

Master in Data Science (MDS)

Multivariate Analysis (MVA) Multiple Factor Analysis

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Outline



- Data Introduction
- 2 Equilibrium and global PCA
- Studying groupsGroup representationPartial points representationSeparate analyses
- Further topicsQualitative dataContingency tablesInterpretation aids

Sensory description of Loire wines



- 10 white wines from the Loire valley: 5 Vouvray 5 Sauvignon
- sensory descriptors: acidity, bitterness, citrus odor, etc.



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	O.fruity	O.passion	O.citrus		Sweetness	Acidity	Bitterness	Astringency	Aroma.intensity	Aroma.persistency	Visual.intensity	Grape variety
S Michaud	4.3	2.4	5.7		3.5	5.9	4.1	1.4	7.1	6.7	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	Sauvignon
S Trotignon	5.1	4.0	5.3		3.0	6.1	4.1	2.4	6.1	6.1	3.0	Sauvignon
S Buisse Domaine	4.3	2.4	3.6		3.9	5.6	2.5	3.0	4.9	5.1	4.1	Sauvignon
S Buisse Cristal	5.6	3.1	3.5		3.4	6.6	5.0	3.1	6.1	5.1	3.6	Sauvignon
V Aub Silex	3.9	0.7	3.3		7.9	4.4	3.0	2.4	5.9	5.6	4.0	Vouvray
V Aub Marigny	2.1	0.7	1.0	•••	3.5	6.4	5.0	4.0	6.3	6.7	6.0	Vouvray
V Font Domaine	5.1	0.5	2.5		3.0	5.7	4.0	2.5	6.7	6.3	6.4	Vouvray
V Font Brûlés	5.1	8.0	3.8		3.9	5.4	4.0	3.1	7.0	6.1	7.4	Vouvray
V Font Coteaux	4.1	0.9	2.7		3.8	5.1	4.3	4.3	7.3	6.6	6.3	Vouvray

Sensory description of wines: comparing juries FIR BUNIVERSITAT POLITÈCNICA BARCELONATECH

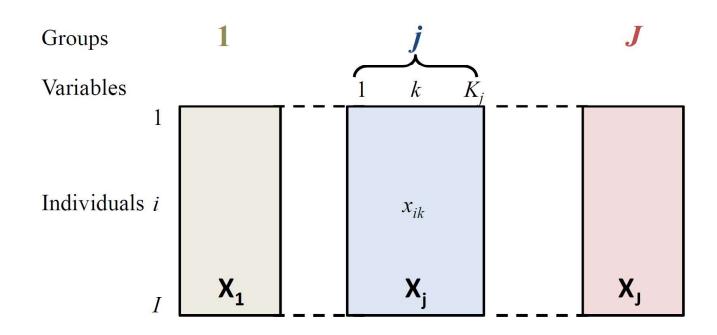


- 10 white wines from the Loire valley: 5 Vouvray 5 Sauvignon
- sensory descriptors: acidity, bitterness, citrus odor, etc.
- tasting note of 60 consumers: overall appreciation

	Expert (27)	Student (15)	Consumer (15)	Appreciation (60)	Grape variety (1)
Wine 1					
Wine 2					
Wine 10					

- How to characterize the wines?
- Are wines described in the same way by the different juries?
- Are there specific responses from certain juries?





Examples with quantitative and/or qualitative variables:

- genomics : DNA, expression, proteins
- questionnaires: student health (product consumption, psychological state, sleep, age, sex, etc.)
- Economics: annual economic indices



 Study the similarity between individuals with respect to the whole set of variables AND the relationships between variables

Take the group structure into account

- Study the overall similarities and differences between groups (and the specific features of each group)
- Study the similarities and differences between groups from an individual's point of view
- Compare the characteristics of individuals from the separate analyses
- ⇒ Balance the influence of all of the groups in the analysis

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Balancing the influence of each group of



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

MFA is a weighted PCA:

- calculate the 1st eigenvalue λ_1^j of the jth group of variables (j = 1, ..., J)
- do an overall PCA on the weighted table :

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

 X_j corresponds to the jth normalized or standardized table

Balancing the influence of each group of



Before weighting

After weighting

	Expert	Student	Consumer	•	Expert	Student	Consumer
λ_1	11.74	7.89	7.17	-	1.00	1.00	1.00
λ_2	6.78	3.83	2.59		0.58	0.49	0.36
λ_3	2.74	1.70	1.63		0.23	0.22	0.23

- Same weights for all variables from the same group : group structure is preserved
- For each group, the variance of the principal dimension (first eigenvalue) is equal to 1
- No group can generate the first axis on its own
- A multi-dimensional group will contribute to more axes than a one-dimensional group

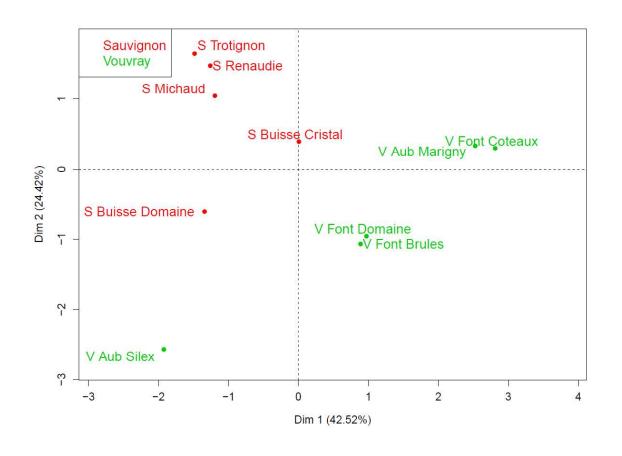
MFA - a weighted PCA



- ⇒ Same plots as in PCA
 - Study similarities between individuals in terms of the set of variables
 - Study relationships between variables
 - Characterize individuals in terms of variables
- ⇒ Same outputs (coordinates, cosine, contributions)
- ⇒ Add individuals and variables (quantitative, qualitative) as supplementary information

Individuals plot

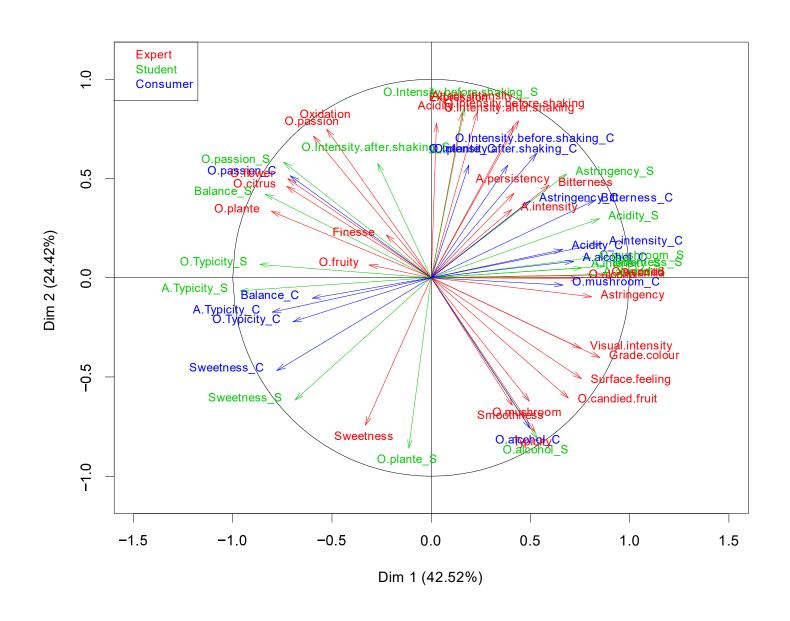




- The 2 grape varieties are well-separated
- The Vouvray are more varied in terms of sensory perception
- Several groups of wines . . .

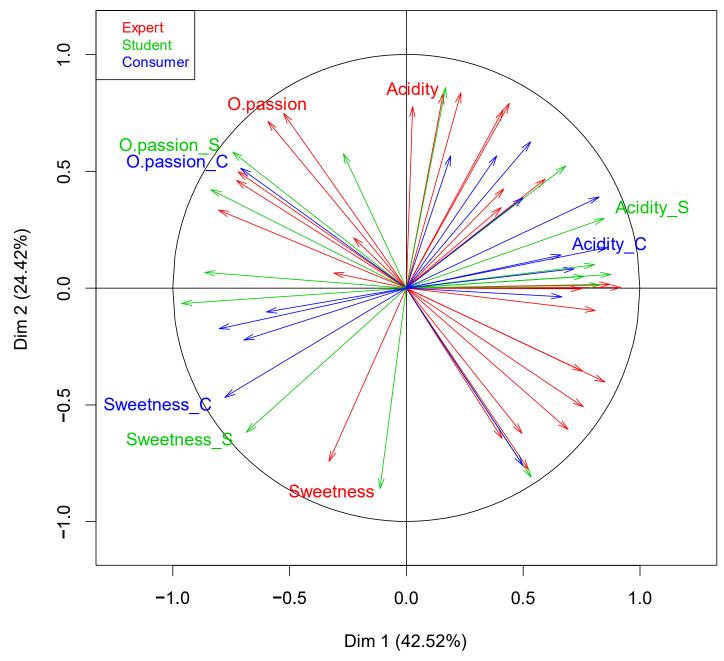
Variables plot





Variables plot





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First MFA component



In PCA (reminder) :
$$\underset{v_1 \in \mathbb{R}^I}{\operatorname{arg\,max}} \sum_{k=1}^K cov^2(x_{.k}, v_1)$$

$$\operatorname{arg\,max}_{v_1 \in \mathbb{R}^I} \sum_{j=1}^J \sum_{k \in K_j} \operatorname{cov}^2 \left(\frac{x_{.k}}{\sqrt{\lambda_1^j}}, v_1 \right) = \operatorname{arg\,max}_{v_1 \in \mathbb{R}^I} \sum_{j=1}^J \underbrace{\frac{1}{\lambda_1^j} \sum_{k \in K_j} \operatorname{cov}^2(x_{.k}, v_1)}_{\mathcal{L}_g(K_i, v_1)}$$

 $L_g(K_j, v_1)$ = projected inertia of all the variables of K_j on $v_1 \Rightarrow$ The first principal component of the MFA is the variable which maximizes the link with all groups, in the L_g sense.

$$0 \leq L_g(K_j, v_1) \leq 1$$

 $L_g = 0$: all variables in the jth group are uncorrelated with v_1

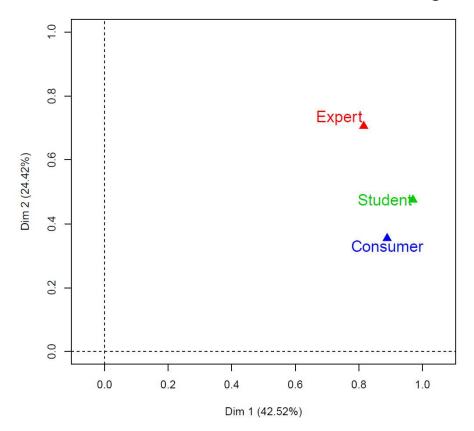
 $L_g = 1 : v_1$ the same as the 1st principal component of K_j

Group plot



 \Rightarrow Using L_g to plot groups

The jth group has coordinates $L_g(K_j, v_1)$ and $L_g(K_j, v_2)$



- 1st axis is the same for all groups
- 2nd axis is due to the Experts group
- 2 groups are close to each other when they induce the same structure
- ⇒ This plot provides a synthetic comparison of the groups
- ⇒ Are the relative positions of individuals similar from one group to the next?

Measuring how similar groups are



 The L_g coefficient measures the connection between groups of variables :

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

• The L_g coefficient as an indicator of a group's dimensionality

$$\mathcal{L}_{g}(\mathit{K}_{j},\mathit{K}_{j}) = rac{\sum_{k=1}^{\mathit{K}_{j}} (\lambda_{k}^{j})^{2}}{(\lambda_{1}^{j})^{2}} = 1 + rac{\sum_{k=2}^{\mathit{K}_{j}} (\lambda_{k}^{j})^{2}}{(\lambda_{1}^{j})^{2}}$$

$$RV(K_j, K_m) = \frac{\mathcal{L}_g(K_j, K_m)}{\sqrt{\mathcal{L}_g(K_j, K_j)} \sqrt{\mathcal{L}_g(K_m, K_m)}} \qquad 0 \le RV \le 1$$

RV = 0: all variable in K_j and K_m are uncorrelated

RV = 1: the two point clouds are homothetic

Partial points representation



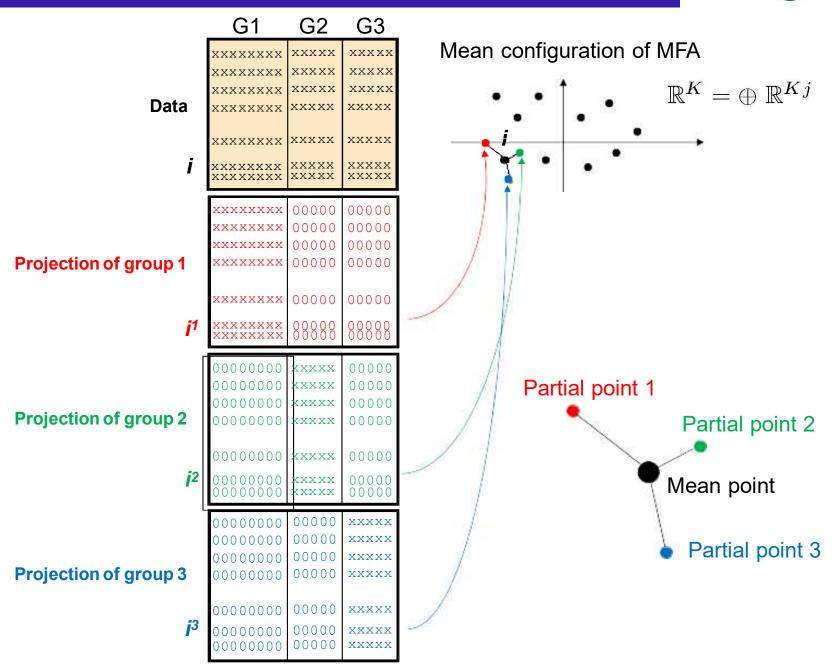
⇒ Comparing groups in terms of individuals

⇒ Comparing descriptions provided by each group in a shared space

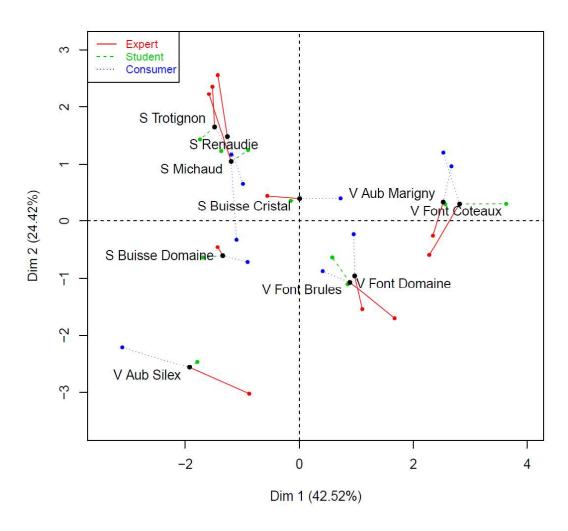
⇒ Are there specific individuals related to certain groups of variables?

Projections of partial points









- Partial point = representing an individual as seen by a group
- An individual is at the barycenter of its partial points

Putting MFA into practice



- Define the structure of the dataset (group composition)
- ② Define the active groups and supplementary elements
- Standardize the variables or not?
- Run the MFA
- 6 Choose the number of dimensions to interpret
- 6 Simultaneous analysis of the individuals and variables plots
- Group study
- 8 Partial analyses
- Use indices to enrich the interpretation

The MFA function of the FactoMineR package

Conclusion



- MFA: a multi-table method for quantitative variables, qualitative variables, and frequency tables
- MFA balances the influence of each table
- Represents the information brought by each table in a shared setting
- Classical outputs (individuals, variables)
- Specific outputs (groups, separate analyses, partial points)



For more information about MFA, have a look at these videos:

https://www.youtube.com/watch?v=MOI0Aw1TTFE

https://www.youtube.com/watch?v=kGSjHD3yG84

https://www.youtube.com/watch?v=OVtNX6Or1FI

https://www.youtube.com/watch?v=Vumu7OoFHdA

https://www.youtube.com/watch?v=7HHuKsl2 fk

Husson F., Lê S. & Pagès J. (2017) Exploratory Multivariate Analysis by Example Using R 2nd edition, 230 p., CRC/Press. **Pagès, J.** (2014). Multiple Factor Analysis by Example Using R. CRC Press.