrow$ partitioning before AHC
  - compute k-means with approximately 100 clusters
  - AHC on the weighted barycentres obtained from the k-means
    $\Rightarrow$ top of the tree is approximately the same

Practice with R

```
res.hcpc <- HCPC(res.mfa)


##### Example of clustering on categorical data
data(tea)
res.mca <- MCA(tea,quanti.sup=19,quali.sup=20:36)
plot(res.mca,invisible=c("var","quali.sup","quanti.sup"),cex=0.7)
plot(res.mca,invisible=c("ind","quali.sup","quanti.sup"),cex=0.8)
plot(res.mca,invisible=c("quali.sup","quanti.sup"),cex=0.8)
dimdesc(res.mca)

res.mca <- MCA(tea,quanti.sup=19,quali.sup=20:36, ncp=10)
res.hcpc <- HCPC(res.mca)
```

CARME conference

International conference on Correspondence Analysis and Related MEthods

Agrocampus Rennes (France), February 8-11, 2011

R tutorials for corresp. ana. and related methods of visualization:

- S. Dray: multivariate analysis of ecological data with `ade4`
- O. Nenadić & M. Greenacre: correspondence analysis with `ca`
- S. Lê: from one to multiple data tables with `FactoMineR`
- J. de Leeuw & P. Mair: multidimensional scaling using majorisation with `smacof`

Invited speakers: Monica Bécue, Cajo ter Braak, Jan de Leeuw, Stéphane Dray, Michael Friendly, Patrick Groenen, Pieter Kroonenberg

Bibliography

- Escofier B. & Pagès J. (1994). Multiple factor analysis (AFMULT package). *Computational Statistics and Data Analysis*, 121-140.
- Greenacre M. & Blasius J. (2006). *Multiple Correspondence Analysis and related methods*. Chapman & Hall/CRC.
- Husson F., Lê S. & Pagès J. (2010). *Exploratory Multivariate Analysis by Example Using R*. Chapman & Hall.
- Jolliffe I. (2002). *Principal Component Analysis*. Springer. 2nd edn.
- Lebart L., Morineau A. & Warwick K. (1984). *Multivariate descriptive statistical analysis*. Wiley, New-York.
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Packages' bibliography

http://cran.r-project.org/web/views/Multivariate.html
http://cran.r-project.org/web/views/Cluster.html

- *ade4* package: data analysis functions to analyse Ecological and Environmental data in the framework of Euclidean Exploratory methods
http://pbil.univ-lyon1.fr/ADE-4
- *ca* package (Greenacre and Nenadic) deals with simple, multiple and joint correspondence analysis
- *cluster* package: basic and hierarchical clustering
- *dynGraph* package: visualization software to explore interactively graphical outputs provided by multidimensional methods
http://dyngraph.free.fr
- *FactoMineR* package
http://factominer.free.fr
- *hopach* package: builds hierarchical tree of clusters
- *missMDA* package: imputes missing values with multivariate data analysis methods

FactoMineR

A website with documentation, examples, data sets:
`http://factominer.free.fr`

How to install the Rcmdr menu:
copy and paste the following line of code in a R session

```
source("http://factominer.free.fr/install-facto.r")
```

A book:
Husson F., Lê S. & Pagès J. (2010). *Exploratory Multivariate Analysis by Example Using R*. Chapman & Hall.